Influence of growth direction and strain conditions on the band line-up at GaSb/InSb and InAs/InSb interfaces

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Abstract

First-principles full potential linearized augmented plane wave (FLAPW) calculations have been performed for lattice-mismatched common-atom III-V interfaces. In particular, we have examined the effects of epitaxial strain and ordering direction on the valence band offset in [001] and [111] GaSb/InSb and InAs/InSb superlattices, and found that the valence band maximum is always higher at the InSb side of the heterojunction, except for the common-anion system grown on an InSb substrate. The comparison between equivalent structures having the same substrate lattice constant, but different growth axis, shows that for comparable strain conditions, the ordering direction slightly influences the band line-up, due to small differences of the charge readjustment at the [001] and [111] interfaces. On the other hand, strain is shown to strongly affect the VBO; in particular, as the pseudomorphic growth conditions are varied, the bulk contribution to the band line-up
changes markedly, whereas the interface term is almost constant. On the whole, our calculations yield a band line-up that decreases linearly as the substrate lattice constant is increased, showing its high tunability as a function of different pseudomorphic growth conditions. Finally, the band line-up at the lattice matched InAs/GaSb interface determined using the transitivity rule gave perfect agreement between predicted and experimental results.

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I. INTRODUCTION

In the last few years “band offset engineering” (i.e. the possibility of tuning the electronic and transport properties of semiconductor heterojunctions through modifications of their valence band offset (VBO) induced by strain, growth process, number of layers etc.) has attracted great attention for both scientific and technological reasons [1]. Only recently, however, have lattice mismatched heterostructures begun to realize their potential, due to new developments in preparation techniques which finally allowed pseudomorphic crystal growth without misfit dislocations [2]. In a parallel way, some theoretical works [3,4,6–11] focused on strained heterojunctions, but still much effort is needed to understand what mainly affects the band line-up at the interface.

In this work, we consider homopolar isovalent heterostructures. In particular, we examine III-V superlattices (SLs), namely the common-anion system GaSb/InSb (lattice mismatch of 5.7 %) and the common-cation system InAs/InSb (lattice mismatch of 6.4 %), concentrating on the effect of ordering direction and strain conditions determined by SL pseudomorphic growth on a given substrate. Ab-initio self-consistent full potential linearized augmented plane wave FLAPW [12] local density calculations were performed for (GaSb)₃/(InSb)₃ and (InAs)₃/(InSb)₃ SLs, grown along the [001] (tetragonal symmetry) and [111] (trigonal symmetry) directions, in which the interface was represented by three alternating layers of each binary constituent (12 atoms in each unit cell). In what follows, it is important to keep in mind that if strain is not taken into account, the valence bands in unstrained GaSb and InSb are predicted to line-up (therefore giving zero VBO), whereas the unstrained InSb topmost valence band is expected to be 0.51 eV higher in energy than that in unstrained InAs (see Ref. [5] and references therein).

As pointed out by Mailhot and Smith [13,14], [111] ordered strained-layer SLs show large polarization fields oriented along the growth direction, which lead to a shift in the electronic energy levels. However, this effect is negligible for ultrathin SLs, such as those examined in the present work. Moreover, the effect completely vanishes for [001] ordered SLs, due to the
symmetry properties of the strain tensor. Finally, we neglect interdiffusion processes which lead to interfacial composition changes (i.e. we consider an atomically abrupt geometry) and relaxations at the interface of the anion-cation distance (bulk bond length away from the interface are considered equal to those immediately next to it): this, in fact, is expected to introduce little modification of the charge rearrangement at the junction and hence of the VBO.

