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Self-consistent calculation of properties of GaAs-AlAs superlattices with homopolar interfaces

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A variational method in terms of Wannier functions is used to study the structural and electronic properties of thin GaAs-AlAs superlattices with homopolar interfaces. We compute self-consistently ionic relaxations, charge transfers, potential barriers, interactions between Wannier functions, and band structures for several [001]- and [111]-oriented superlattices. The results of our localized scheme are compared with experimental information, as band discontinuities, for thick superlattices.

I. INTRODUCTION

In the last few years much progress has been made in the technology of artificial crystals constituted by periodic layers of two semiconductors. These superlattices (SL's) show, under certain conditions, very interesting properties such as extremely high carrier mobility[1] or negative differential resistance.[2] A SL which has received a great deal of attention is GaAs-$Al_xGa_{1-x}As$ grown by molecular-beam epitaxy. Several experimental techniques[3-17] have been used to study the vibrational and electronic properties of this system. The Kroning-Penney model has been extensively used to interpret the phenomenology. Such models can be adequate when the layer thickness is large enough to consider that regions with bulk properties of each semiconductor exist. However, for a general value of x, the theoretical analysis is more difficult in that systems where ultrathin layers form the SL. Fortunately, in such cases the experments have been performed in samples where $x=1$.[7-10] This makes possible a calculation of the properties of these $(GaAs)_m$-$(AlAs)_n$ SL's where m and n are the number of layers of each semiconductor in a period of the crystal. Some efforts[18-23] have been made to study such systems by means of model Hamiltonians. However, to our knowledge, just one self-consistent calculation[24] has been carried out for [110]-oriented GaAs-AlAs SL's.[25] This implies heteropolar interfaces with properties which can be different compared to the homopolar ones of the experimental samples which have been grown in the [001] direction. The aim of this paper is to analyze several SL's with polar interfaces, both (001) and (111) by means of a self-consistent calculation of their electronic and structural properties. Besides the electronic self-consistency, similar to that obtained in the computations published for other interfaces,[24,25] we extend the self-consistency to the ions which are free to move in order to reach their equilibrium positions. The method is a minimization of the total energy in terms of a localized basis which makes easier its comparison with calculations where a tight-binding model Hamiltonian is used. Since the experiments are usually performed in [001] SL's, we will devote more attention to this case. In particular, we will analyze several systems with different layer thickness in order to see when the SL can be considered as a junction of the two semiconductors or as a completely new crystal.

In Sec. III the method, which has been used elsewhere for some other problems, is sketched and applied to GaAs and AlAs perfect crystals as a starting point of the study of the SL's. Sections III and IV are devoted to the analysis of the results for [001] and [111] SL's, respectively. Some conclusions are drawn in Sec. V, particulary on the comparison between different systems.

II. THE METHOD

Since the method has been applied elsewhere for other problems,[26-31] we just give a brief outline of it. In order to describe the electronic structure of the crystal, we use a Wannier-function (WF) representation.[32] This localized basis presents an important advantage in our case of fully occupied bands. By means of a unitary transformation between the eigenstates of the valence bands and the WF of these bands, both the charge density and the kinetic energy can be written in terms of the WF.[27,28] Therefore, within a local approximation, the total energy of the semiconductor can be expressed as a function of the valence WF and an ionic pseudopotential. A self-consistent solution is obtained by a minimization of that total energy as a function of a set of variational parameters included in a set of trial WF's. The whole scheme to get trial WF's from localized functions which must be orthogonalized was proposed by Kohn[32] and it is simple enough to allow the calculation of different crystal properties.[26-31] In particular, it has been used to study stacking faults in silicon[29] by a model where a fictitious SL is used. Satisfactory results were obtained so that we will follow here the same procedure and only a few technical points need more attention.

