

**Bulk and surface electronic bandstructure
 of ternary II-VI compounds.**

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Abstract

Ternary alloys of wide gap semiconductors are gaining much interest due to their potential applications specially in optical devices. In a random substitutional semiconductor either the cation sites or the anion sites are randomly occupied. The influence of these local fluctuations in occupation on the electronic states of the alloy should depend on the localization of the states in question. To illustrate the effect of alloy fluctuations, we have performed a Green's function calculation of the electronic bandstructure in bulk and in the surface (001) of $Cd_xZn_{1-x}Te$. Our method allows us to study the local density of states layer by layer and thus we follow the states from the surface to the bulk.

Method

We use the tight-binding method to construct the bulk Hamiltonian, which in turn is used to build the surface Hamiltonian. We assume first-neighbors interaction. For a zinc-blende crystal, a good description of the valence bands can be obtained by including s and p orbitals but in order to reproduce the lowest conduction bands it is appropriate to introduce an excited s state, s^* [1].

We take into account the effect of the spin-orbit interaction through the expression

$$H_{so} = \frac{\hbar}{2m} \frac{1}{2c} (\nabla V \times p) \cdot \sigma \quad (1)$$

and thus we have a basis of 10 Bloch functions [2] ($SP^3 S^*$ with two spin orientations) of the form

$$\psi_k(r) = N^{-1/2} \sum_j \exp(i k \cdot r_j) \varphi(r - r_j) \quad (2)$$

and a 10×10 Hamiltonian matrix with elements

$$\langle \varphi_n | H | \varphi_m \rangle = \sum_j \exp(i k \cdot \rho_j) \int \varphi_n(r) H \varphi_m(r - \rho_j) d^3r \quad (3)$$

After diagonalization, we obtain the dispersion relation, $E(k)$, for the bulk. Now, to describe the surface, we use the same tight-binding method, but the Hamiltonian matrix will be composed of submatrices representing the coupling between layers. Each principal layer is labeled with the index n where $n=0$ represents the surface principal layer. The unity can be written as

$$I = |n-1\rangle \langle n-1| + |n\rangle \langle n| + |n+1\rangle \langle n+1| \quad (4)$$

Each term of the Hamiltonian (H_{nm}) is a 20×20 matrix, describing the interaction of the atomic layers within the principal layers m and n .

To obtain the Green's function, we start from

$$(\omega - H)G = I \tag{5}$$

$$\langle m | (\omega - H)G | n \rangle = \delta_{mn} \tag{6}$$

The expression for the surface Green's function (G_{00}), in terms of the transfer matrix (T), defined as $T = G_{00} H_{00}^+$, is

$$(\omega - H_{00} - H_{01} T)G_{00} = I \tag{7}$$

For the bulk Green's function projected on a layer, we have

$$G_B^{-1} = (G_{00}^{-1} - H_{01}^+ \bar{T}) \tag{8}$$

Where \bar{T} is the transfer matrix of the dual surface. Following the iterative scheme of López Sancho *et al* [3], we can obtain the T matrices. Using the method of Cunningham [4], we integrate over the reduced Brillouin zone to get the density of states, given by

$$N(E, k) = -\frac{1}{\pi} \text{Im Tr } G(E, k) \tag{9}$$

Results

In table 1. we compare the obtained values of energy (for CdTe and ZnTe) in high symmetry points within the Brillouin zone, with experimental and theoretical data reported in the literature. The values for the fundamental gaps were accurately reproduced.

We do not include the bowing parameter in the calculation of the bandstructure of the alloy for different concentrations, because the fundamental gap of these compounds seems to show a linear behaviour as a function of the concentration [5]. As shown in Fig. 2, the eigenvalues for the alloy stand within the limits for the pure materials.

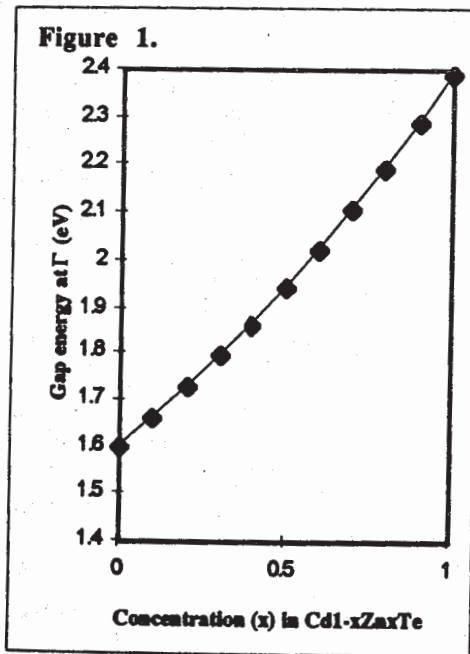


Table 1.

Comparison of our results with experimental and theoretical data, at some high symmetry points in the Brillouin zone

	ZnTe		CdTe	
Γ				
	2.39*	2.39+	1.69*	1.59**
	-0.91*	-0.91+	-0.91*	-0.89**
	-13.0*	-13.0++	-10.75*	-11.07**
X				
	-1.93*	-1.93+	-8.9*	-9.12**
	-2.4*	-2.4+	-4.29*	-5.05**
	-5.5*	-5.5+	-2.19*	-1.98**
	3.09*	3.05++	-1.73*	-1.6**
L				
	-11.98*	-12++	-4.1*	-4.73**
	-5.23*	-5.5++	-1.32*	-1.18**
	-1.46*	-1.1++	-0.77*	-0.65**
	2.64*	2.38++	2.09*	2.82**

- * Our results
- ** Reference [6]
- + Reference [7]
- ++ Reference [8]

Figure 2.

