Evolution of the band-gap and band-edge energies of the lattice-matched Ga In As Sb/ Ga Sb and Ga In As Sb/ In As alloys as a function of composition

Rita Magri, Alex Zunger, and H. Kroemer

Citation: Journal of Applied Physics 98, 043701 (2005); doi: 10.1063/1.2010621
View online: http://dx.doi.org/10.1063/1.2010621
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/98/4?ver=pdfcov
Published by the AIP Publishing

Evolution of the band-gap and band-edge energies of the lattice-matched GaInAsSb/GaSb and GaInAsSb/InAs alloys as a function of composition

Rita Magri[a)]
I N F M (INFM)- [3] D F , M R E , M 41100, I

Alex Zunger
N R E L , G , C 80401

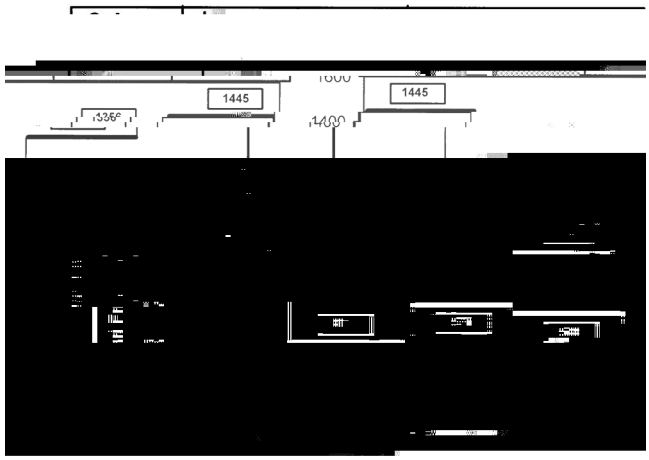
H. Kroemer
D E C E , C B (C B), B , C 93106

Recei ed 29 No ember 2004; accepted 8 Jul 2005; published online 16 August 2005

Using atomistic pseudopotential calculations e predict the e olution of the alence-band ma imum energ $E_{\Box}$, and conduction-band minimum energ E , for a compositionall graded quaternar Ga_{13} In As Sb_{13} allo lattice matched to GaSb or InAs as a function of , or, equi alentl , as a function of distance from the substrate. We nd up ard-conca e bo ing for both E and $E_{\Box}$, in contradiction ith simple interpolati e models. A transition from staggered t pe II to broken-gap t pe III lineup relati e to GaSb is predicted to occur at =0.81 and =0.92 on a GaSb substrate, and at =0.59 and =0.62 on an InAs substrate. In the latter case, the quaternar allo has a minimum gap at =0.85 and =0.87. *2005 A I P .*
DOI: 10.1063/1.2010621

I. INTRODUCTION

The materials belonging to the 6.1 lattice-constant famil of semiconductors InAs, GaSb, and AlSb are becoming increasingl important for a large ariet of applications, ranging from transistors both bipolar and eld-effect transistors FETs , to infrared detectors, photomi ers, resonant tunnel diodes, and superlattices for quantum cascade lasers and other applications.[1] All these heterostructure de ices in- ol e at least t o of the three semiconductors of the famil . The t o dominant properties in such heterointerfaces are the fact that: i GaAs, InAs, InSb, and GaSb ha e an unusual set of band alignments[2,3] Fig. 1 spanning t pe-I straddling arrangement in GaAs/InAs, GaSb/InSb, and GaSb/GaAs, as ell as t pe-III broken-gap arrangement in InAs/InSb and InAs/GaSb; and ii b simultaneousl adjusting the allo composition , in a particular fashion = , it is possible to maintain a ed lattice constant , for the entire Ga_{13} In As Sb_{13} composition range. For e ample, one can select a function = so that , $\equiv$ $_{GaSb}$, thus the allo can be gro n lattice matched on a GaSb substrate. This can be accomplished b starting ith GaSb, then adding both a fraction of In and a fraction of As in a graded fashion e.g., 1% composition change per monola er , reaching e entuall the ternar $InAs_{0.89}Sb_{0.11}$ hich is lattice matched to GaSb. Gi en i and ii abo e, it is interesting to inquire ho ould the allo band gap E , and the alence as ell as the conduction-band edges $E_{\Box}$, and E , depend on the composition , under lattice-matched conditions. To in estigate the beha ior of band lineups under compositional grading is important: for e ample, high-speed bipolar transistors increasingl emplo designs in hich the energ gap in the base regions decreases from emitter to collector to speed up the o of minorit carriers. In fact, the technolog of transistors based on Si/Ge allo s[4] ielding the fastest Si-based transistors is entirel based on this principle. But the amount of grading is limited b the se ere 4% lattice mismatch bet een Si and Ge. In a GaSb-to-InAs graded base, strain can be a oided using the quaternar s stem, and much larger energ -gap gradients could be emplo ed. In order to design such a de ice, ho e er, it is essential to kno ho e actl the energ gap aries along the