The procedure begins with a set of sp^3 Slater-type orbitals (STO's) centered at the positions where ionic pseudopotentials are placed to describe the effect of the nuclei and core electrons. In order to have a good starting point for the SL calculation we have previously computed the WF and lattice constant for GaAs and AlAs perfect semiconductors in a zinc-blende structure. We apply our method with the ionic pseudopotentials used for the [110] GaAs-AlAs superlattice.[24] The parameters of the STO involved in the valence WF and the lattice constants are the results we are interested in, because this information is required as a starting point in the SL calculation. Moreover, the value of the lattice constant is a test of the correctness of our approach. We have obtained 5.556 and 5.544 Å for the lattice parameters of AlAs and GaAs, respectively, when the necessary sums[26,28] running over the reciprocal lattice contain the terms corresponding to $|\vec{g}| \leq 8\pi/a$. The agreement with the experimental values,[33] 5.660 and 5.653 Å, respectively, improves when more $\vec{g}$ vectors are included, but in the SL case that means a numerical task beyond our possibilities, so that we take that maximum value of $|\vec{g}|$ in our calculations. The other result we need is the valence WF. They are built up from trial functions for each bond given by

$$f_{\vec{v}_i}(\vec{r})=\sin\lambda\phi_{\vec{v}_i}(\vec{r})+\cos\lambda\phi_{\vec{v}_i}\left[\vec{r}-\frac{a}{4}\vec{v}_i\right], \tag{2.1}$$

where $\phi_{\vec{v}_i}(\vec{r})$ is a sp^3 STO centered at one ion and pointing along the bond direction labeled by $\vec{v}_i$. Besides the variational parameter λ which gives the relative weight of each one of the two sp^3 orbitals, other parameters varying in the minimization are the exponents of the STO. Table I shows our results for all those variational parameters for AlAs and GaAs with zinc-blende structure with the calculated lattice constant given above.

Once the perfect crystal has been analyzed, the results there obtained are used to start the SL calculation. The ions are placed at their ideal positions in a perfect SL with a lattice constant which is the average of the two above obtained for each zinc-blende crystal. With this choice no mismatch of the two lattices is allowed which is a good approach because of the very similar parameters of these semiconductors. For this lattice constant, the total energy is self-consistently computed. The calculation is repeated for several lattice constants around that initial value so that a more precise minimization is achieved. In a final step the process is completed by allowing ionic relaxation at the interfaces which is a feature never calculated for these SL's. Each one of these steps is fulfilled in the following way. The valence WF of the superlattice are variationally computed with the same procedure from a set of linear combinations of sp^3 STO. Now the symmetry along the superlattice direction has been broken so that both the exponents of the orbitals and the mixture coefficients can be different for each bond. That implies many variational parameters and consequently a rather cumbersome numerical task. Therefore, we adopt the approach which gave us excellent results in the case of the stacking fault of silicon.[29] Only the parameters of the atoms at the interfaces are treated as variable, fixing the corresponding ones in the inner layers at their bulk values as previously calculated for the zinc-blende structure. In order to test the results of this enormously simplified approach we have made particular calculations by

TABLE I. Parameters obtained for the valence WF's of AlAs and GaAs with zinc-blende structure. The STO of Ga and As have the functional form corresponding to states of the fourth atomic shell and the orbitals of Al the form corresponding to the third atomic shell (Refs. 26 and 27).

AlAs		GaAs	
λ	1.014	λ	1.042
β_{4s}^{As}	2.470	β_{4s}^{As}	2.478
β_{4p}^{As}	1.705	β_{4p}^{As}	1.691
β_{3s}^{Al}	1.559	β_{4s}^{Ga}	2.270
β_{3p}^{Al}	1.038	β_{4p}^{Ga}	1.494

minimizing with respect to the parameters of the inner layers. The total energy decreases so little with this degree of freedom in which no significant variation appears, that this simplified approach can be considered as rather effective. In this scheme, the computation starts by taking, for the interface bonds, the bulk parameters as the initial values for the minimization procedure. As far as other technical points are concerned, they are treated as detailed in Ref. 29, in particular the expressions for the total energy and the special-points scheme used to perform integrals in reciprocal space.

