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THE EFFECT OF A METAL INTRALAYER ON THE HETEROJUNCTION BAND OFFSET: EXTRINSIC AND INTRINSIC CHARGE NEUTRALITY LEVELS

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The effect of an Al metal intralayer on the ZnSe–Ge heterojunction band offset has been theoretically analysed using a consistent tight-binding calculation. In our analysis we show: (i) first, that the heterojunction band offset is basically modified by the first metal monolayer deposited at the interface; (ii) the changes in the band-offset are mainly due to the modifications introduced in the charge neutrality levels of the semiconductors forming the junction. This implies that extrinsic charge neutrality levels are responsible for the actual heterojunction band offsets.

We have also considered different geometries for the first stages of the Al deposition at the interface. Our analysis of the band offset and the core level shift of the Al intralayer allows us to propose a model for the geometry of the growing metal.

1. Introduction

The purposes of this paper is to analyse theoretically the heterojunction barrier formation and its dependence on metal intralayers [1–4]. More especifically, we want to address theoretically the following point: how an heterojunction band offset evolves from an ideal semiconductor–semiconductor interface to the limit of a semiconductor–metal–semiconductor junction for a thick metal intralayer. Our approach follows the previous work developed in our group and analyses the interface electronic properties within a consistent tight-binding Hamiltonian [5,6]: this model is intimately related to the metal induced gap states model of Heine [7], further developed by other groups [8–12].

In our specific calculation we shall analyse the ZnSe–Ge heterojunction and assume to have an Al intralayer between the two semiconductors. There exists some experimental [1,3] and theoretical work [2,13] on this interface and our work also tries to make contact with the data for its band offset and the core level shifts as obtained for the Al levels at the interface [3].

The two main issues we shall discuss in this paper are the following ones: (i) first, how the band offset and the charge neutrality levels of both semiconductors depend on the intralayer metal thickness; this point will be discussed in section 2; (ii) in section 3, we shall discuss the effect of the interface geometry on the electronic properties of the junction.

The main conclusion of this paper is that the semiconductor charge neutrality levels depend on the electronic properties of the interface. Following this result, we shall introduce the concept of the extrinsic and intrinsic charge neutrality levels of a semiconductor [14]: this means that the intrinsic charge neutrality level of a semiconductor can be modified depending on the interface conditions, similar to the Fermi level of a doped semiconductor, which can fluctuate around the intrinsic Fermi energy.

2. From a thin to a thick metal intralayer

In this section we address one of the two main issues raised above, namely, how the heterojunc-

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tion electronic interface properties depend on the thickness of the metal intralayer.

For the sake of simplicity, we consider in this paragraph the geometry shown in fig. 1. The first Al layer is defined by assuming that the Al-atoms are bonded to the Se-atoms of the semiconductor first layer, and that the Al monolayer forms an ideal Al(110) fcc face. More Al layers are assumed to follow the ideal Al fcc crystal structure. In the next section we shall analyse other interface geometries; the one taken here has been chosen based on chemical arguments [3], suggesting that the Al atoms should be bonded to Se. In any case, the geometry considered in this section should be only taken as a model chosen for the sake of simplicity in order to analyse the band offset dependence on the intralayer metal thickness.

In this section we have analysed for the chosen geometry the following cases: (i) first of all, we have considered the ZnSe–Al–Ge interface by changing the number of Al layers from 0 to 5; (ii) then, we have proceeded to analyse the following Schottky interfaces, ZnSe–Al and Ge–Al, changing the number of Al layers form 1 to 5. The results for both cases allow us to show how the heterojunction band offset is intimately related to the Schottky barriers of the independent metal–semiconductor interfaces, and to the ideas behind the induced density of interface states (IDIS) model [5].

In our method of calculation we have followed a consistent tight-binding approach [5,6]. In this method the different parameters defining the basic hamiltonian have been taken from independent sources. Thus, the ZnSe and Ge parameters have been taken from Vogl et al. [15] and their energy levels referred to vacuum using the experimental semiconductor affinities. For Al, we have followed ref. [13], with some slight changes in the Al–Al parameters that have been calculated using a modified Harrison's prescription [16] more appropriate for the Al-crystal structure. We should comment

