Theoretical calculation of band-edge discontinuities near a strained heterojunction: Application to (In,Ga)As/GaAs

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Energy-band lineups at [100] GaAs/(In,Ga)As heterojunctions are calculated using a self-consistent tight-binding treatment. We distinguish (i) the modification of bulk band structures due to strain, and (ii) a shift of one bulk structure with respect to the other, due to charge transfer across the interface. The main result is that, for a system strained to the GaAs lattice parameter, depending on the indium concentration, light and heavy holes can be localized either both in the same layer, or in the two different layers. Comparison with different experiments provides fairly good agreement.

Some strained superlattices like the $In_xGa_{1-x}As$/GaAs system are important heterostructures for high-speed and optoelectronic device applications. Because of this, and the interest in understanding the physics of strained quantum-well structures (QWS's) and superlattices, several experimental studies of this system have been performed in the last few years.[1-8] Recent theories that consider charge-transfer effects at the heterojunction interface provide reasonable agreement with experiment for unstrained systems. These theories include the *ab initio* self-consistent pseudopotential calculations by Van de Walle and Martin,[9] the "midgap" theories by Tersoff[10] and by Cardona and Christensen,[11] and also tight-binding calculations.[12,13] The agreement between the theories and published experimental results is not as good for systems with lattice mismatch (except for the first-principles study on Si/Ge in Ref. 9). Until now, the only *ab initio* calculation of the InAs/GaAs band offset has been mentioned in Ref. 11 but has not been published. The self-consistent tight-binding description of unstrained [100] heterostructures has recently provided theoretical values for band offsets that agree fairly well with experimental data (0.496 eV for GaAs/AlAs, 0.390 eV for CdTe/HgTe, and 0.451 eV for GaSb/AlSb).[14] The main reason for this agreement is that realistic electronic bulk structures and dielectric constants are used in this calculation. In this paper we show how we can extend this technique to strained structures.

For device application, different systems are interesting: (In, Ga)As/GaAs on a GaAs substrate, that provides QWS's with a band gap smaller than GaAs (which cannot be obtained with any GaAs lattice-matched system): and $In_xGa_{1-x}As/In_yGa_{1-y}As$ on an InP substrate that provides gaps smaller than in InP lattice-matched materials. In order to estimate band offsets in these systems, we first give the results for GaAs/InAs, under different strains, the whole system being strained in the direction parallel to the interface plane to (i) the GaAs lattice parameter, (ii) the InAs lattice parameter, and (iii) an intermediate configuration, the InP lattice parameter. In these systems the strain is either (i) and (ii), confined to one side of the heterojunction, or (iii), shared by both sides. We discuss the effect of the strain and estimate roughly the effect of indium concentration on band lineups. Finally, we compare our calculated results and published experimental data, showing that all available experiments can be explained satisfactorily with our single calculation.

Despite the lattice mismatch ($\sim 7\%$) between GaAs and InAs, high-quality strained single- and multiple-quantum-well structures as well as superlattices can be grown, provided the thickness of the strained layers is kept small enough to avoid a misfit dislocation generation.[3,15,16] In such layers the lattice mismatch is entirely taken up by elastic strain. Then the effect of the strain in the QWS's can be considered in terms of atomic rearrangement: the in-plane parameter is imposed by the substrate or the buffer layer that determines the biaxial stress in each layer. From a tight-binding point of view, this atomic rearrangement induces a modification of off-diagonal interactions,[17] and also[18] a modification of atomic-level parameters. The biaxial stress can be decomposed as the sum of a purely hydrostatic part plus a uniaxial part. Equations (1) give the modifications of the band edges in a bulk crystal under biaxial stress, related to the a and b deformation potentials,[17]