In spite of the fact that the following sections are devoted to the analysis of different SL's, we can advance here the general trend of the results. The main variation obtained with the minimization corresponds to the mixture parameter λ at the interface as well as to the coefficients, obtained in the orthogonalization procedure, of each WF given in terms of the bond orbitals (2.1). However, the exponents of the STO do not vary significantly. Such a result could be expected because something similar happens in a much more drastic situation as that of the change from free atoms to ions forming a crystal.[26,27]

III. [001] SUPERLATTICES

In this section we discuss the results obtained when the method above described is applied to SL's oriented along the [001] direction which are of experimental interest. We concentrate upon $(\mathrm{GaAs})_m$-$(\mathrm{AlAs})_m$ systems with $m=1$, 2, and 3 in order to analyze the effect of layer thickness on the properties of the SL's. Experimental information[8] for such very thin SL's indicates that these crystals must be considered as three-dimensional (3D) with properties rather different from those of thicker SL's where two-dimensional (2D) configuration appears. Our results allow us to analyze how the transition in the 3D-2D behavior occurs and, in particular, the way in which transfer of charge and ionic relaxation takes place at the interface of thicker SL and heterojunctions.

Figure 1 shows the supercell used in the calculation for $m=3$. Similar supercells are taken for $m=1$ and $m=2$. Straight lines joining the ions represent the bonds [Eq. (2.1)] from which a set of trial WF's is built up as described above. As in many other systems[26-31] our results show that each valence WF can be associated with one of those bonds because its weight in the neighboring bonds decreases very quickly. Therefore, we refer hereafter sometimes to a particular valence WF as a particular bond. As mentioned above we start by self-consistently solving the problem of a perfect (without ionic relaxations at the interface) SL in order to determine the size of the supercell. This can be represented by the bond length l_m in each case $(\mathrm{GaAs})_m$-$(\mathrm{AlAs})_m$. We get $l_1=2.404$ Å, $l_2=2.370$ Å, and $l_3=2.380$ Å, values which are very close to $l_{\mathrm{GaAs}}=2.401$ Å and $l_{\mathrm{AlAs}}=2.406$ Å obtained in zinc-blende structure. This can be taken as a satisfactory test of the consistency of our SL calculations. Once the bond length has been determined for the inner ions, the distance between ionic layers at the interface is allowed to vary looking for equilibrium positions. Such a step is made only for $m=3$ because it does not mean a new variational freedom in the other two cases where all the ions can be considered as being at an interface. For $m=3$ we obtain that both the distances Al-As and Ga-As at the interface increase by 2.5% of their bulk value. This implies that the period of

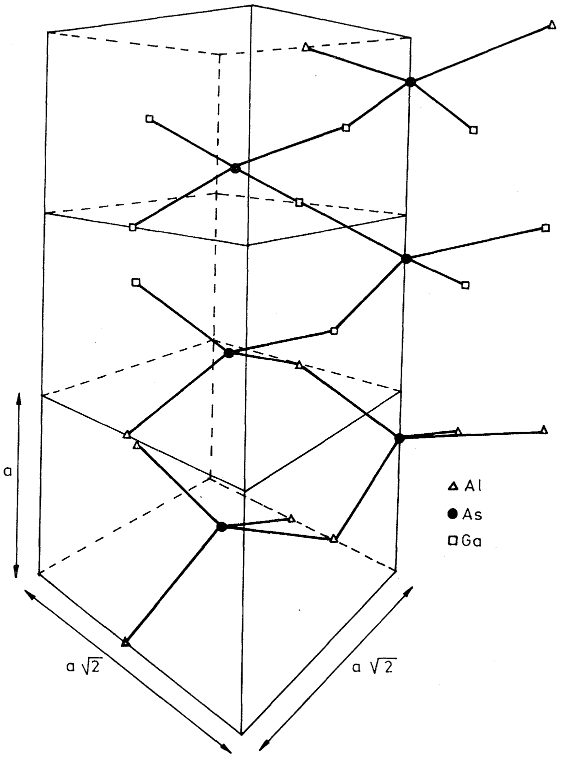

FIG. 1. Supercell used in the calculation of the structure of a $(\mathrm{GaAs})_3$-$(\mathrm{AlAs})_3$ SL oriented along the [001] direction. Heavy lines represent the bonds [Eq. (2.1)] from which WF's are built up. Parameter a is the lattice constant of the corresponding zinc-blende crystal.

TABLE II. Values of the mixture parameter λ for bonds in the bulk and at the interface for different superlattices. λ_A is for the combination in Al—As bonds, and λ_G for Ga—As bonds [Eq. (2.1)].