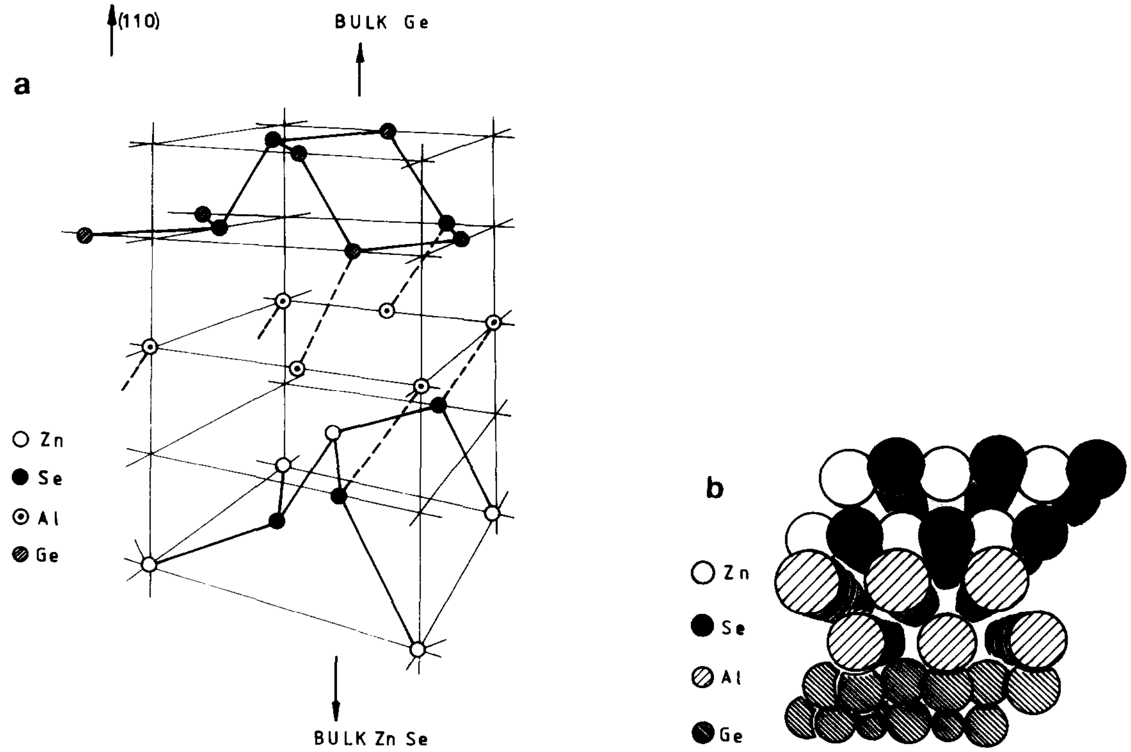

Fig. 1. Geometry of the model for the ZnSe–Al–Ge (110) junction used in section 2: (a) with one monolayer of Al (schematic) and (b) with two monolayers of Al (notice that Al layers follow the ideal Al fcc crystal structure).

Table 1
Parameters (in eV) defining the Se–Zn, Ge–Ge, Se–Al, Zn–Al, Ge–Al and Al–Al interactions and the atomic levels

	Se–Zn	Ge–Ge	Se–Al	Zn–Al	Ge–Al	Al–Al
V_{ss}	−1.55	−1.70	−1.61	−1.61	−1.68	−0.59
V_{s1p2}	1.51	2.37	1.83	2.46	2.29	1.43
V_{s2p1}	2.74	2.37	2.55	1.90	2.37	1.43
V_{pps}	3.75	2.85	3.13	3.13	2.73	2.35
V_{pppi}	−0.75	−0.82	−0.67	−0.67	−0.70	0.00
V_{s1^*p2}	1.12	2.26	1.48	1.83	2.10	1.47
V_{2p^*p1}	1.71	2.26	1.92	1.56	2.21	1.47
V_{ss^*}	0.00	0.00	0.00	0.00	0.00	−1.03

	Se	Zn	Ge	Al
E_s	−11.84	0.02	−3.91	1.34
E_p	1.51	5.99	3.58	6.09
E_{s^*}	7.59	8.99	8.36	9.23

that although this tight binding approach is going to give a poor description of metallic Al, the Al–Al parameters have been fitted to give an appropriate description of the metal density of states at the Fermi level: as the metal-induced gap states model shows [5], the interface barrier formation is intimately related to this metal density of states which is well described in our approach. Moreover, introducing appropriate changes in the Al–Al hopping parameters [13,16], do not modify the main conclusions of this paper and only introduce slight shifts (around ±0.15 eV) in the heterojunction band offset. Table 1 gives the tight-binding parameters for the different interface atoms: in general, the hopping integrals between two atoms are defined for their covalent distance; small changes around this distance are taken into account by scaling the hopping integrals with the d^{-2} law. In our calculation the diagonal elements of table 1 are modified by introducing a diagonal perturbation in each atom as calculated by a Hartree consistency: in this procedure the diagonal perturbations are related to the transfer of charge at the interface [6]. We also mention that the tight-binding Hamiltonian has been solved using a decimation technique [17] that allows us to project the total Hamiltonian into a few layers around the interface; in this procedure, we solve this reduced Hamiltonian, and calculate the density of states and the induced charge in each atom of the interface.

