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Heterojunction valence-band-discontinuity dependence on face orientation

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Band offsets for the (100), (110), (111), and $(\bar{1}\,\bar{1}\,\bar{1})$ orientation of the GaAs-AlAs and CdTe-HgTe heterojunctions have been investigated by use of a self-consistent tight-binding method. Our results show an important face dependence for the band offsets of the CdTe-HgTe heterojunction (≈ 0.20 eV), although differences for the GaAs-AlAs interface are negligible. We conclude that for high-ionicity semiconductors there is a slight dependence of the charge neutrality level on the face orientation.

The formation of semiconductor interfaces is a current problem receiving a lot of attention from the experimental and the theoretical points of view.[1] As regards the metal-semiconductor junction, two models have received widespread attention in order to explain the barrier formation: the metal-induced-density-of-states (MIDOS) model[2] and the defect model.[3] As regards heterojunctions, the most recent evidence[4] favors the equivalent of the MIDOS model,[5] that is, the interface-induced-density-of-states (IIDOS) model. In this case, the band offset for the heterojunction is determined by the rearrangement of the electronic charge around the abrupt interface between the two semiconductors. In its simplest form, the IIDOS model proposes that heterojunction discontinuities are determined by the alignment of the semiconductors charge neutrality levels.[5] In its most elaborate form, the IIDOS model calculates the band offsets by means of a self-consistent local-density (SCLD) formalism.[6,7] At an intermediate level of sophistication, a self-consistent tight-binding (SCTB) method has been proposed[8-10] to calculate the induced interface dipoles and the heterojunction band offsets. The advantage of this last SCTB method is that it keeps a great simplicity compared with the SCLD formalism, and introduces in the calculation the main effects associated with the charge neutrality conditions and the charge neutrality levels.[5,8,10]

In Table I, we present recent theoretical results calculated for different (110) interfaces by use of the methods mentioned above, within the IIDOS model. Notice the good agreement found between the SCTB[11] and the SCLD[7] methods: The band offsets found for III-V semiconductors agree within 0.1 eV. For ZnSe junctions differences are larger probably as a result of the high semiconductor ionicity, and the different treatment of the semiconductor bands. On the other hand, the agreement found between theory and experiments is good enough to conclude that the basic mechanism forming the interface barrier is well understood.

In this paper we address the problem of the band offsets dependence on the face orientation. In the simplest approach within the IIDOS model,[5] band offsets are assumed to be independent of the face orientation; on the other hand, as far as we know only a SCLD calculation[7] for different faces of a GaAs-AlAs junction has been presented. Here, we use the SCTB approach to analyze that face dependence. In particular, two typical III-V and II-VI heterojunctions having a common anion are considered, the GaAs-AlAs junction (an interface that has re-

TABLE I. Theoretical and experimental values (in eV) of the valence-band discontinuities for different (110) heterojunctions.

Heterojunction	SCTB method[a]	SCLD method[b]	Charge neutrality conditions[c]	Experimental
GaP-Si	0.64	0.61	0.45	0.80[d]
GaAs-Ge	0.61	0.63	0.32	0.35,[d] 0.55[e]
AlAs-Ge	0.94	1.05	0.87	0.95[d]
AlAs-GaAs	0.32	0.37	0.55	0.38,[f] 0.56[g]
ZnSe-Ge	1.70	2.17	1.52	1.40,[h] 1.52[i]
ZnSe-GaAs	1.01	1.59	1.20	1.10[i]

[a]From Ref. 11.
[b]From Ref. 7.
[c]From Ref. 12.
[d]From Ref. 7.
[e]From Ref. 13.
[f]From Ref. 14.
[g]From Ref. 15.
[h]From Ref. 16.
[i]From Ref. 17.

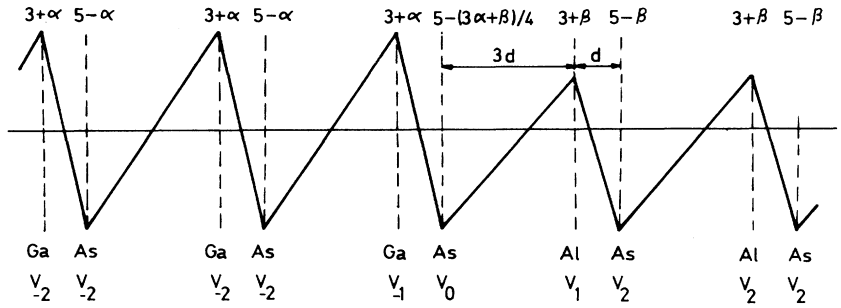

FIG. 1. Shows ideal charges and the electrostatic potential for the (111) interface of GaAs-AlAs, after averaging in the sense parallel to the interface. Mean ionic charges are assumed to be located in a plane, α and β measure the electronic charge transferred between ions in GaAs and AlAs, respectively.

ceived a lot of attention in recent years[9,14]) and the CdTe-HgTe junctions (a case that has been recently discussed from the point of view of the common anion rule[12,18]). For those heterojunctions we shall consider the typical (110), (100), (111), and $(\bar{1}\bar{1}\bar{1})$ faces and analyze their band offsets. The GaAs-AlAs $(\bar{1}\bar{1}\bar{1})$ interface configuration appears in Fig. 1, and the $(\bar{1}\bar{1}\bar{1})$ interface means the following configuration: -Ga-As-Al-As- . . . .