		Bulk	Interface
	$m=1$		$\lambda_A=1.005$ $\lambda_G=1.043$
$(GaAs)_m$-$(AlAs)_m$ (001)	$m=2$	$\lambda_A=1.014$ $\lambda_G=1.042$	$\lambda_A=0.991$ $\lambda_G=1.040$
	$m=3$	$\lambda_A=1.014$ $\lambda_G=1.042$	$\lambda_A=0.974$ $\lambda_G=1.046$
$(GaAs)_3$-$(AlAs)_3$ (111)		$\lambda_A=1.015$ $\lambda_G=1.046$	$\lambda_A=0.999$ $\lambda_G=1.048$

$(GaAs)_3$-$(AlAs)_3$ SL's is 1.008 times that of the ideal one. Let us now discuss the values of the variational parameters at this minimum of the total energy. No significant variations exist for the exponents of the STO with respect to the bulk values. The main changes at the interface are those of the mixture of parameters λ appearing in Eq. (2.1).

Table II gives our results for such parameters for the three SL's under study. The comparison between bulk and interface values shows that the combination between Ga and As orbitals does not change significantly. The main variation is that of the mixture of Al and As orbitals. The connection of these results with physical properties is far from straightforward because the main change produced in going from perfect crystals to SL's is not in the orbitals' shape but in the way in which these orbitals combine to give the WF of the system. In other words the effect of the SL is essentially contained in the orthogonalization procedure. Therefore, it is better to analyze directly physical results as the charge density or the potential self-consistently calculated for the SL's. Figure 2 shows the potential average parallel to the interface plane for $(GaAs)_3$-$(AlAs)_3$. The mean value of $V(z)$ is 6 meV higher in the GaAs region than in the AlAs one. Similar results are obtained here for $m=2$ and by Pickett *et al.*[24] for the [110]-oriented SL. The reason of this induced potential barrier is easily understood in terms of the charge transfer. In order to visualize this transfer, Figs. 3 and 4 show, for $m=2$ and 3, respectively, the difference between the SL charge density and the charge of each perfect crystal placed at the adequate spatial region. In both cases a net charge is transferred from AlAs to GaAs. Such a result could be expected from the Pauling's scale of electron negativities[34] where Ga has a higher value than Al, so that the latter tends to transfer electrons to the

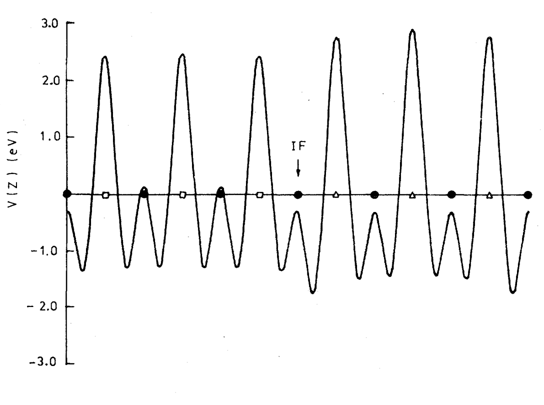

FIG. 2. Self-consistent potential averaged parallel to the interface (IF) for $(GaAs)_3$-$(AlAs)_3$ SL's oriented along the [001] direction. Layers of ions are represented by ● for As, △ for Al, and □ for Ga.

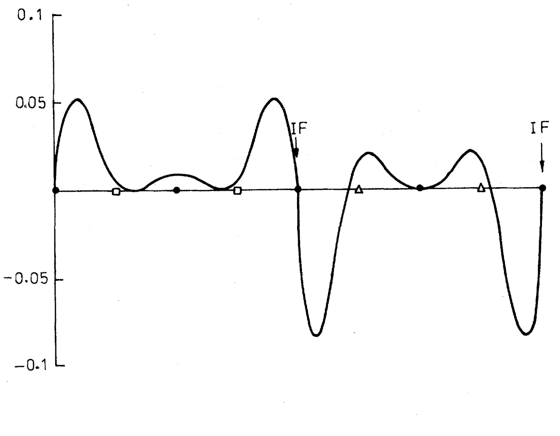

FIG. 3. Charge transfer in electrons per ion (see text) self-consistently computed for $(GaAs)_2$-$(AlAs)_2$ SL's in the [001] direction. Layers of ions are represented by ● for As, △ for Al, and □ for Ga.