II. COMPUTATIONAL AND STRUCTURAL PARAMETERS

Most of the computational parameters are common to those used previously for [001] and [111] ordered (1x1) SLs [17], except for the wave function cut-off ($k_{\text{max}} = 2.7$ a.u.). [17] Tests performed by increasing the $k_{\text{max}}$ up to 3.1 showed a change in the VBO of less than 0.01 eV. There is, however, an important difference with respect to the calculations performed for ultrathin ($n = 1$) SLs regarding the cation $d$-shell: in the present work, the Ga $3d$ and In $4d$ electrons are treated as part of the core and not as valence electrons (previous works [4] demonstrated a slight dependence (about 0.03 eV) of the VBO in common-cation systems on the $d$-shell treatment) - which results in a strong reduction of the computational effort. Furthermore, the core charge spilling out of the Ga and In muffin tin spheres was treated using an exact overlapping charge method, thus minimizing the error introduced by the treatment of semicore states.

The structural parameters (reported elsewhere [17]) are determined according to the macroscopic theory of elasticity (MTE), whose validity in predicting the correct structure for the determination of the VBO is established [11]. Our choice is also justified by the results obtained in the case of ultrathin SLs [17], which were found to be in good agreement with those obtained from total energy minimization.

In order to study the dependence of the VBO on the strain, we examined different strain conditions for (AC)$_3$/(BC)$_3$-type [001] ordered SLs (the common cation case (AB)$_3$/(AC)$_3$ is treated in an analogous way): (i) pseudomorphic growth of a BC epilayer on an AC substrate;
(ii) “free standing mode”, equivalent to a system grown on an $A_{0.5}B_{0.5}C$ substrate (denoted in the following as “Av. subs.”); and (iii) pseudomorphic growth of an AC epilayer on a BC substrate.

On the other hand, the dependence of the VBO on the ordering direction is studied through a comparison of the [001] and [111] ordered SLs grown on a fixed substrate with average lattice constant, but different crystallographic orientations. This choice of the substrate and the consequent lattice relaxation, leads to a small difference (about 1.4 %) between the lattice constants of the binary constituents along the [001] and [111] growth direction.

III. RESULTS AND DISCUSSION

In analogy with the common experimental approach followed in photoemission measurements, we have evaluated the VBO using core electron binding energies as reference levels \cite{18}. We have chosen the $s$-levels of the common atom C (i.e. Sb in the common-anion system and In in the common-cation system). Note that other choices of core levels for different atoms (i.e. Ga and In in the common-anion system, As and Sb in the common-cation system) would produce a VBO value differing from those reported here by at most 0.06 eV, which has thus to be considered as our numerical uncertainty.

The calculation of the VBO, $\Delta E_v$, is done according to the following expression:

$$\Delta E_v = \Delta b + \Delta E_b$$

where the interface term $\Delta b$ indicates the relative core level alignment of the two C atoms at opposite sides of the interface (one belonging to the AC side and the other to the BC side), while $\Delta E_b$ indicates the binding energy difference (relative to the valence band maximum (VBM)) of the same core levels evaluated in the binary constituents, opportunely strained to reproduce the elastic conditions of the SL.

First of all, we focus our attention on the elastically relaxed “Av. subs.” [001] and [111] ordered SLs. We should now notice that there are two inequivalent interfaces along the [111]
growth axis \([13]\); for example, in the common-anion SL, we can have the ordering direction parallel either to the InSb interface bond or to the GaSb interface bond. Our results indicate that the \(\Delta b\) term is essentially the same (within 0.02 eV) in the two different situations, suggesting that the effect due to the particular geometry at the interface is very small.

Table I lists the contributions due to the interface \((\Delta b)\) and to the strained bulks \((\Delta E_b)\) and the resulting values of the VBOs \((\Delta E_v)\) as a function of the ordering direction; the superscripts \((nr)\) and \((r)\) indicate respectively the non-relativistic and relativistic \((i.e.\) spin-orbit coupling treated in a perturbative approach) calculations.