Our main results for the ZnSe–Al–Ge interface are summarized in table 2, where the diagonal perturbations for each layer as calculated in our Hartree procedure, the Fermi energy and the valence band offset are given as a function of the number of Al intralayers. We have also calculated the charge neutrality level (ϕ^0) of each semicon-

Table 2
Diagonal perturbations (in eV) on the last ZnSe layer, in the Al-intralayers and in the two last layers of Ge, as a function of the number of Al monolayers in a ZnSe–Al–Ge heterojunction (the Fermi energy, the heterojunction band offset and the charge neutrality levels of ZnSe and Ge are given referred to the ZnSe valence band top)

Layers	ZnSe	Al	Al	Al	Al	Al	Ge	Ge	E_{Fermi}	ΔE_v	ϕ^0_{ZnSe}	ϕ^0_{Ge}
–	−0.06	–	–	–	–	–	−0.18	−0.27		1.70	1.82	1.88
1	0.02	−1.03	–	–	–	–	0.38	0.14	2.67	2.11	2.64	2.64
2	−0.15	−0.43	−0.36	–	–	–	0.58	0.27	2.61	2.24	2.60	2.57
3	−0.16	−0.55	−0.00	−0.50	–	–	0.55	0.23	2.58	2.20	2.56	2.54
4	−0.13	−0.55	−0.04	−0.05	−0.48	–	0.55	0.22	2.57	2.19	2.55	2.52
5	−0.13	−0.53	−0.04	−0.09	−0.00	−0.47	0.56	0.24	2.58	2.20	2.56	2.53

Table 3

Diagonal perturbations (in eV) in the last ZnSe layer and in the Al layers as a function of the number of Al monolayers (we also give the interface Fermi energy and the charge neutrality level with respect to the top of the ZnSe valence band)

Layers	ZnSe	Al	Al	Al	Al	Al	E_{Fermi}	ϕ^0_{ZnSe}
1	−0.18	−1.27	–	–	–	–	2.43	2.36
2	−0.09	−0.52	−0.69	–	–	–	2.58	2.56
3	−0.12	−0.54	−0.03	−0.76	–	–	2.64	2.63
4	−0.14	−0.53	−0.02	−0.12	−0.81	–	2.60	2.59
5	−0.17	−0.57	−0.08	−0.16	−0.16	−0.86	2.54	2.53

ductor for a given interface: notice that the total electronic charge below the neutrality level defines a neutral condition in the semiconductor. This condition yields, therefore, the neutrality level of each semiconductor for any ZnSe–Al–Ge interface; the case of an ideal ZnSe–Ge interface has to be treated in a different way, since the density of states in the absolute energy gap is zero. In this case, we calculate the difference between the charge neutrality levels of both crystals by imposing neutrality conditions on local terms: this means that the diagonal perturbations on each atom are adjusted to give a local charge neutrality condition; then both charge neutrality levels are aligned and we can calculate their energy difference. On the other hand, the Ge charge neutrality level has been taken from ref. [18] (Notice that he ZnSe–Ge band offset given by the charge neutrality levels in ref. [18] is in very good agreement with our calculations.)

From the results of table 2 we find that the band offset for the ideal ZnSe–Ge heterojunction is 1.70 eV (experimentally this figure is 1.44 [3]), while this value changes to 2.11, 2.24, 2.20, 2.19 and 2.20 eV, when the number of monolayers increases one by one. These results show that the changes introduced in the valence band offset by the Al deposition are practically saturated with a single monolayer.

We have also analysed the ZnSe-Al and the Ge–Al interfaces to see how the ZnSe–Al–Ge heterojunction band offset can be related to the barriers of the Schottky junctions. Tables 3 and 4 show the diagonal perturbations for each layer, the Fermi energy and the charge neutrality levels for the Ge–Al and ZnSe–Al interfaces as a function of the number of Al layers deposited on the semiconductor. In table 5 we compare the band offsets as a function of the number of Al intralayers for the ZnSe–Al–Ge heterojunction as given in table 2 and as calculated by aligning the Fermi levels of the two interfaces, Ge–Al and ZnSe–Al. The agreement between both figures for more than a monolayer is quite good, although differences of up to 0.1 eV appear for the 5 Al layers case, due to the accuracy of our calculation (estimated to be around 0.05 eV). This result shows that, even for an Al monolayer, the heterojunction band offset can be approximately described as the superposition of two Schottky junctions.