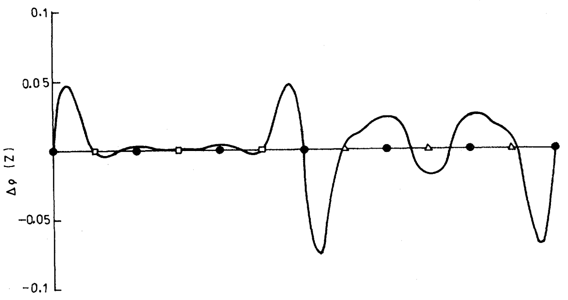

FIG. 4. Charge transfer in electrons per ion (see text) self-consistently computed for $(GaAs)_3$-$(AlAs)_3$ SL's in the [001] direction. Layers ions are represented by ● for As, △ for Al, and □ for Ga.

former. This effect is mainly concentrated at the interface and it has a clear implication in the interaction between localized orbitals. In our scheme we work with the interaction between WF $a_i(\vec{r})$ given by

$$\epsilon_{ij}(\vec{R})=\langle a_i(\vec{r})\,|\,H\,|\,a_j(\vec{r}-\vec{R})\rangle\;, \qquad (3.1)$$

where H is the self-consistent Hamiltonian, $\vec{R}$ a lattice vector, and i,j label two WF's of the set associated with the valence bands.[26,29] In order to compare with simple tight-binding models it is enough to look at the interaction of a WF with itself because a WF essentially contains atomic orbitals of two first neighbors. Table III shows that magnitude for different WF's in the $(GaAs)_3$-$(AlAs)_3$ SL's. The conclusion drawn from these results is that the self-interaction of Ga—As bonds at the interface tends to be an average of the two bulk values in consistency with a simple tight-binding model proposed by Schulman and McGill.[20] However, that is not the case of the self-interaction of the Al—As bond at the interface which is significantly lower than the bulk values. This clear difference with the simple tight-binding model is associated with the change of the mixture parameter λ mentioned above and shown in Table II.

Let us finally discuss our results for the band structure. Once the self-consistent potential has been obtained, the valence spectrum is computed by diagonalizing the Hamiltonian represented in a basis of Bloch sums of WF's.[26] Then, the calculation is rather simple because the size of the matrix is just $8m \times 8m$. Table IV gives the eigenstates at the valence-band edges for the three SL's we are concerned with. The main result is the well-known[18,20,21] splitting of some meV of the upper valence states at Γ. As it was obtained by Pickett *et al.*[24] in their self-consistent calculation for [110] GaAs-AlAs SL's, we get a nondegenerate upper state, but since the width of our SL is too small, such a state is not concentrated at the GaAs region. Therefore, it cannot be considered as a 2D SL state as the ones experimentally observed in thicker SL's.[3–6] A magnitude which gives the trend of the band structure as a function of the SL thickness is the valence-band width. Table IV shows an increase of this width as m increases. We also obtain a similar increase for the total energy per atom, a magnitude that, to our knowledge, is not possible to compare with any experimental information.

IV. [111] SUPERLATTICES

No experimental or theoretical information exists, to our knowledge, for SL's grown in the [111] direction. We have applied our method to such a system because, together with the [001] SL's above discussed, they contain the two common polar interfaces. Moreover, we will use the results here obtained to analyze, in the next section, the valence-band discontinuities at semiconductor heterofunctions.

Figure 5 shows the supercell used to calculate the properties of a $(GaAs)_3$-$(AlAs)_3$ [111] SL's with the same approach as that discussed above for the [001] case. Again we start with the ions placed at the ideal bulk positions and minimize the energy as a function of the bond length l. We get $l=2.403$ Å which is practically the average of $l_{\mathrm{GaAs}}=2.401$ Å and $l_{\mathrm{AlAs}}=2.406$ Å obtained in Sec. II for perfect zinc-blende crystals. Once this bulk bond

TABLE III. Self-interaction (in a.u.) of different WF's around the interface of the superlattice $(GaAs)_3$-$(AlAs)_3$ grown in the [001] direction.