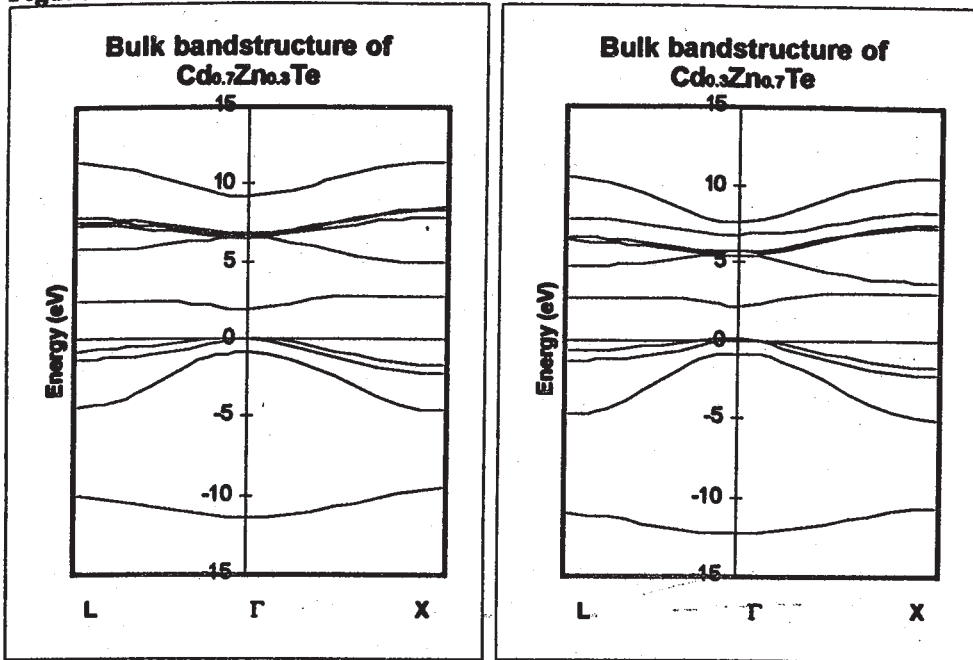
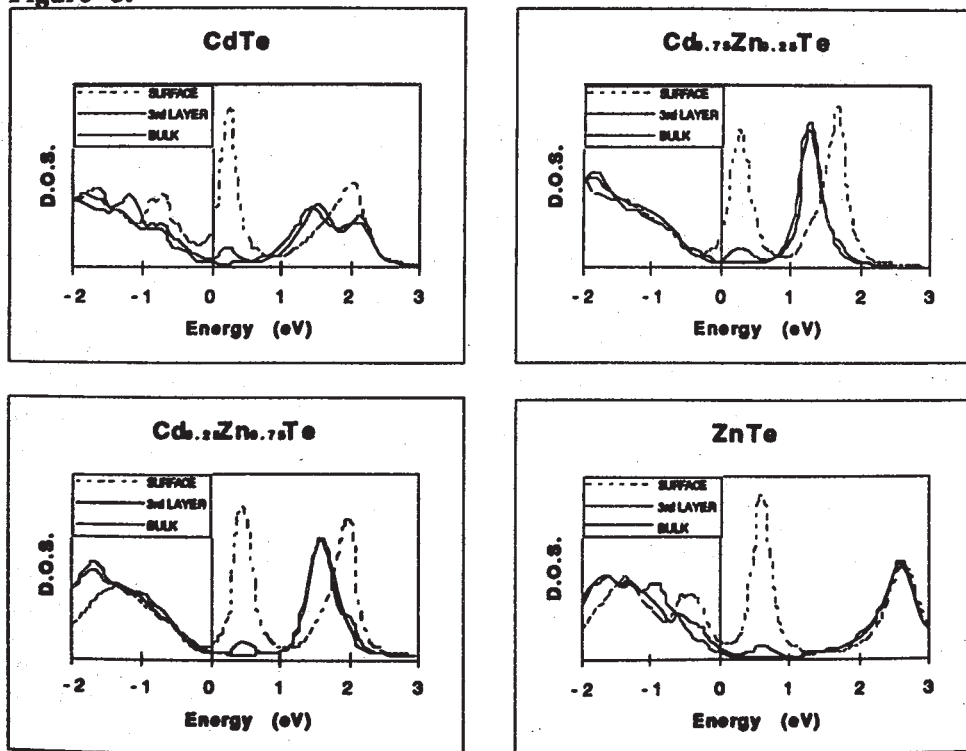


Figure 3.



As seen in Fig.2, the bandstructures of the alloys keep the main features of the binary compounds with larger concentration. For $\text{Cd}_{0.3}\text{Zn}_{0.7}\text{Te}$ the gap is 2.1 eV and for $\text{Cd}_{0.7}\text{Zn}_{0.3}\text{Te}$ is 1.8 eV.

Fig. 3 shows the surface projected bulk density of states and the surface density of states for the third principal layer and for the surface, for the binary compounds and for $x=0.75$ and 0.25 in $\text{Cd}_x\text{Zn}_{1-x}\text{Te}$.

From the figure it is clear that two new states appear when we take the effect of the surface into account. We detected the first surface state for all the different concentrations and found that it moves to higher energies when we change x from zero to one shifting from 0.25 eV in CdTe to 0.6 in ZnTe. As with the bulk energy gap, the increment in energy with x , is linear. A Second new state is clearly found in the conduction band for CdTe at 0.2 eV, this state shifts to the conduction band edge as x increases. For $x=1$, ZnTe, this second state coincides with the band edge. Instead of it in this pure material appears a new state at the valence band edge.

We report two new surface states in the studied alloys.

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