We are now in the position of discussing which are the physical effects introducing the band offset changes when Al is deposited between ZnSe and

Table 4

Diagonal perturbations (in eV) in the last Ge layer and in the Al layers as a function of the number of Al monolayers (we also give the interface Fermi energy and the charge neutrality level with respect to the top of the Ge valence band)

Layers	Ge	Al	Al	Al	Al	Al	E_{Fermi}	ϕ^0_{Ge}
1	0.15	−1.40	–	–	–	–	0.50	0.48
2	0.31	−0.63	−0.91	–	–	–	0.43	0.38
3	0.34	−0.67	−0.22	−0.94	–	–	0.41	0.36
4	0.32	−0.67	−0.22	−0.32	−1.02	–	0.40	0.35
5	0.35	−0.65	−0.21	−0.30	−0.34	−1.03	0.44	0.39

Table 5
Heterojunction band offset (in eV) as obtained by direct calculation (table 2) and by application of the figures given in tables 3 and 4, as a function of the number of Al monolayers for a ZnSe–Al–Ge heterojunction

	Layer				
	1	2	3	4	5
ΔE_v	2.11	2.24	2.20	2.19	2.21
$\phi_{ZnSe-Al} - \phi_{Ge-Al}$	1.93	2.15	2.23	2.20	2.10

Ge. According to the previous discussion, one can think of the ZnSe–Al–Ge interface as the superposition of two Schottky barriers: the ZnSe–Al and the Ge–Al barriers. As discussed in ref. [3], this back-to-back Schottky barriers case would introduce a change in the heterojunction band offset due to the finite interface screening: in our calculation this effect should appear as the difference between the interface Fermi energy and the charge neutrality levels of the semiconductors (ϕ^0). As table 2 shows, ϕ^0_{ZnSe} and ϕ^0_{Ge} do not coincide with E_F, this effect yielding a change in the valence band discontinuity of the order of magnitude of 0.05 eV, in good agreement with the comments of ref. [3]. This value is, however, very small compared with the total heterojunction band offset change introduced by Al, as shown in table 2. The results of this table show that the main contribution to the band offset change comes from the modifications introduction by the deposition of Al in the charge neutrality levels of ZnSe and Ge, that are shifted by around 0.7 and 0.15 eV, respectively.

From these results, we conclude that upon Al-deposition the ZnSe–Ge heterojunction band offset is formed in such a way that the charge neutrality levels of both semiconductors are still practically aligned (with an accuracy of ±0.05 eV), in agreement with the charge neutrality model [5]; the differences between the band offsets of the ZnSe–Al–Se and ZnSe–Ge heterojunctions being mainly due to the modifications in the charge neutrality levels appearing in both semiconductors upon deposition of the metal intralayer. In this respect, we should also mention that the charge neutrality levels given in tables 3 and 4 are in good agreement with the ones given in table 2, showing again that the barrier heights of each Schottky barrier is determined by the extrinsic charge neutrality level of each semiconductor. We should talk about extrinsic charge neutrality levels, since the semiconductor charge neutrality level may be dependent on the interface conditions, as our calculation shows.

We also conclude that the heterojunction barrier formation is determined basically by the interface layers of both semiconductors for an ideal interface, and by the first Al intralayer deposited in the junction. These conclusions are consistent with other independent results obtained for Schottky barriers [19]: in this case we have also found that the Schottky barrier is practically formed with the deposition of one or two metal layers on the semiconductor.

3. The interface geometry of the metal intralayer

In previous section we have analysed the barrier formation of the heterojunction for a specific interface geometry. The aim of that discussion was to show that the band offset is basically determined by the first Al intralayer deposited in the junction. In this section, we shall discuss the offsets associated with the changes of the interface geometry and try to make contact with the available experimental evidence.