[a] Electronic mail: magri@unimo.it

gradient. It is also important to determine hat ill be the nature of the bo ing up ards or do n ards of the conduction-band minimum CBM and the alence-band ma imum VBM and at hich composition , ould the s, stem Ga_{13} In As Sb_{13} matched to GaSb or InAs re ert from t, pe II staggered to t, pe III broken gap . Would the band gap of the quaternar, ha e a minimum at some intermediate ? It is of fundamental importance to ans er these questions since quaternar, allo, s at different compositions pro ide the de ice engineer ith a larger e ibilit, in the tuning of de ice characteristics such as band gaps and band offsets bet een the components. Unfortunatel, , hile most of the band-structure parameters of binar, and ternar, III V s, stems are kno n,[5] no analogousl, detailed informations about the quaternar, s, stem can be found in the literature.

The paper is organi ed as follo s. In Sec. II e use elasticit, , to determine the lattice-matching condition = of the quaternar, allo, Ga_{13} In As Sb_{13} ith the substrate, GaSb or InAs, and compare the results ith the usuall, emplo, ed appro imations based on Vegard's La . In Sec. III e present our atomistic empirical pseudopotential method EPM used to sol e the band structure of the narro gap quaternar, Ga_{13} In As Sb_{13} random allo, . In Sec. IV e sho our results for the alence- and conduction-band edges $E_{\square}$ and E as a function of the allo, composition = for Ga_{13} In As Sb_{13} gro n both on GaSb and InAs, and compare the results ith the interpolati e models idel, used b, the de ice engineers' communit, .[5] In Sec. V e determine the fraction of In and of As ia = , in the quaternar, allo, s gro n on GaSb or InAs at hich the transition from a staggered to a broken-gap lineup ith the substrate takes place. Finall, , in Sec. VI e compare our theoretical predictions for band alignments and band gaps ith the a ailable e perimental data present in the literature.

II. FINDING VARIOUS SUBSTRATE-MATCHING $X = F(Y)$ CONDITIONS

Here e contrast Vegard-like appro imations[6] ith atomistic strain minimi ing predictions.[7]

A. Vegard's law

The simplest Vegard-like appro imation for a quaternar, is

$$, = {}_{\mathrm{InAs}} + 1\,3 \quad {}_{\mathrm{GaAs}} + 1\,3 \quad {}_{\mathrm{InSb}} + 1\,3 \quad \square\ 1\,3 \quad {}_{\mathrm{GaSb}}. \qquad 1$$

The condition , ≡ , ith = $_{\mathrm{GaSb}}$ or ith = $_{\mathrm{InAs}}$ leads to the function = $_{\mathrm{Vegard}}$ for hich Ga_{13} In As Sb_{13} is lattice-matched to GaSb. Other appro imations include the linear =0.89 rule obtained b, considering the quaternar, allo, Ga_{13} In As Sb_{13} as the solid solution[5] of GaSb and the lattice-matched ternar, $InAs_{0.89}Sb_{0.11}$ allo, , that is GaSb InAs

InSb+GaAs is the correct description since In Sb plus Ga As bonds are the majorit, .

