

Tight-binding hamiltonians for the study of the electronic structure of the valence band of the II-VI binary/ternary-alloy interfaces

D. Olgún, R. Baquero

Departamento de Física,

Centro de Investigación y de Estudios Avanzados del IPN

Apdo. Postal. 14-740, 07000 México D.F.

We present an electronic band structure calculation of the valence band of the II-VI binary/ternary—alloy interfaces. We use the empirical tight-binding method and the surface Green's function matching method. For the ternary alloys we use our previously set Hamiltonians. They describe well the band gap change with composition obtained experimentally. With this data, we go on to describe the interface states. At the interface domain, we find three non-dispersive- and two interface-states besides the known bulk bands. We make use of the available theoretical calculations for the (001)-oriented surfaces of the binary compounds and for the binary/binary interfaces to compare our new results with.

Keywords: II-VI alloys; electronic band structure: tight-binding method.

1. Introduction

In previous work, we have studied the electronic band structure of the valence band for the (001)-surface of several II-VI wide band gap semiconductors [1, 2], and different binary heterostructures [3]. We have obtained the (001)-projected electronic band structure for both, surfaces and binary interfaces using the known Surface Green's Function Matching (SGFM) method [4].

In the (001)-surfaces in addition to the well known bulk bands and surface resonances, we have described three different structures in the valence band region, the so—called surface induced bulk states B_h, B_l , and B_s . Later we found that this kind of induced states appear at the interface domain as well. Therefore, more generally, we found that any frontier can induce these states. For that reason we have redefined them as frontier-induced semi-infinite medium (FISIM) states since they are not, strictly speaking, *bulk* (infinite medium) states. These FISIM states do not show dispersion as a function of the wave vector \mathbf{k} for the surfaces studied. This is theoretically and experimentally shown for the (001)-oriented CdTe surface [1, 2, 5, 6]. For the binary/binary (001)-oriented II-VI compound interfaces, in contrast, they show some clear dispersion [3].

The interest of this work is the study of the evolution of the FISIM states from a non-dispersive character to a dispersive one as stress and different crystal composition enters into play. We show that, if we select a ternary alloy to produce little stress and change only slightly the composition, the FISIM states do exist on both sides of the interface but do not show as much dispersion. So the existence of the FISIM states is due to the existence of a frontier alone and the amount of dispersion is related to the existing stress at the interface and on the chemical character of the interface partner.

We will present in this work the valence band of the (001)-CdTe/CdSe_{0.15}Te_{0.85} interface in detail, and we will concentrate in particular in the FISIM states. The method used is discussed in our previous work [1-3]. Here we only summarize the relevant features of it, in Section II, for completeness; Section III is devoted to discuss our results. We give our conclusions in section IV.

2. The Method

To describe the interface between two semiconductor compounds, we make use of tight-binding Hamiltonians. The Green's function matching method takes into account the perturbation caused by the surface or interface exactly, and we can use the bulk tight-binding parameters (TBP) [7, 8, 9]. We use the method in the form cast by García-Moliner and Velasco [4]. These authors give the Green's function for the interface, G_I , by

$$G_I^{-1} = G_{s(A)}^{-1} + G_{s(B)}^{-1} - I_B H^i I_A - I_A H^i I_B \quad (1)$$

where $G_{s(A)}$ and $G_{s(B)}$ are the surface Green's function of medium A and B, respectively. $-I_A H^i I_B$ and $-I_B H^i I_A$ are the Hamiltonian matrices that describe the interaction between the two media.

The tight-binding Hamiltonians for the II-VI ternary alloys are described in detail in Ref.[10]. Briefly speaking, we have used the tight-binding method and, with certain conditions, the virtual crystal approximation to study the ternary alloys. We have included an empirical bowing parameter in the s-on site TBP of the substituted ion. This procedure gave us the correct behaviour of the band gap value with composition [10]. More exactly for the TBP of the ternary alloy, we take

$$E_{a,a}(x) = xE_{a,a}^{(1)}, \quad \mathbf{a}, \mathbf{a}' = s, p^3, s^*, \quad i = 1, 2 \quad (2)$$

for all but the s-on site TBP of the substituted ion. In eq. 2 $E^{(1,2)}_{\mathbf{a},\mathbf{a}}$ are the TBP of the compound (1 or 2); α, α' are the atomic orbitals used as the basis set.

For the s-on site TBP of the substituted ion we use the following expression

$$E_{s,v}(x, b_v) = E_{s,v}(x) + x(1-x)b_v, \quad v = a, c \quad (3)$$

where $E_{s,v}(x)$ is given by eq. (2) and b_v is the empirical bowing parameter per each different substitution (anion (a) or cation-substitution (c)). We have used $b_a = -0.195$ in this work, which is the same value used in Ref. [10].