Margaritondo et al. [3,20] have shown that the ZnSe–Ge band offset can be modified with the

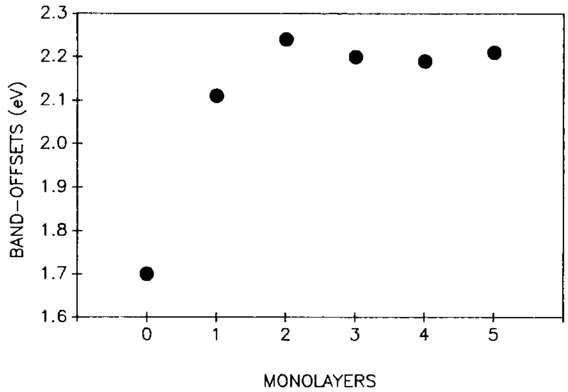

Fig. 2. Theoretical results for ΔE_v as a function of the number of Al intralayers.

deposition of an Al intralayer, the saturation values for the change in ΔE_v being around 0.3 eV. In fig. 2, we show our theoretical results of section 2 for the change of ΔE_v as a function of the number of Al intralayers: the saturation discussed above is apparent (in reasonable agreement with ref. [3]), but the maximum change of ΔE_v is in our case around 0.5 eV, a little larger than the experimental data. Another piece of experimental information given in ref. [3] is the core level shift appearing in Al for the 2p orbital after its deposition on ZnSe: this shift is around 2.3 eV larger at the interface than in metallic Al. This figure seems to be not too much dependent on the deposition of Ge at the interface, at least for a small Al coverage. Our results of section 2 tend to show that the core level shift [21] in Al, for the geometry discussed there, is not more than 1 or 1.3 eV at small coverages, a