To decide hat atomic arrangement is thermod, namicall, the more appropriate one for Ga_{13} In As Sb_{13} , one can proceed as in Ref. 9 and minimi e the energ, functional,

$$E_{\text{tot}} \quad , \quad \mathbf{R} \, , \; = 1, \ldots, N \quad = E_{\text{chem}} \quad ,$$
$$\mathbf{R} \, , \; = 1, \ldots, N \quad + E_{\text{strain}} \quad ,$$
$$\mathbf{R} \, , \; = 1, \ldots, N \quad , \qquad 3$$

here indicates that E_{tot}, E_{chem}, and E_{strain} are functionals of the atomic con, gurations obtained b, differentl, arranging the cations Ga, In and the anions As, Sb on the N sites of a inc-blende lattice. In Eq. 3

$$E_{\text{chem}} = \frac{1}{2} \quad E \quad _3 \, , \qquad 4$$

here $_3$ is the number of bonds of t, pe 3 , and E is the

to be adjusted in order to minimi e the elastic energ . This leads to a strong dependence of the calculated bond lengths, bond angles, and a is at the minimum elastic energ on the initial distribution of atoms ithin the 512 unit cell. In the case of the ternar allo one has to adjust onl t o kind of bonds In As and In Sb and the three different kind of bond angles, thus the nal minimum energ con guration is less sensiti e to the initial choice of the atomic positions.

To each ed In fraction , there corresponds a small range of possible As compositions for hich the quaternar allo is lattice matched to its substrate. B a eraging o er a number of different atomic con gurations e calculate the quaternar allo lattice parameter , hich satis es the matching condition ith the substrate. The lattice parameter , obtained using the atomistic calculations turns out to be different from the Vegard-like beha ior gi en b Eq. 1 . This is true e en in the simpler case of ternar allo s, as seen in Fig. 4 hich compares the lattice constant of the ternar InAs Sb_{1-3} allo gi en b Vergard's la dashed line ith that obtained b the atomistic calculation a eraged o er a large number of different atomic con gurations, full dots . The lattice parameter predicted b the atomistic elasticit departs from the linear Vegard trend mostl around composition =0.5, here the In As and In Sb

, it does not ha e the band-gap error problem,[17] thus the band gaps are in good agreement ith the e perimental alues. , because of the small cutoff needed in $v_{\square}\,\mathbf{G}$ the method is much faster computationall , and thus can treat s stems ith hundreds and thousands of atoms per unit cell. This is essential for the description of random allo s here the con gurational and atomic disorder effects are rele ant. Such effects are often neglected b the irtual cr stal ap-pro imation VCA currentl emplo ed together ith self-consistent DFT-LDA calculations.[18]