$$
\begin{aligned}
&\Delta(E_c-E_v^{\mathrm{av}})=3a\epsilon_h+a(\epsilon_u^{xx}+2\epsilon_u^{zz})\ ,\\
&E_{v2}-E_v^{\mathrm{av}}=\tfrac{1}{3}\Delta_0-b(\epsilon_u^{xx}-\epsilon_u^{zz})\ ,\\
&E_{v1}-E_v^{\mathrm{av}}=-\tfrac{1}{6}\Delta_0+\tfrac{1}{2}b(\epsilon_u^{xx}-\epsilon_u^{zz})+\tfrac{1}{2}[\Delta_0^2+2\Delta_0 b(\epsilon_u^{xx}-\epsilon_u^{zz})+9b^2(\epsilon_u^{xx}-\epsilon_u^{zz})^2]^{1/2}\ ,\\
&E_{v3}-E_v^{\mathrm{av}}=-\tfrac{1}{6}\Delta_0+\tfrac{1}{2}b(\epsilon_u^{xx}-\epsilon_u^{zz})-\tfrac{1}{2}[\Delta_0^2+2\Delta_0 b(\epsilon_u^{xx}-\epsilon_u^{zz})+9b^2(\epsilon_u^{zz}-\epsilon_u^{zz})^2]^{1/2}\ ,
\end{aligned}
\tag{1}
$$

where E_{v1}, E_{v2}, E_{v3} are the tops of the three upper valence bands, E_v^{av} their average value Δ_0 the spin-orbit splitting at the top of the valence band for unstrained bulk, and the hydrostatic ϵ_h and uniaxial ϵ_u^{xx} and ϵ_u^{zz} (with x the growth axis) strain components are given by

$$\begin{aligned}
\frac{a_\perp}{a_\parallel} &= \left[1+2\frac{C_{12}}{C_{11}}\right]\frac{a_0}{a_\parallel}-2\frac{C_{12}}{C_{11}}\,, \\
\epsilon_u^{zz} &= \frac{1-a_\perp/a_\parallel}{1+a_\perp/a_\parallel+C_{11}/C_{12}}\,, \\
\epsilon_u^{xx} &= -\left[\frac{C_{11}+C_{12}}{C_{12}}\right]\epsilon_u^{zz}\,, \\
\epsilon_h &= \frac{a_\parallel}{a_0}\left[\frac{1}{1+\epsilon_u^{zz}}\right]-1\,,
\end{aligned} \tag{2}$$

where a_0 is the lattice parameter of the unstrained bulk, $a_\parallel$ is the imposed in-plane parameter, $a_\perp$ is the deduced interplane parameter, and C_{11} and C_{12} are the elastic constants of the material. Equation (2) is obtained by simple identification of macroscopic deformations in a material under biaxial stress, and in a material that has been first hydrostatically stressed and then uniaxially stressed. The ratio $a_\perp/a_\parallel$ is obtained by writing that the (y,z) surfaces are not stressed ($\sigma_{xx}=0$). At this point it is important to notice that the atomic rearrangement also induces a modification of the Madelung sums in the self-consistent solving of Poisson's equation (see Ref. 18 for details).

Using the self-consistent tight-binding description given in Ref. 18 and the heterojunction treatment described in Ref. 14, we have self-consistently calculated the band-edge alignment in the three systems made by a well of a few (1–8) layers of InAs between two semi-infinite GaAs crystals, with an in-plane lattice parameter strained to (i) the GaAs value, (ii) the InAs value, and (iii) the InP value. First, we have checked that, for a given strain, the width of the well has no influence on the band offset: As soon as the well is made by two layers or more, the obtained offset does not vary substantially. In Fig. 1 one can observe the band alignment obtained at GaAs/InAs heterojunctions for the three considered strain configurations. We can separate the offset of a strained heterojunction into two components: ΔE_v^{av}, the discontinuity of the average top of the valence bands resulting from charge transfers at the interface (which of course varies with the strain), and the splittings of the top of valence band in each strained bulk material, given in Eq. (1). An important result that can be observed in Fig. 1 is that the ratio $\Delta E_c/\Delta E_v^{av}$ strongly depends on the strain as it varies from $\frac{87}{13}$ for (i) to $\frac{63}{37}$ for (ii), with an intermediate value of $\frac{74}{26}$ for (iii). Figure 1 also clearly shows that the three cases considered correspond to three different localization of holes: In (i) both light and heavy holes are confined in InAs layers, whereas in (ii) and (iii) heavy holes are confined in InAs layers and light holes in GaAs layers.