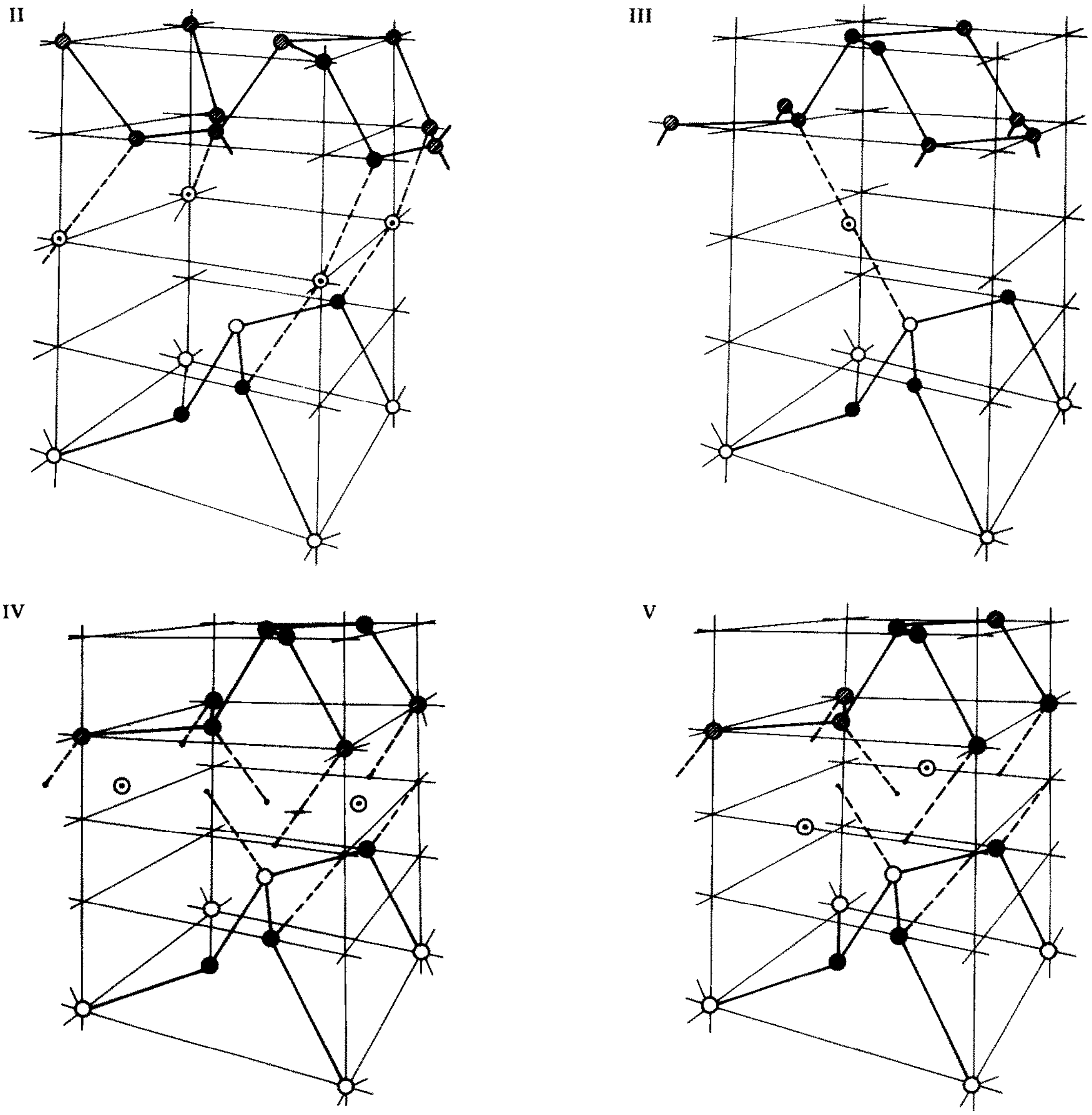

Fig. 3. Different geometries for the ZnSe–Al–Ge junction with half a monolayer of Al (II–V) and with a monolayer of Al (VI–VII). The numbers II–VII are referred to the cases discussed in the text (section 3).

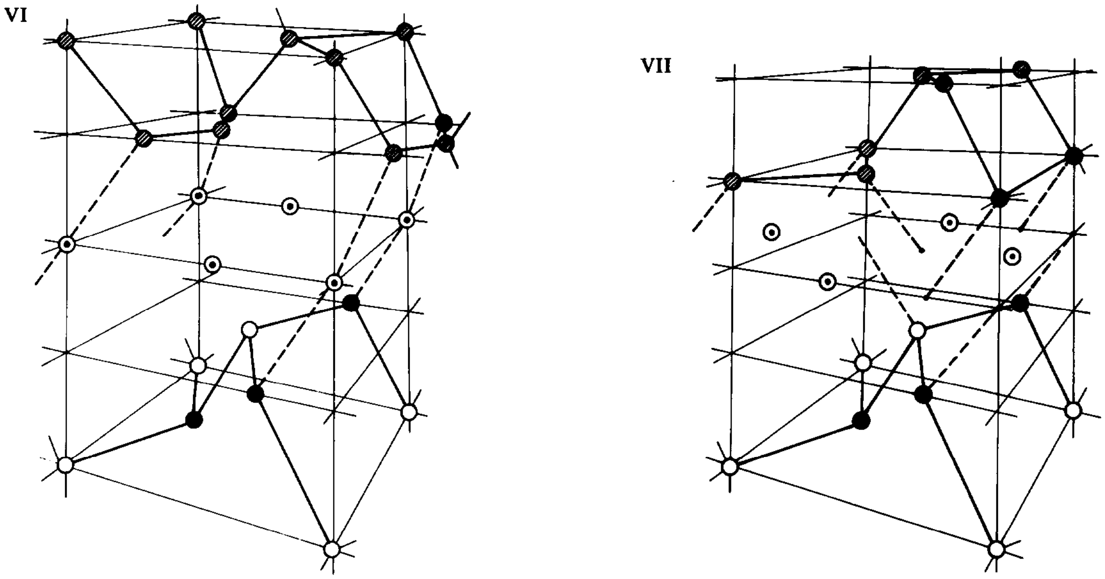

Fig. 3. Continued.

value not too much consistent with the experimental evidence.

These discrepancies have prompted us to analyse other interface geometries trying to find: (i) first of all, how interface barriers and core level shifts depend on the chosen atomic arrangement; (ii) then, to find out which is the most likely geometry and the interface chemical bonds at the heterojunction.

In this section we analyse different geometries and different metal coverages, but we only consider the metal coverages to be less than, or equal to, a monolayer. According with previous section, the heterojunction band offset can be expected to be practically saturated in that limit.

Fig. 3 shows the different geometries we have considered in this section. In four cases, we have assumed to have an Al half monolayer, with the Al atoms bonded to the semiconductor surface in different ways, while in other three cases we have considered a full Al monolayer (one of these cases coincide with the one analysed in section 2). Let us first discuss the Al half monolayer geometries: In case II Al is bonded to Se, in case III to Zn, and in cases IV and V is located at an intermediated position (see fig. 3).