We note that the interface term has a positive sign, indicating that the Sb-core levels are deeper at the GaSb (InAs) side of the common-anion (common-cation) interface, compared to the corresponding levels at the InSb side. Further, the first contribution \((\Delta b)\) is seen to be sensitive to the crystallographic ordering (the two values for \([001]\) and \([111]\) growth axis differ by 0.1 eV both in the common-anion and the common-cation systems), while the second contribution to the VBO \((\Delta E_b)\) is almost uninfluenced by the ordering direction. On the whole, we do not observe a marked dependence of the VBO on the crystallographic ordering at the interface. Since it is well-known for lattice matched structures \([20,21]\) that the band line-up is independent of interface orientation, the VBO change we find in going from the \([001]\) to the \([111]\) ordered SLs has to be related only to the appreciable mismatch which causes a different relaxation of the interface bond-lengths.

Let us now look at the role of the mismatch in determining the band line-up. Our results for \([001]\) systems with different pseudomorphic growth conditions are shown in Table II, where the notation is analogous to that of Table I. Note that the interface term \(\Delta b\) is very similar in the same SL grown on the three different substrates, implying that the charge readjustment at the interface is almost independent of the strain conditions. This is confirmed by the results obtained with a small change (by as much as 0.6 \%) of the bond length at the interface: the calculated \(\Delta b\) is consistent with the one obtained for MTE structures within 0.03 eV.

On the other hand, the \(\Delta E_b\) term \((i.e.\) the bulk contribution to the VBO) varies
dramatically, showing that the core level binding energies in the strained binary suffers an appreciable change when growing the SL on different substrates. In fact, the energy of the topmost valence level (and hence the binding energy \( E_b \)) is determined by the interplay of the spin-orbit coupling and the non-cubic “crystal field” \(^{22}\). In particular, the second of these two effects is critically dependent on strain conditions, and is thus the origin of the large difference between the \( \Delta E_b \) in Table \( \text{[I]} \). Furthermore, what is remarkable about Table \( \text{[I]} \) is the clear trend shown by the VBO as a function of the substrate lattice constant: the smaller the \( a_{\text{sub}} \), the more the InSb topmost valence level is raised with respect to the VBM of the other SL constituent.

In order to understand more fully the action of the strain on the VBO, we have also estimated the band line-up with respect to unstrained binaries for the [001] interfaces. Thus, we substituted in Eq.(1) the \( \Delta b \) value obtained for [001] interfaces (which was found to be almost independent of strain effects) and the \( \Delta E_b \), evaluated starting from the zincblende bulk unstrained constituents (i.e. disregarding the effect of strain on the binary’s VBM). Taking into account the spin-orbit coupling, we obtain \( \Delta E_{v}^{\text{rel}} = 0.03 \) eV and \( \Delta E_{v}^{\text{rel}} = 0.49 \) eV for the GaSb/InSb and InAs/InSb heterojunctions, respectively. These results match perfectly those reported in Ref. \( \text{[5]} \) and the above mentioned valence bands perfect alignment for the common anion system and \( \Delta E_{v}^{\text{rel}} = 0.51 \) eV for the common cation case, showing that, if strain is not correctly taken into account, completely different results are found.

It is important to notice that the strain acting on the energy of the topmost valence band level is also responsible for the spatial localization of this state. We find, in fact, that in all of the common anion (common cation) structures, the hole carriers are mainly localized on the InSb side of the heterojunction, while in the GaSb/InSb system grown on an InSb substrate we find a complementary situation. This is clear from the decreasing trend of the VBO as the lattice constant is increased and from the sign change in the InSb substrate case (showing that the VMB in GaSb is higher in energy than in InSb).

Figures \( \text{[I]} \) and \( \text{[2]} \), for common-anion and common-cation interfaces respectively, illustrate
the linear dependence (see the solid line in the figures) of the VBO on the lattice parameter which determines the SL pseudomorphic growth. Thus, the two figures show that the GaSb/InSb and InAs/InSb SLs provide a good opportunity for tuning their VBO: a range of about 0.5 eV for common-anion and of 0.7 eV for common-cation systems is covered by varying the strain conditions determined by the substrate.