	Ga		As		Ga		As		Al		As		Al
$\epsilon_{ii}(\vec{R}=0)$		0.1772		0.1771		0.1767		0.1582		0.1711		0.1723	

TABLE IV. Eigenstates in $\Gamma\equiv(0,0,0)$ and $J=(2\pi/a)\,(\frac{1}{2},\frac{1}{2},0)$ at the valence-band edges of a [001] SL. The other eigenvalues of the valence bands are not required in our discussion so they are omitted in order to simplify the table. Numbers in parentheses stand for degenerancies. Result are given in eV with origin at the mean potential for each superlattice.

$(GaAs)_1$-$(AlAs)_1$		$(GaAs)_2$-$(AlAs)_2$		$(GaAs)_3$-$(AlAs)_3$	
Γ	J	Γ	J	Γ	J
9.906	8.773	9.928	9.006	9.918	8.860(2)
9.893(2)	8.245	9.921(2)	8.781	9.909(2)	8.705
7.128(2)	6.443	8.257(2)	8.751	8.951(2)	8.571
−2.490	−1.058	−2.526	−1.102	−2.579	−1.110

length has been determined, the interface ions are allowed to relax looking for a deeper minimum of the energy. In contrast with the [001] SL's where a net relaxation was obtained, now the distance between Al and As interface planes increases by 0.5%, but the distance between Ga and As interface planes decreases by the same amount. In other words, no relaxation appears at this interface where just the As plane slightly moves towards the Ga plane but the Al-Ga distance does not change. In spite of this difference our results for the variational parameters are rather similar in both systems. Again the only change at the (111) interface is that the mixture parameter λ for Al—As bond significantly decreases with respect to bulk values as shown in Table II. This similitude implies that charge transfer and differences of mean potentials appear in this [111] SL in the same way as in the [001] one. The charge density that AlAs transfers to GaAs implies that the mean value of $V(z)$ at GaAs is 8 meV higher than the mean value of $V(z)$ at AlAs. Since a figure of $V(z)$ or the averaged transfer charge would be very similar to Fig. 4, we give here a different picture of the same questions by showing in Fig. 6 the contour plots of the total charge density around the interface.

All these results bring to the conclusion that [001] and [111] SL's are very similar, the main difference being that the former shows ionic relaxation at the interface and the latter does not. One more difference appears when one analyzes the spectrum of the [111] SL. Now the upper state at Γ, placed 10.07 eV higher than the mean value of the SL potential, is doubly degenerate and is localized at the GaAs region. Since this type of localized state has been experimentally observed in thicker [001] SL's our result suggests that the transition from 3D to 2D behavior appears before in [111] SL's than in [001] ones where we have not obtained states localized in the GaAs region.

V. CONCLUSIONS

We have used a self-consistent localized scheme in terms of WF's to analyze the structural and electronic properties of several GaAs-AlAs SL's grown in the [001] and [111] directions. From the structural point of view, we have found that these SL's with polar interfaces differ from each other in that [001] ones present ionic relaxation while [111] ones do not. Nevertheless, that difference is not very important because the relaxation around the As ions of the (001) interface just affects to the

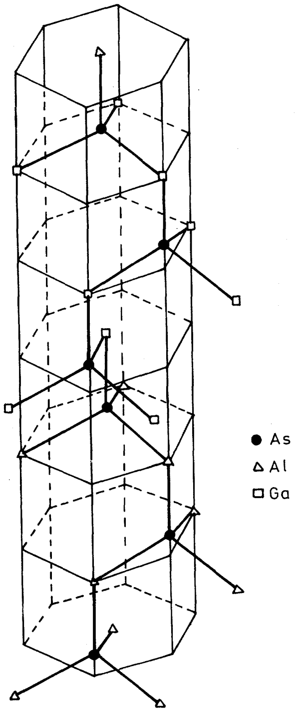

FIG. 5. Supercell used in the calculation of the structure of a $(GaAs)_3$-$(AlAs)_3$ SL oriented along the [111] direction. Heavy lines represent the bonds [Eq. (2.1)] from which WF's are built up.