The results for the Al half monolayer cases are given in table 6: in each case we give the diagonal perturbation at each layer, the Fermi energy and the valence band offset; for each position we also include the results for the ZnSe–Al interface, assuming that no Ge layer is deposited at the junc-

Table 6

Diagonal perturbations (in eV) in the last ZnSe layer, in the Al-intralayer and in the two last layers of Ge, for half a monolayer of Al in a ZnSe–Al and a ZnSe–Al–Ge heterojunctions for the different geometries discussed in the text (we also give the Fermi energy and the change in the heterojunction band offset due to the Al intralayer, the ZnSe valence band top is the energy origin

Geometry	ZnSe	Al	Ge	Ge	E_{Fermi}	$\delta(\Delta E_v)$
II	-0.38	-2.71	–	–	2.95	–
	-0.50	-2.32	0.81	0.80	2.83	1.07
III	-0.07	-3.50	–	–	0.37	–
	-0.15	-3.83	-1.64	-1.67	0.33	-1.40
IV	-0.28	-1.09	–	–	2.69	–
	-0.30	-1.59	0.37	0.60	2.81	0.86
V	-0.18	-1.44	–	–	2.20	–
	-0.28	-1.59	0.40	0.47	2.54	0.74

tion. These results show a value for ΔE_v too large when compared with the experimental evidence. For the case III, with Al bonded to Zn, the value of ΔE_v is -1.40, even with an opposite sign to the value found experimentally. The difference between cases II and III can be better appreciated by looking at the Fermi energy and at the local density of states shown in fig. 4: these results show how the ZnSe surface states are playing the crutial role under the Al intralayer deposition. These results suggest, in agreement with ref. [3], that Al cannot be bonded to Zn; the other three cases, however, yield similar changes in the band offset: they are a little too large although they show the right sign. We can discriminate among these three cases by considering the value of the core level shift as calculated for the ZnSe–Al interface [21]. The values given in table 6 suggests that Al is bonded to Se as corresponds to the II-position: this is in good agreement with the comments of Margaritondo et al. [3] about the formation of a Se–Al compound. We should keep in mind, however, that the calculated value of ΔE_v is too large for this half monolayer: this suggests that in the growing mechanism, islands – with a full monolayer geometrical configuration to be

Table 7
Diagonal perturbations (in eV) in the last ZnSe layer, in the Al-intralayer and in the two last layers of Ge, for a monolayer of Al in a ZnSe–Al–Ge heterojunction for the different geometries discussed in the text (we also give the Fermi energy and the change in the heterojunction band -offset due to the Al intralayer, the ZnSe valence band top is the energy origin)

Geometry	ZnSe	Al	Ge	Ge	E_{Fermi}	$\delta(\Delta E_v)$
I	0.02	−1.03	0.38	0.14	2.67	0.41
VI	−0.49	−1.75	−0.09	−0.12	2.29	0.15
VII	−0.55	−1.93	−0.26	0.02	2.14	0.29

