SURFACE STATES OF CdTe (100)

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Abstract

We have established the bulk band structure of CdTe using the tight binding method. We used in our description an orthogonal basis, $s p^3 s^*$, in order to take into account the orbitals in the valence band in detail and the conduction band at its right energy. We have included the spin-orbit coupling (SO), necessary to describe the splitting of the states near the valence band. Using the tight-binding parameters of Schulman we set 1.6 eV for the gap and 0.9 eV for the SO splitting. A little correction to the tight binding parameters allowed us to obtain the experimental gap value (1.48 eV) keeping for the SO splitting (0.9 eV) also in agreement with experiment.

In this work we study the (100) CdTe direction in detail. In particular, we look at the branch of states starting at -4.4 eV from the top of the valence band at $\Gamma$, a result established by Niles and Höchst via photoemission spectroscopy. We obtained for the first time a theoretical description of this branch and made an analysis of the relevant states.

Introduction.

In recent experiments Niles and Höchst [1] described the band structure of the (100) CdTe direction. They gave values for the energy of the valence band between 0.0 eV and -5.0 eV in the $\Gamma - X$ direction, on the first Brillouin zone. They compared their results with theoretical bulk band structure calculations. In particular, they found discrepancy between experiment and theory in that there is a band at -4.4 eV that does not appear in the theoretical calculations but does appear in their photoemission experiments.

In their work, Niles and Höchst suggest that the valence band has its origin in the high density of states around the $X_\phi$ point, apparently not treated properly in the non local pseudopotential calculation of Chelikowsky and Cohen [2].

We calculated the band structure of CdTe bulk, using the tight binding method in the Slater-Koster formalism [3], with an orthogonal basis of five atomic orbitals, $s p^3 s^*$, where the $s^*$ state is introduced to simulate the excited states in the conduction band [4]. We used the Surface Green Function Matching method [5] and calculated the surface Green function ($G_s^{-1} = (E - H_{00}) - H_{01} T$), where we use the
definitions and conventions of reference [10]). We looked for the poles of the real part of the Green function, which correspond to the eigenvalues of the energy. In this way we found the band reported by Niles and Höchst. Our result suggest that the disagreement comes from a deficient description of the $X$ point of the Brillouin zone in the pseudopotential calculations, as suggested by Niles and Höchst.

Further we found that the band beginning at $-4.4$ eV in $\Gamma$ has its origin in the hybridized states that form the bond Cd-Te. This is a band with very little dispersion.

**Results and Discussion.**

Figure 1 shows the experimental (100) CdTe band structure results obtained by Niles and Höchst [1] compared to the bulk band calculations of Chelikowsky and Cohen [2], and Humphreys and Srivastava [6].

Figure 2 shows the band structure obtained with the tight binding method using the Schulman parameters [7], which we readjusted to reproduce the values of the energy in $\Gamma$ and $X$ reported by experiment. We have obtained the band starting at $-4.4$ eV in $\Gamma$, and that spreads out in the $\Gamma - X$ direction, directly from the poles of the real part of the bulk Green function [8].

![Figure 1](image1.png)

**Fig. 1.** Comparison of the experimentally determined valence band along (100) direction of CdTe with band-structure calculations, after Niles and Höchst (Ref. [1]).

![Figure 2](image2.png)

**Fig. 2.** Band-structure calculation of the valence band in this work, showing the valence state at $-4.4$ eV.

In the figures 3 and 4 we plot the poles of the bulk and surface Green functions. In this figures we can see that the state at $-4.4$ eV, reported by Niles and Höchst,
appears in the bulk Green function and not in the surface Green function. This means that the state is not a surface state. We studied the two surfaces. One terminated in the cation and the other in the anion. We can see that the result is the same for both surfaces (figure 3). Therefore, the band reported by Niles and Höchst is of bulk origin.

![Fig. 3. Poles of the Bulk Green Function. In this plot we can see the state at -4.4 eV and how it spreads out in the $\Gamma - X$ direction. We are plotting results for both surfaces on the compound (i.e. anion and cation termination).](image)

![Fig. 4. Poles of the Surface Green Function. In this plot we are plotting the same surfaces that in the Fig. 3.](image)

The same surface has been studied by Rodríguez et al. [9], but they don't discuss in detail neither the position nor the origin of the bands in the valence bands, a point we make clear in our work.

**Conclusions.**

Using the tight binding method with an orthogonal basis of five atomic orbitals, $s p^5 s^*$, we calculated the band structure in bulk of the compound CdTe. We have also calculated the (001) direction electronic band structure both with a Cd and Te termination. We have used the Surface Green Function Matching method. We were able to explain the Niles and Höchst experiment, as a state that coming from a bulk state hybridized from the 5s Cd and 5p$_z$ Te electronic states. This state appears in our calculation in the bulk projected bands in the (100) direction at the experimental energy of -4.4 eV in $\Gamma$ and spreads out in the $\Gamma - X$ direction in
two bands, very near each other in energy, that almost reach the X-point on the Brillouin zone.

References.