To compare our theoretical result with the pioneer experimental result of Kowalczyk *et al.*[1] on the

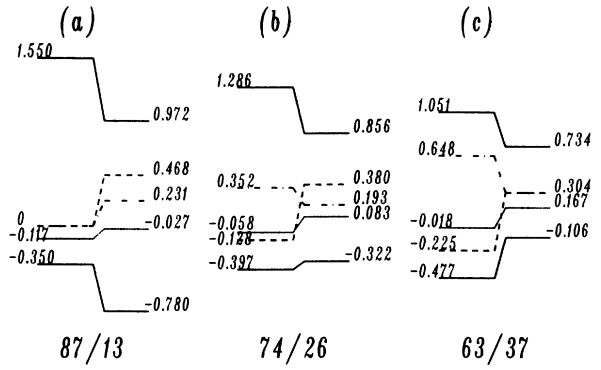

FIG. 1. Band alignment at GaAs/InAs heterojunctions strained to (a) the GaAs parameter (5.654 Å), (b) the InP lattice parameter (5.869 Å), and (c) the InAs lattice parameter (6.058 Å). At the top of the valence band the dotted curve corresponds to E_v^{av}, the dashed curve to heavy holes, the dashed-dotted curve to light holes, and the solid curve to the third top of valence band. GaAs is always on the left-hand side. The values of $\Delta E_c/\Delta E_v^{av}$ are indicated in each case. Energies are given in eV. The valence-band splittings are those obtained in the tight-binding approximation and then are different from those obtained with experimental deformation potentials (see the text).

InAs/GaAs(100) heterojunction, it is not possible to talk in terms of ΔE_v, as Ref. 1 neglects the effect of strain (in the InAs layer) on the valence band. However, if we assume that our atomic levels are rigidly bound to core levels, and using experimental values of unstrained materials $(E_{\text{Ga }3d}^{\text{GaAs}}-E_v)=18.81\pm0.02$ eV and $(E_{\text{In }4d}^{\text{InAs}}-E_v)=17.43\pm0.02$ eV, we can deduce from our calculated value of the "unstrained ΔE_v," 0.235 eV, a theoretical value of $\Delta E_{\text{cl}}=1.61\pm0.05$ eV, which agrees fairly well with the experimental determination, i.e., 1.55 ± 0.02 eV.

The estimated numerical accuracy of our calculated ΔE_v^{av} is about a few meV. The greatest limitation of our calculation is bound to the fact that our tight-binding predictions for the uniaxial deformation potentials "b" differ somewhat (Ref. 19) from experimental values.[20] This point has been discussed in Ref. 18. We have numerically estimated the influence of this error on ΔE_v^{av} and have found a few tenths of a meV. The error on the splittings of the top of the valence band is much more important. A more reliable way to deduce offsets in our strained systems would be then to use our calculated ΔE_v^{av}, and to add the splittings given in (1), where the exact experimental values of b are injected. This we do in the forthcoming cases.

Most of the available experiments about the GaAs/$In_xGa_{1-x}As$ systems correspond to alloys with $x\neq1$. It is possible to deduce from our results corresponding to $x=1$ the band configuration for every $x\neq1$: In a virtual potential approximation, ΔE_v^{av} varies linearly with indium concentration (this result seems to correspond to the actual situation and has been observed in different systems[21]). The splittings $E_{vi}-E_v^{av}$ in $In_xGa_{1-x}As$ can be calculated using (1). In this way we

TABLE I. Band-alignment data for the $In_{0.05}Ga_{0.95}As/GaAs$ system strained to GaAs. The notation is that given in Ref. 7.