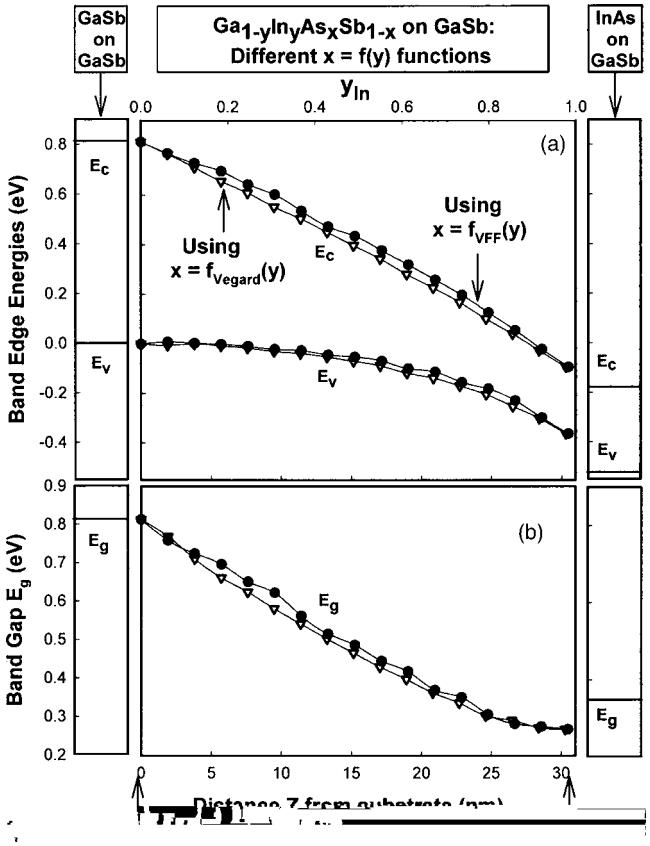


FIG. 6. Comparison of: a the alence- and conduction-band edges and b band gaps of the quaternar, Ga_{13} In As Sb_{13} /GaSb allo, calculated using the Vegard-like lattice-matching functions = Vegard do n ard empt, triangles ith the = VFF e tracted b, the atomistic VFF calculations full circles .

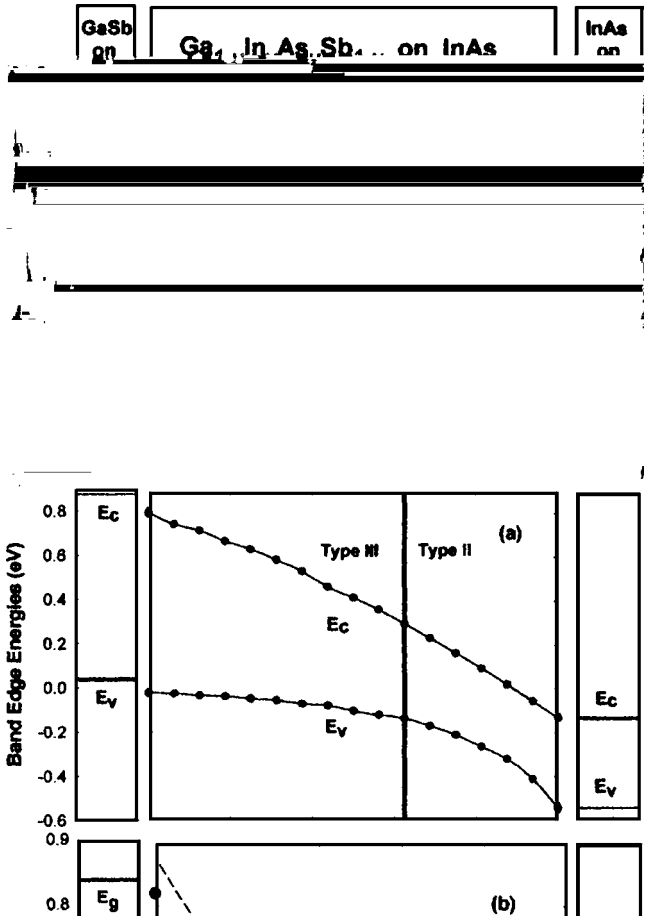


FIG. 7. a

de ice application, the free passage of electrons from the InAs conduction band to the GaSb alence band could be either desirable Ohmic contacts bet een and or it could be a nuisance. The strong positi e bo ing of the alence-band edge found in this ork see Figs. 5 7 sho s that grading should be a oided at all cost if interband transport is desirable, but ould be er, bene, cial to the opposite objecti e.

To understand the une pected negati e bo ings of the conduction-band edges in Figs. 5 and 7 e , rst note that the, are displa, ed ith respect to the standard[5] linear interpolation of band edges of GaSb and $InAs_{0.89}Sb_{0.11}$ for the GaSb substrate, Fig. 5 , and InAs and $GaAs_{0.08}Sb_{0.92}$ for the InAs substrate, Fig. 7 . These reference materials ha e almost e clusi el, Ga Sb and In As bonds ith a er, small percentage of In Sb bonds for the GaSb substrate or Ga As bonds for the InAs substrate . This choice of end-point reference materials is different from the usual practice in ternar, allo, s, such as InAs Sb_{13} here the bo ing is aluated relati el, to the linear interpolation InAs + 1 3 InSb of the t o end-point materials InAs and InSb. The latter is a consistent choice since the ternar, allo, has the same bonds In As and In Sb as the end points. But in the quaternar, allo, Ga_{13} In As Sb_{13} four bonds Ga Sb, In As, In Sb, and Ga As are present, , et the, are not considered hen the quaternar, is considered as the superposition of GaSb and $InAs_{0.89}Sb_{0.11}$ for the GaSb substrate or as the superposition of InAs and $GaAs_{0.08}Sb_{0.92}$ for the InAs substrate .