Let us now compare our results with other theoretical predictions, obtained from model [6,23], semi-empirical [24] and **ab-initio** [10] calculations, as illustrated in Figures 1 and 2. Note that all the predicted values agree with those of the present work (except those of Ref. [23]), within their uncertainty of a few hundredths of an eV [6] and our error bars, respectively. Incidentally, we observe that a similar disagreement between **ab initio** results and those obtained by Cardona and Christensen [23] was also found in other III-V isovalent heterojunctions, such as GaP/InP [10] and GaAs/InAs [11]. Furthermore, the linear trend of the band offset as a function of the strain found in the present work is in excellent agreement with the predictions of other theoretical work [6,23] and is reasonably expected to reproduce the real situation.

So far, we have completely omitted a discussion of the conduction band offset ($\Delta E_c$), due to well known failures of LDA in predicting the correct band gap energies. However, we should now point out that, using an approximate estimate of empirical band gaps (see Ref. [17] for details), we can obtain information on the different kinds of band line-ups as growth conditions are changed. In fact, we find a type I alignment for all the [001] common anion interfaces, while [111] GaSb/InSb shows a type II staggered alignment (partial overlap of the band gaps). On the other hand, for [001] common cation grown both on an InAs and on an average substrate, we find a type II broken gap line-up, with the InAs conduction band minimum lower in energy than the InSb VBM. Finally, the [001] InAs/InSb grown on InSb and the [111] InAs/InSb heterojunctions contain a semimetallic compound (InAs), thus leading to a type III alignment.

Starting from the results obtained from **ab initio** calculations [10,11,4,25] for different [001] oriented strained layer interfaces (with similar lattice mismatch and grown on a sub-
strate having lattice constant averaged over those of the constituents), it is interesting to
discuss the VBO trend as a function of the atomic species involved. We compare the value
obtained for the common anion GaSb/InSb (lattice mismatch of 5.7 % and $\Delta E_v = 0.07$
eV, in good agreement with $\Delta E_v = 0.04$ eV reported in Ref. [4]), with those obtained
for GaP/InP [10] (lattice mismatch of 7.4 % and $\Delta E_v = 0.01$ eV) and for GaAs/InAs [11]
(lattice mismatch of 5.7 % and $\Delta E_v = 0.00$ eV). Taking into account that these results are
obtained by different computational methods and are therefore affected by different error
bars, it appears that, under similar strain conditions, the VBO is almost uninfluenced by
the change of both anions in the common anion systems. Therefore, since the $\Delta b$ term
is expected to be constant (due to similar ionicity difference of the constituents), these re-
sults seem to suggest that also the $\Delta E_b$ term has to be similar in all the GaX/InX (X=P,
As, Sb) structures. A similar $\Delta E_v$ is also found, if we compare our results for InAs/InSb
(lattice mismatch of 6.4 % and $\Delta E_v = 0.54$ eV) with GaAs/GaSb (lattice mismatch of 7.2
%), where both cations are changed ($\Delta E_v = 0.65 \pm 0.1$ eV [23]). This observation can be
explained, considering the anionic character (see Ref. [10], Ref. [17] and references therein)
of the topmost valence level in the binary constituents, which determines the binding en-
ergy contribution ($\Delta E_b$) to the valence band offset: for example, provided that the state of
strain is similar in the constituent materials grown on an average substrate, we don’t expect
a strong difference in the band line-up if we change the cation at both sides of the common
cation interface.

From the experimental point of view, the high mismatch (about 6 %) between the lattice
constants of the two SL constituents results in great difficulty to grow the SL systems,
without misfits and dislocations. Only recently, an InSb quantum-well has been realized in
GaSb [2]; starting from photoluminescence peak emission energy data and from calculations
based on a standard finite square-well model [23,24] (taking into account strain [28,29]), a
VBO of 0.16 eV was obtained that is quite different from the one, 0.34 eV, reported in Table
[1]