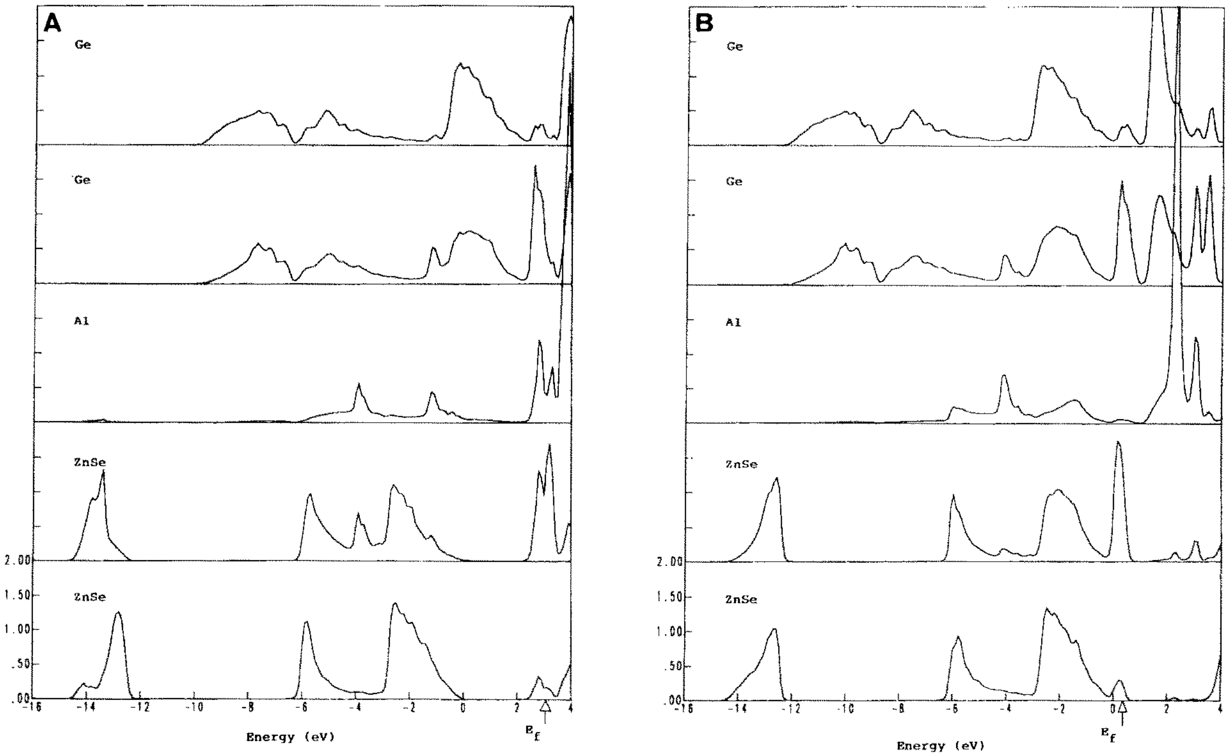

Fig. 4. Local density of states at different layers in a ZnSe–Al–Ge junction with half Al monolayer for two cases discussed in section 3: (A) case II and (B) case III. $E = 0$ is the top of the ZnSe valence band.

discussed below – must be formed reducing the value found for ΔE_v in the case II of table 6. This is also supported by the results of ref. [3] where the core level photoemission spectra shows a broad Al 2p peak and a shoulder that are associated with different Al environments in the interface for the first stages of Al deposition.

The results we have obtained for the Al monolayer cases are shown in table 7. For comparison we also include the case discussed in section 2 (the case I of table 7). From this table it is apparent that cases VI and VII give a better agreement with the data of ref. [3] than case I, both for the valence band offset and for the core level shift of Al. In particular, notice that the case VI has a geometry similar to the case of section 2, the only difference being the coordination of the Ge atoms to Al: with this coordination we find a reasonable value for the core level shift (about −1.8 eV) and a slightly smaller band offset. For the case VII, the core level shift is even a little larger, around −1.9 eV, and the band offset presents a quite good agreement with the experimental evidence. The actual theoretical analysis does not allow us to reach a conclusive point of view (notice that our results have been obtained by assuming all the atoms of the same layer to have the same core level shift) and to discriminate between cases VI and VII; moreover, it is a plausible assumption to think that both geometries may appear at the ZnSe–Al–Ge interface.

Putting together the results for the Al half monolayer and the full monolayer we conclude that the deposition of Al on ZnSe and the further deposition of Ge may proceed in the following way: (i) At low Al coverages, the Al atoms are bonded to the Se atoms. This explains the high shift [3] of the 2p core level of Al. (ii) At further deposition, the Al atoms must form islands having the geometry shown in figure 3 for the cases VI and VII; this explains the heterojunction band offset shifts found for the submonolayer regime. (iii) For the deposition of a full Al monolayer, we can expect to have a disordered geometry showing a combination of the case VI and VII of fig. 3. In these cases, the calculated band offset and the Al core level shift present a good agreement with the experimental evidence of ref. [3].

Once we have discussed how our theoretical analysis can be used to analyse the interface geometry, we turn our attention to one of the two main issues raised in the introduction: how the interface geometry affects the electronic properties of the junction. The results shown in tables 6 and 7 show conclusively that the ZnSe–Ge band offset depends dramatically on the interface geometry; in similarity to the discussion of section 2, we also conclude that the semiconductor charge neutrality level is a function of the interface geometry and the chemical bonds formed between the intralayer and the semiconductors forming the heterojunction.

4. Conclusion

The main conclusion of this paper is that the heterojunction band offsets can be changed by introducing intralayers between the semiconductors of the junction. The analysis of this paper shows conclusively that this effect in ZnSe–Al–Ge is basically due to the changes introduced by the metal intralayer in the semiconductor charge neutrality levels. It is, therefore, important to introduce the concept of the extrinsic charge neutrality level: this implies that intrinsic values may be modified by the actual interface conditions. Although in a zeroth-order approximation, the intrinsic levels yield a reasonable value of the band offset for ideal interfaces, we suggest that the band offsets for heterojunctions with intralayers have to be calculated specifically in every case, taking into account the shift in the charge neutrality level.

Finally, we should also stress that the analysis given in this paper is a good example showing how the actual interface geometry can be deduced from the experimental data about the band offsets and the core level shifts of the atoms deposited at the interface.

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