To illustrate ho bo ing depends on reference energies, e sho in Fig. 8 for the quaternar, allo, gro n on InAs b, the solid circles the energ, ΔE = ; of the EPM-calculated conduction-band minimum E ith respect to the con entional reference energ, E^{TR} of ,

$$\Delta E^{TR} = \quad ; \quad = E \text{ Ga}_{13} \text{ In As Sb}_{13}/\text{InAs } 3\, E^{TR} \quad , \tag{9}$$

here

$$E^{TR} = E \text{ InAs} + 1\,3 \quad E \text{ GaAs}_{0.08}\text{Sb}_{0.92}/\text{InAs} \; . \tag{10}$$

We see that $\Delta E^{TR} \Delta 0$, impl, ing negati e bo ing $\Delta 0$ as also seen b, the solid circles in Fig. 7 a . To see that this $\Delta 0$ is merel, an artifact of selecting E^{TR} of Eq. 10 as a reference, e also sho in Fig. 8 the energ, of the conduction-band minimum solid circles ith respect to the alternati e reference energ, E^{BR} of constituents,

$$E^{BR} = E^{InAs} + 1\,3 \quad E^{GaAs} + 1\,3 \quad E^{InSb} + 1\,3 \quad \square\ 1\,3 \quad E^{GaSb}. \qquad 11$$

Gi en

$$\square E^{BR} = \quad ; \quad = E\ \ Ga_{1\,3}\ In\ As\ Sb_{1\,3}\ /InAs\ \ 3\ E^{BR} \quad , \qquad 12$$

e see that $\square E_c^{BR} \square 0$, impl, ing a bo ing $\square 0$, as normall, e pected. Since the reference $E^{BR} \quad \square E^{TR}$ e see that

$$E \quad = E \quad = 0\ 3\ \frac{\square^{\ 2}}{+\square}. \qquad 13$$

The parameters $\square$ and $\square$ for GaSb, InAs, GaAs, and InSb are gi en in Ref. 5. For the quaternar, allo, ith In composition and As composition e estimated the $\square$ and $\square$ parameters using a linear interpolation of the binar, $\square$ and $\square$ alues, using an e pression of the form as in Eq. 1 . We can see in Fig. 5 b that the =0 K translated e perimental data lie bet een the dashed line corresponding to the relation for E at =0 K proposed in Ref. 5 and our calculated alues, and there is a difference of the order of about 30 meV at =0.16 among the band-gap alues measured b, different groups. Our calculated alues are al a, s slightl, than the e perimental data for $\square$0.1 and the de iation bet een e periment and theor, seems to increase ith increasing In and As content. Unfortunatel, , in the energ, range 0.30 $\square$ $\square$0.70, here the differences bet een the predictions of the atomistic calculations and of the interpolati e schemes are larger, the quaternar, allo, presents a miscibilit, gap.[28] Until recentl, onl, t o lattice-matched regions ith indium content 0$\square$ $\square$0.28 and $\square$0.70 ere successfull, gro n and onl, for these compositions measurements of the band gaps ha e been performed. Reference 28 reports the measurement of a minimum gap E =0.34 eV at =77 K and E =0.26 eV at =300 K, smaller than the gap of InAs, for the quaternar, allo, ith $\square$0.70. Our calculations predict gaps from 0.27 to 0.35 eV in the range $\square$0.75 in reasonable agreement ith the e perimental alues.

E perimental alues of E of Ga

ACKNOWLEDGMENTS

One of the authors R.M. ackno ledges the European