Unfortunately, a similar disagreement between theoretical and experimental data, ob-
tained using different techniques, was found also for other homopolar isovalent III-V interfaces, such as the GaAs/InAs (see Ref. [11] and references therein) and GaP/InP ($\Delta E_v = 0.01$ eV, the theoretical result [10] against $\Delta E_v = 0.60$ eV, the experimental results from photoluminescence [30]) systems, that are reasonably close to the common-anion one studied here. In particular, in a recent work focused on GaAs/InAs SLs, Ohler et al. [31] obtained (from ultraviolet photoelectron spectroscopy measurements of the cation $d$-core levels) a $\Delta E_v$ value in disagreement (by as much as 0.3 eV) with theoretical predictions [6,7,9,11]. Notwithstanding some differences between the experimental and theoretical VBO values, many important observations discussed above are confirmed by Ohler et al. experimental work [31]. For example, the linear trend found [31] for $\Delta E_v$ (in GaAs/InAs SLs) as a function of $a_{\text{sub}}$ agrees with theoretical predictions [11] and with our results; further, the independence of the $\Delta_b$ term on the strain conditions discussed above, is experimentally confirmed [31] by the trend of the In $4d/2$ and Ga $3d_{3/2}$ core-level binding energy difference, which is almost unaffected by the different substrate used in growing the heterostructure.

As a last comment, we think that it worthwhile to remark that the linear trend found in Ref. [11] for the GaAs/InAs VBO’s as a function of the growth conditions leads to a slope that is almost equal to that of Fig. 1 for GaSb/InSb systems. Starting from the band offset transitivity rule - which is well established (to within 0.02 eV) [16] for [001] common-atom superlattices - we can derive the VBO for the InAs/GaSb system, an almost lattice matched interface (the two lattice constants differ only by 0.6 %). This system is attracting more and more attention recently for its unusual type II broken-gap band line-up. Through a linear interpolation of the common-anion band offsets as a function of the substrate lattice constant, we have calculated the VBO for the GaSb/InSb system as if grown on an InAs substrate. As evidenced above (see Fig. 1), the linear approximation is expected to be reasonably valid; furthermore, in this case the extrapolation is obtained for a lattice constant ($a_{\text{InAs}}$) which differs by only 0.7 % from one of our self-consistent results ($a_{\text{GaSb}}$). We thus report in Fig. 3 our calculated VBO for the common-cation SL on an InAs substrate and the extrapolated value for the ideal common-anion SL grown on an InAs
substrate. Using the transitivity rule, we obtain:

$$
\Delta E_v(InAs/GaSb) = \Delta E_v(InAs/InSb)_{InAs-sub.} - \Delta E_v(InSb/GaSb)_{InAs-sub.}
$$

so that $$\Delta E_v(InAs/GaSb)_{InAs-sub.} = 0.88 - 0.40 = 0.48 \text{ eV}.$$ This result is in good agreement with the available experimental values (0.46 eV [32], 0.51 eV [33]).

**IV. CONCLUSIONS**

In summary, we have studied the valence band offsets in [001] and [111] GaSb/InSb and InAs/InSb interfaces by means of *ab-initio* FLAPW calculations, focusing our attention on its dependence on ordering direction and strain conditions. Our results indicate that, under the same strain conditions, the former has quite a small effect on the band line-up mainly due to the different structural relaxation of the interface atoms at the [001] and [111] heterojunctions. On the other hand, a much more important effect is due to pseudomorphic growth on different substrates: the high tunability of the VBO (about 0.5 eV and 0.7 eV for common-anion and for common-cation SLs, respectively) is evidenced by its linear decreasing trend as the substrate lattice constant is increased, mainly due to the bulk contribution to the band line-up. Finally, the transitivity rule was used to determine the InAs/GaSb valence band offset and good agreement between theory and experiment was obtained.