	This work	Expt.
$\Delta E_c/\Delta E_{gh}$	0.41	0.40±0.04
ΔE_{vh} (meV)	10	35,41[a]

[a]Reference 7; the two values corresponding to the two samples which are reported.

have first considered the $In_{0.05}Ga_{0.95}As/GaAs$ system strained to GaAs experimentally studied in Ref. 7. Table I summarizes the comparison between our results and those obtained in Ref. 7. The difference between the calculated (20 meV) and experimentally deduced (36 and 41 meV) ΔE_{vh} is about 20 meV, which is greater than our numerical accuracy for $x=0.05$, which would be of the order of a few meV. However, the discrepancy is small enough that we cannot consider that our calculation really contradicts (Ref. 7). At this point it is important to notice that a slight shift in indium concentration, such as 7% In instead of 5%, will shift up the ΔE_v^{av} by 4 meV and will also make the difference between E_{hh} and E_v^{av} greater by 6 meV, so that the theoretical ΔE_{vh} for $Ga_{0.93}In_{0.07}As$ becomes 30 meV. We can note that both in the experimental and theoretical cases the small difference between ΔE_{vh} (20–40 meV), the heavy-hole band offset, and ΔE_{lh} (26 meV), the splitting between light and heavy holes, does not allow us to derive a definite conclusion about light-hole localization: Whether they are localized in GaAs or in $Ga_{1-x}Al_xAs$, the well or barrier height is only about 10 meV.

We have also considered $In_{0.15}Ga_{0.85}As/GaAs$ strained to GaAs (Refs. 2, 5, 6, and 8) (these different works being rather coherent). Our predictions are in excellent agreement with the results of Ref. 2 since we obtain $\Delta E_{vh}=56$ meV and $\Delta E_{vl}=-15$ meV when experiment gives $+52$ and -18 meV. It is interesting to note that a superlattice such as $GaAs/In_xGa_{1-x}As$ strained to GaAs can form a type-I superlattice for both light and heavy holes when $x=1$, and, on the contrary, form a type-II superlattice for light holes, remaining type I for heavy holes when $x<1$ (as here when $x=0.15$).

We have also considered the $In_{0.40}Ga_{0.60}As/In_{0.63}Ga_{0.37}As$ system strained to InP already observed in Ref. 22. The band configuration obtained is summarized in Fig. 2. The photoluminescence experiments performed in Ref. 22 do not allow us to deduce the band offset precisely, but the configuration we have obtained corresponds to what is assumed to interpret the observed excitonic transitions.

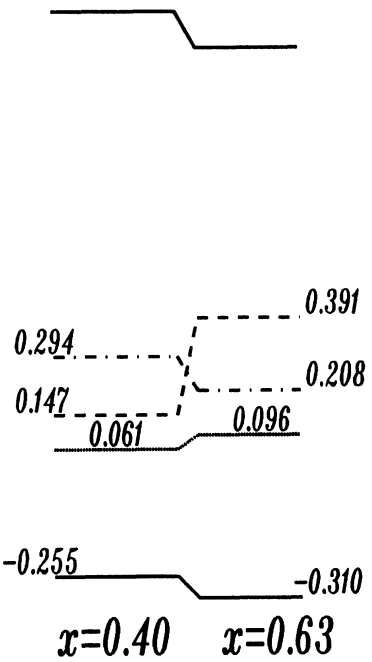

FIG. 2. Band alignment at $In_{0.40}Ga_{0.60}As/In_{0.63}Ga_{0.37}As$ heterojunction strained to the InP parameter. The same notations as in Fig. 1 are used. Left-hand side $x=0.40$, right-hand side $x=0.63$.

In conclusion, here we have extended a tight-binding calculation of band offsets to strained structures. The strains are straightforwardly taken into account. We have theoretically shown that the ratio $\Delta E_c/\Delta E_v^{av}$ (where ΔE_v^{av} is the average top of the valence bands) and the localization of light and heavy holes strongly depend on strains and indium concentration. Comparison with available experimental data is quite satisfactory.

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[20]The experimental deformation potentials given in *Landolt-Börnstein: Numerical Data and Functional Relationships in Science and Technology,* edited by O. Madelung (Springer-Verlag, Berlin, 1982), are $a=-9.2$ eV and $b=-2$ eV for GaAs and $a=-6$ eV and $b=-1.8$ eV for InAs.

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