As explained elsewhere,[9,11] we describe the semiconductor band structures by means of a tight-binding model using sp^3s^* orbitals. For the GaAs-AlAs and the CdTe-HgTe junctions we use the parameters of Refs. 19 and 20, respectively. Notice that the parameters of Ref. 20 include spin-orbit coupling. In the case of the (110) face, we need those parameters coupling the last layers of both crystals. They have been obtained by taking an average of the interactions for each crystal; the validity of this approximation is clear from the point of view that the cations are not so different. Nevertheless, we have checked the effect of different models for these interactions and we find corrections to ΔE_v smaller than 5%. In this way, the interface Hamiltonian is completely defined except for some diagonal levels which shall be discussed below.

As regards the method of calculation we only mention that we compute the interface Green's function of the system projected onto each layer by means of a decimation technique.[8] In this way, we reduce the whole crystal Hamiltonian to an effective one having a dimension related to the number of different orbitals included in the effective interface.

We turn now to a discussion of how self-consistency is introduced in our SCTB method by considering a (111) face. In Fig. 1, we show the ideal charges at the different semiconductor layers, after averaging in the sense parallel to the surface (the particular case of GaAs-AlAs is considered). The charges shown in Fig. 1 define the initial case. Notice that that case corresponds to the ideal charges of each infinite crystal except for the common anion having an average of the ideal charges for the two crystals. For this initial case, different orbital levels are defined using the parameters of the two ideal crystals,[19,20] in such a way that we refer the levels of the orbitals of a crystal to each other by means of the mean sp^3 level of the common anion. This completely defines the initial Hamiltonian. (Notice that with this procedure we do not change the differences $E_s - E_p$ in each atom.)

The ideal charges shown in Fig. 1 are not consistent, however, with the orbitals levels calculated as explained above. This means that the initial Hamiltonian, as defined above, does not yield the interface charges shown in Fig. 1. Then, we introduce perturbations around the interface (V_{-2}, V_{-1}, V_0, V_1, and V_2 in Fig. 1) and impose Hartree consistency between those potentials and the charges induced at the interface, $\delta n_{-2}, \ldots, \delta n_2$, with respect to the ideal case. Notice that these induced charges are calculated using the initial Hamiltonian perturbed with V_i. That consistency completely defines the total interface Hamiltonian, i.e., the initial plus the diagonal perturbations V_i.

A similar procedure has been followed for the other faces. Our results for the different GaAs-AlAs and CdTe-HgTe interfaces are given in Table II. Case (b) is the full self-consistent calculation, while case (a) is obtained by using a zeroth-order approximation equivalent to determining the diagonal perturbations at the interface V_i by imposing the condition of no transfer of charge from the ideal case [this defines the solution equivalent to aligning the charge neutrality levels,[10] while in case (b) some charge is allowed to be transferred from one semiconductor to the other, depending on the relative semiconductor electronegativities].

The important results of our calculations are the following: (i) For the AlAs-GaAs heterojunction we find a very slight dependence of the band offsets on the face orientation, the maximum difference appearing between the (110) and (100) orientations, for which the band offsets

TABLE II. Band offsets (in eV) for AlAs-GaAs and CdTe-HgTe heterojunctions as a function of the interface orientation: (a) charge neutrality conditions, (b) full SCTB calculation.

Calculation	(110)	(100)	(111)	$(\bar{1}\bar{1}\bar{1})$
	GaAs-AlAs junctions			
(a)	0.36	0.44	0.46	0.40
(b)	0.32	0.38	0.37	0.35
	CdTe-HgTe junctions			
(a)	0.30	0.49	0.43	0.43
(b)	0.28	0.46	0.40	0.41

differ in 0.05 eV. The mean value of the offsets for different faces is about 0.35 eV, in very good agreement with SCLD calculations.[7] We notice that in Ref. 7, Van de Walle and Martin also find a practically face-independent band offset (the accuracy of both calculations is ± 0.05 eV), in agreement with Van de Walle and Martin calculations and, to our knowledge, the only experimental evidence[21] where different faces are investigated for this interface. (ii) For the CdTe-HgTe heterojunction, our results show a larger dependence on the face orientation, the differences between the (110) and the (100) faces being about ≈ 0.20 eV, a change that could be easily observed experimentally. Notice that the mean value for the band offsets of different faces is about 0.4 eV, in good agreement with recent theoretical predictions;[12] the value for the (111) face, 0.40 eV, is also in good agreement with the recent experimental evidence.[18] As stressed by Tersoff[12] and Kowalczyk[18] these results show the failure of the common anion rule. A final comment should be made showing the advantage of using the consistent tight-binding method for analyzing simple rules connected with the heterojunction behavior (see Priester, Allan, and Lanoo[10] also). In a recent paper Tersoff[12] has suggested that the band offset discontinuity for heterojunctions with a common anion depends on the energy levels of the cations forming the interface, in particular, he has suggested a substantial change on the band offset if the cation atomic s eigenvalues are changed with respect to the ideal interface. We have checked that suggestion for the CdTe-HgTe (111) interface by changing the s eigenvalue of Hg by 1 eV; this means that the difference $E_s - E_p$ is almost similar for both cations. Proceeding in the way explained above for the SCTB method, we have found $\Delta E_v \approx 0.03$ eV, in good agreement with Tersoff's discussion.[12] This obviously reflects the effect of the sp^3 orbitals on the semiconductor charge neutrality levels.

In conclusion, we have presented consistent tight-binding calculations for different faces of the GaAs-AlAs and CdTe-HgTe heterojunctions. Our results show an important face dependence for the band offsets of the CdTe-HgTe heterojunction, although differences for the GaAs-AlAs interface are negligible. We conclude that the independence of the charge neutrality level with the face orientation can only be taken as a reasonable zeroth-order approximation, this rule having an accuracy for semiconductors of high ionicity not better than 0.12 eV.

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