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TABLES

TABLE I. Interface term ($\Delta b$), strained bulk term ($\Delta E_b$) and valence band offset ($\Delta E_v$) for elastically relaxed (GaSb)$_3$/(InSb)$_3$ and (InAs)$_3$/(InSb)$_3$-average substrate-superlattices as a function of the ordering direction ($\Delta E_b^{(nr)}$ and $\Delta E_v^{(nr)}$) and including ($\Delta E_b^{(r)}$ and $\Delta E_v^{(r)}$) spin-orbit effects). Energy differences (in eV) are considered positive if the level relative to the InSb layer is higher in energy with respect to the GaSb (InAs) layer in the common-anion (common-cation) system.

|       | $\Delta b$ | $\Delta E_b^{(nr)}$ | $\Delta E_b^{(r)}$ | $\Delta E_v^{(nr)}$ | $\Delta E_v^{(r)}$ |
|-------|------------|----------------------|----------------------|----------------------|----------------------|
| (GaSb)$_3$/(InSb)$_3$ | [001] | +0.19 | -0.21 | -0.12 | -0.02 | +0.07 |
|       | [111] | +0.29 | -0.27 | -0.13 | +0.02 | +0.16 |
| (InAs)$_3$/(InSb)$_3$ | [001] | +0.07 | +0.27 | +0.47 | +0.34 | +0.54 |
|       | [111] | +0.17 | +0.30 | +0.51 | +0.47 | +0.68 |

TABLE II. Interface term ($\Delta b$), strained bulk term ($\Delta E_b$) and valence band offset ($\Delta E_v$) for (GaSb)$_3$/(InSb)$_3$ and (InAs)$_3$/(InSb)$_3$ [001] superlattices as a function of the substrate lattice parameter neglecting ($\Delta E_b^{(nr)}$ and $\Delta E_v^{(nr)}$) and including ($\Delta E_b^{(r)}$ and $\Delta E_v^{(r)}$) spin-orbit effects). Energy differences (in eV) are considered positive if the level relative to the InSb layer is higher in energy with respect to the GaSb (InAs) layer in the common-anion (common-cation) system.

|       | $\Delta b$ | $\Delta E_b^{(nr)}$ | $\Delta E_b^{(r)}$ | $\Delta E_v^{(nr)}$ | $\Delta E_v^{(r)}$ |
|-------|------------|----------------------|----------------------|----------------------|----------------------|
| (GaSb)$_3$/(InSb)$_3$ | GaSb-subs. | +0.20 | +0.10 | +0.14 | +0.30 | +0.34 |
|       | Av. subs. | +0.19 | -0.21 | -0.12 | -0.02 | +0.07 |
|       | InSb-subs. | +0.18 | -0.47 | -0.34 | -0.29 | -0.16 |
| (InAs)$_3$/(InSb)$_3$ | InAs-subs. | +0.09 | +0.65 | +0.79 | +0.74 | +0.88 |
|       | Av. subs. | +0.07 | +0.27 | +0.47 | +0.34 | +0.54 |
|       | InSb-subs. | +0.05 | -0.04 | +0.18 | +0.01 | +0.22 |
FIGURES

FIG. 1. Valence band offset (in eV) for GaSb-InSb SLs as a function of the substrate lattice parameter. Our results (together with their error bars) are evidenced by filled squares ([001] SLs) or filled circles ([111] SLs) and solid line. The dotted line shows the behaviour of unstrained GaSb and InSb. Empty squares: Ref. [23]; empty diamonds: Ref. [6]; filled diamond: Ref. [24]; empty circles: Ref. [10].

FIG. 2. Valence band offset (in eV) for InAs/InSb SLs as a function of the substrate lattice parameter. Symbols are the same as those in Fig. 1.

FIG. 3. Valence band offset (in eV) for InAs/GaSb interface, obtained using the transitivity rule.
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FIG. 1

Substrate lattice constant

GaSb/InSb

Valence Band Offset (eV)

FIG. 2

Substrate lattice constant

InAs/InSb

Valence Band Offset (eV)
$\Delta E_v = 0.48 \text{ eV}$
(InAs subs.)

$\Delta E_v = 0.40 \text{ eV}$
(InAs subs.)

$\Delta E_v = 0.88 \text{ eV}$
(InAs subs.)