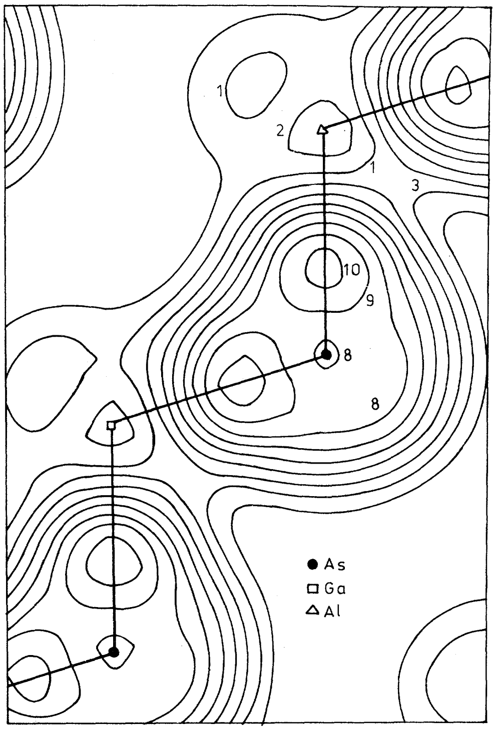

FIG. 6. Total charge density at the interface of a $(GaAs)_3$-$(AlAs)_3$ SL oriented along the [111] direction. Units are in electrons per ion.

first Ga and Al planes on each side both increasing by 2.5% their distance to the anion. Such small relaxation has no significant effect on the electronic properties. In any case, this relaxation is a purely interface effect so that it seems quite natural to consider that the displacements here obtained can be valid for thicker SL's and heterojunctions.

Since we work with a localized scheme the influence of an interface does not enter too much into the deep layers of each semiconductor. Therefore, $(GaAs)_m$-$(AlAs)_m$ SL's for both orientations, when $m=3$, already show bulklike behavior in the central layer of each semiconductor. For instance, our results for these $m=3$ cases allow us to see how AlAs transfers a small amount of electronic charge to GaAs, so that a potential barrier between both semiconductors appears. At this point, it is very tempting to use this barrier Δ between mean potentials to estimate the shift of the electronic structure of GaAs with respect to AlAs for thicker SL's or even an heterojunction of semi-infinite semiconductors. The best magnitude to measure this shift is the difference ΔE_v between the top of the AlAs and GaAs valence bands which requires the position of that level E_v for both bulk semiconductors. In order to be consistent with our approach, we have computed that level in a SL framework for $(GaAs)_6$-$(AlAs)_0$ and $(GaAs)_0$-$(AlAs)_6$ for both orientations. We have obtained

$$\Delta E_v^{[001]}=\Delta^{[001]}+E_v^{\mathrm{GaAs}[001]}-E_v^{\mathrm{AlAs}[001]}$$
$$=0.282\ \mathrm{eV}\ ,$$
$$\Delta E_v^{[111]}=\Delta^{[111]}+E_v^{\mathrm{GaAs}[111]}-E_v^{\mathrm{AlAs}[111]}$$
$$=0.288\ \mathrm{eV}\ ,$$

which are very similar to each other. The unique experimental information for this magnitude is obtained as an extrapolation for $x\rightarrow 0$ of this shift measured in GaAs-$Ga_xAl_{1-x}As$ thick SL's oriented along the [001] direction.[4] The experimental result is $\Delta E_v=(0.15\pm 0.03)E_g^{\Gamma}$ where E_g^{Γ} is the direct gap at the Γ point of the SL. In this paper we do not concentrate on conduction bands which are required to know E_g^{Γ}, but it is straightforward to use the self-consistent Hamiltonian we have obtained to compute such a magnitude. We find $\Delta E_v=0.135E_g^{\Gamma}$ which compares fairly well with the above-mentioned experimental result. This suggests the possibility of an analysis of thick SL's or heterojunctions by using the information obtained for ultrathin SL's. In particular we plan to use the interactions between WF's calculated here to analyze the spectrum of GaAs-AlAs heterojunctions.

In spite of the similarity of both [001] and [111] SL's with $m=3$, the electronic spectrum shows a significant difference. In the [111] SL's the upper valence state is spatially localized on the GaAs region as it has been experimentally observed for thicker SL's. However, in the [001] SL's no such localization exists in our results. This seems to be consistent with Raman experiments analyzed by a simple model.[10] Nevertheless the experimental information obtained both by Raman spectroscopy and infrared absorption requires a more detailed analysis which we are currently fulfilling.

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