3. Results and Discussion

The system studied has been chosen with a composition (x) as to give a minimum stress at the interface. The induced stress is small, about 1%. This magnitude of the induced stress allows us to ignore its effect in our calculation. The real bulk bands as well as the FISIM states, should lie very closely to our calculated ideal case. We adopt the same convention for the interface domain as in Ref. [3]. That is, we consider nearest neighbors interactions in our bulk Hamiltonians and, as a consequence, four atomic layers as the interface domain, two belonging to medium A and two to medium B. In the alloy case, we consider a pseudobinary compound so that the concept of anion and cation atomic layers remains meaningful. We will project the interface electronic band structure on each atomic layer and we will see how the different states, that we found for the free surface and for the binary/binary interface case, change or disappear at the binary/ternary one.

Figure 1 shows the electronic band structure of the valence band for the interface studied here: (001)-CdTe/CdSe_{0.15}Te_{0.85}. The dispersion relations are found from the poles (triangles in the figure) of the real part of the interface Green's function. The solid-lines are a guide to the eye. These are to be compared to the dispersion curves found for the bulk (infinite medium) case. The calculated energy eigenvalues for the FISIM states are denoted by stars, crosses and points; the dotted lines are intended only as a guide to the eye. We label the FISIM states as B_{lh} , B_{ll} , and B_{ls} . This convention follows the previous free (001)-surfaces study (see Refs. [1, 2]). Furthermore, we have obtained two interface states (empty diamonds). The energy eigenvalues for all the calculated states are given in Table I.

Bands resembling the bulk ones appear in all the projections [1, 2]. The heavy hole (hh) and light hole (lh)

bands show more dispersion at the interface domain than in the semi-infinite medium. They lie usually lower in energy (about 0.7 eV and 0.4 eV, respectively) in all the atomic layers than in the bulk. The spin-orbit band shows almost the same dispersion that in the semi-infinite medium. As we stated above, we find two interface states (IS_1 and IS_2 , in the figure). The first one (IS_1) starts at -1.3 eV in Γ . The interface state eigenvalue varies with \mathbf{k} and seems to disappear near X, probably merging to a bulk band. A second interface state (IS_2), appears at -1.9 eV in Γ . This state presents a substantial dispersion from Γ - X. The way in which it depends on \mathbf{k} is peculiar. We have followed the composition of this state as we go from Γ to X so that we could identify the calculated eigenvalues as belonging to the same eigenstate band. It strongly depends on \mathbf{k} , as strongly as the spin-orbit band. It is worth noticing that from about 0.4 in the Γ - X interval up to X the band almost ceases to depend on \mathbf{k} .

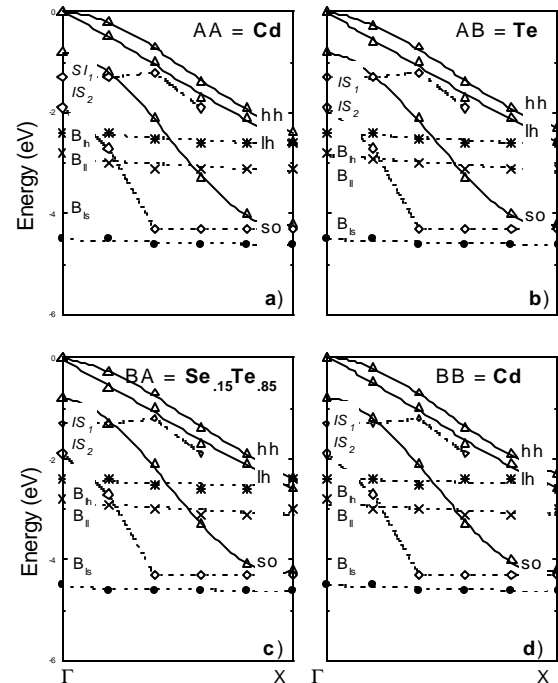


Figure 1: Electronic band structure of the valence band projected on each atomic layer of the (001)-CdTe/CdSe_{0.15}Te_{0.85} interface. The dispersion relations are obtained from the poles (triangles) of the real part of the interface Green's function. The solid lines are a guide to the eye. B_{lh} , B_{ll} and B_{ls} are the calculated FISIM states (the dotted lines, intended to show the dispersion of the bands, are a guide to the eye). We show the interface states IS_1 and IS_2 .

Some final remark about the frontier induced semi-infinite medium (FISIM) states. There are two factors that intervene in the \mathbf{k} dependence of the FISIM states. One is the lattice mismatch and the second is the change in the crystal potential as one goes from one binary semiconductor to the other partner of the interface. We

want to clearly establish the origin of these FISIM states. For that reason we have chosen ternary-alloys that have almost the same lattice constant as the binary partner and we have neglected any difference in the calculations. So our results are a consequence of the existence of a frontier only, no stress is used. First, as we see in Fig. 1, the FISIM states do exist. So they do come from the mere existence of a frontier. A difference with the surface case is that the FISIM states do not lie at the same energy as the bulk bands at X, as it can be seen in the figure and in Table 1, and that they show a slight dispersion. So the conclusions are that the existence of the FISIM states is due to the existence of a frontier and the way they depend on \mathbf{k} is to be attributed to stress at the interface.

Similar comments can be addressed for other CdTe- and ZnSe-ternary-alloy interfaces, as we will show elsewhere [14].

Table 1: Energy-eigenvalues for the heavy hole (hh), light hole (lh), and spin-orbit, bands at Γ and X high-symmetry points as obtained for the interface dominion for (001)-CdTe/CdSe.₁₅Te.₈₅. The values for the FISIM states, B_{lh}, B_{ll}, and B_{ls} are also included.

Atomic layer	Γ -point			X-point		
	Γ_7^v			X ₇ ^v	X ₆ ^v	X ₆ ^v
Cd	-0.8			-2.4	-2.6	-4.2
Te	-0.8			-2.3	-2.6	-4.2
Se. ₁₅ Te. ₈₅	-0.8			-2.4	-2.6	-4.2
Cd	-0.8			-2.3	-2.6	-4.2
	B _{lh}	B _{ll}	B _{ls}	B _{lh}	B _{ll}	B _{ls}
Cd	-2.4	-2.5	-4.5	-2.6	-3.1	-4.6
Te	-2.4	-2.5	-4.5	-2.6	-3.1	-4.6
Se. ₁₅ Te. ₈₅	-2.4	-2.5	-4.5	-2.4	-3.0	-4.6
Cd	-2.4	-2.5	-4.5	-2.6	-3.0	-4.6

4. Conclusions

In conclusion, we have calculated the electronic band structure of the valence band of the (001)-CdTe/CdSe.₁₅Te.₈₅ II-VI binary/ternary-alloy interface. We have used the tight-binding method and the surface Green's function matching method to obtain the electronic band structure projected onto each atomic layer that constitutes the interface dominion. To describe the ternary alloys we have used our tight-binding Hamiltonians obtained in previous work. They give good account of the changes of the band gap with composition obtained experimentally. The system was chosen here so that stress could be ignored

for the particular value of the compositional variable. The calculated valence band electronic structure of the interface shows bulk bands with similar dispersion as the semi-infinite medium (a system with a surface). The FISIM states observed before in the (001)-oriented surfaces and binary/binary interfaces appear also in this case and show an intermediately strong \mathbf{k} -dependence. At the interface domain, the calculated states, both the bulk bands and the FISIM states, have a LCAO composition that is a combination of the corresponding ones of the two media forming the interface.

By avoiding stress we have isolated one of the two factors that give rise to the FISIM states, stress and change in chemical composition. We could establish that the difference in chemical composition is enough to create FISIM states.

We have obtained, further, for the binary/ternary-alloy case two interface states for the CdTe-based heterostructures and one that do not show for the binary/binary interfaces at least in the energy interval that we have considered in a previous work [3].

References

- [1] D. Olgúin and R. Baquero, Phys. Rev. B 50, 1980 (1994)
- [2] D. Olgúin and R. Baquero, Phys. Rev. B 51, 16 981 (1995)
- [3] D. Olgúin, Ph. D. Thesis, CINVESTAV-Mexico (1996).
- [4] F. García-Moliner and V. R. Velasco, Prog. Surf. Sci. 21, 93 (1986); Theory of Single and Multiple Interfaces, World Scientific, Singapore, 1992.
- [5] D. Niles and D. Höchst, Phys. Rev. B 43, 1492 (1991)
- [6] K. -U. Gawlik, J. Brüggmann, S. Harm, C. Janowitz, R. Manzke, M. Skibowski, C. -H. Solterbeck, W. Schattke, and B. A. Orlovski, Acta Physica Polonica A 82, 355 (1992)
- [7] R. Baquero, V. R. Velasco, and F. García-Moliner, Physica Scripta 38, 742 (1988)
- [8] R. Baquero and A. Noguera, Rev. Mex. de Física 35, 638 (1989)
- [9] C. Quintanar, R. Baquero, F. García-Moliner, and V. R. Velasco, Rev. Mex. de Física 37, 503 (1991)
- [10] D. Olgúin, R. de Coss, and R. Baquero, Rev. Mexicana de Física (in press).
- [11] T. M. Duc, C. Hsu, and J. P. Faurie, Phys. Rev. Lett. 58, 1127 (1987)
- [12] R. Baquero, A. Noguera, A. Camacho, and L. Quiroga, Phys. Rev. B 42, 7006 (1990)
- [13] V. R. Velasco, R. Baquero, R. A. Brito-Orta, and F. García-Moliner, Condens. Matter 1, 6413 (1989)
- [14] D. Olgúin and R. Baquero (to be published).