



# Hydrostatic pressure dependence of the direct gap, transverse effective charge and refractive index of CdTe system

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**Abstract--We have determined the pressure dependence of the direct band gap, transverse effective charge and refractive index for CdTe system up to 3 GPa. Using the  $sp^3s^*$  semi-empirical tight-binding method (TB) with the scaling law and the Murnaghan's equation of state, we have shown that all these properties were found to have a sublinearity behavior with the pressure. The results are compared with other works.**

**Index Terms---**Tight binding method, electronic properties, refractive index, CdTe .

## I. INTRODUCTION

RECENTLY, New window materials are used as heterojunction partners on CdTe solar cells. For example both ZnS and  $Zn_xCd_{1-x}O$  thin films can be used as buffer layers on CdTe solar cells, although the ZnS/CdTe heterojunction gave a better photovoltaic efficiency [1]. These results will involve a better understanding of the properties of these window layers and junction formation processes. We know that the valence band offset of any heterostructure at the interface is a fundamental property, and the pressure coefficients have been used to determine the band offset at zincblende semiconductor interfaces [2]. Whence, strain effect upon the band offset must be considered. It is clear then that under stress, the device's optical properties are modified. Therefore, it would be interesting to study and understand the behaviour of electronic and optical properties when stress is applied.

In this paper we study the effect of hydrostatic pressure on the energy band gap, transverse effective charge and refractive index of CdTe. The calculations were performed using an  $sp^3s^*$  semi-empirical tight-binding (TB) method with the scaling law

and Murnaghan's equation of state (EOS) [3]. The calculated results are carefully analysed and compared with the available experimental data and theoretical results.

The paper is organized as follows: in Section 2 we present the calculation framework. In Section 3 we compare and discuss our obtained results. Finally, the conclusion is given in Section 4.

## II. CALCULATION

We use our approach based on the Tight Binding Hamiltonian, described in the Slater-Koster language with  $sp^3s^*$  model [4]. The virtual orbital  $s^*$  is introduced to properly locate in energy the conduction band usually formed by  $d$  states in the II-VI zinc-blende semiconductor compounds. The Hamiltonian is defined by 13 parameters describing the microscopic interactions. These parameters can be obtained by there adjustment to the experimental data given at the high symmetry points  $\Gamma$ , X and L.

In order to study the electronic and optical properties of a strained compounds, we start with the tight binding (TB) description of unstrained compounds that we have discussed above, and used the scaling law which describes the variation of the interaction TB parameters with respect to the interatomic distance  $a$ . In fact, if a stress (hydrostatic, for instance) is applied, the interatomic distances decrease from the  $a_0$  unstrained bulk value to the  $a$  value leading to an enhancement of the interactions. The off-diagonal matrix elements of the Hamiltonian between two atomic orbitals  $i$  and  $j$  centered on an anion and a cation  $V_{ij}^{a,c}(a)$  are assumed to vary according to the law,

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$$V_{ij}^{a,c}(a) = \left[ \frac{a}{a_0} \right]^{-x_{ij}} V_{ij}^{a,c}(a_0)$$

(1)

Where the exponents  $\alpha_j$  are expressed in our formula by [3] :

$$\alpha_{ij}(d) = \log\left(\frac{h_{ijm} \frac{\hbar}{m_0 V_{ij}^{a,c}(d_0) d^2}}{d_0}\right) / \log\left(\frac{d}{d_0}\right) \quad (2)$$

where  $\alpha_j$  are valid only for  $d \neq d_0$  but are negligible for all  $d$  not near to  $d_0$ . We have determined there values numerically for CdTe when  $d \gg d_0$ .

The interatomic distance  $a$  used in Eq. 1 is obtained from Murnaghan's equation of states by :

$$a(P) = a_0 \left[ 1 + \frac{B_0'}{B_0} P \right]^{-\frac{1}{3B_0'}} \quad (3)$$

where  $a_0 = 6.481 \text{ \AA}$  and  $B_0$  and  $B_0'$  are the values of the bulk modulus and of its first pressure derivative at  $P=0$ . There values are 44.5 GPa and 6.4 for CdTe respectively [5].

### I. RESULTS

The TB parameters of CdTe at the equilibrium phase are determined by the fitting procedure to various energy values at  $\Gamma$ , X and L high symmetry points of the Brillouin zone (BZ). The final adjusted TB parameters are published elsewhere [3] and its resulting band structure is displayed in figure 1. The comparison of the calculated energies at  $\Gamma$ , X and L points with other works show a good agreement [6].

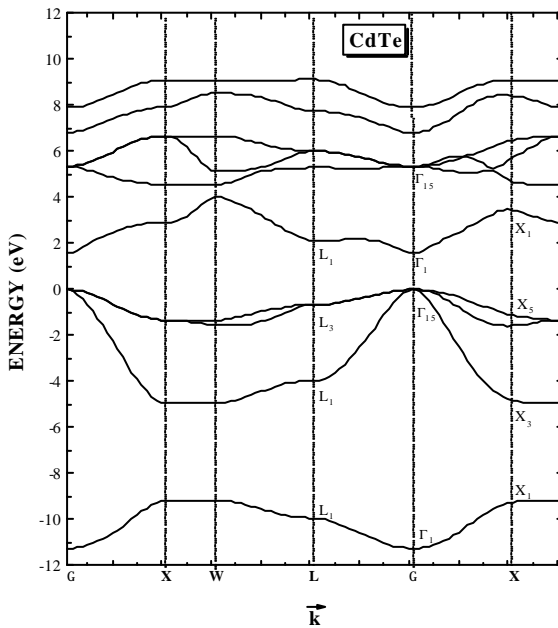


Fig. 1 : Band structure of CdTe.

#### A. Energy gap $E_0$

Using the  $\alpha_j$  value's obtained for CdTe in the eq. (1), we have determined the TB parameters as function of the pressure and the energy gap under pressure effect is obtained up to 3 GPa. The variation is plotted in fig. 2, and shows that the direct gap  $E_0$  increases with increasing pressure. A least square fit of the curve exhibits a sublinearity, yielding for the linear and quadratic energy coefficients :

$$E_0(P) = E_0(P=0) + bP + cP^2 \quad (4)$$

In table 1, we have given our calculated coefficients compared with the empirical pseudopotential method (EPM) [6,7], linear muffin tin orbital (LMTO) [8] calculation and experimental data [9]. We have obtained a good agreement between the data for the pressure shift of  $E_0$ .

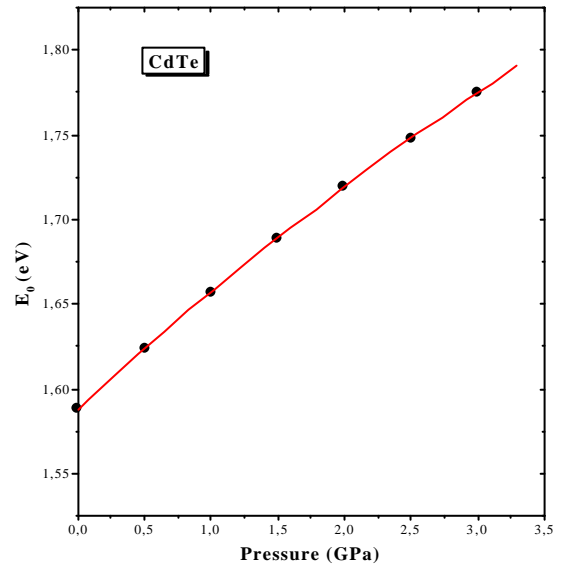


Fig. 2 : Pressure dependence of the direct band gap for CdTe

TABLE I  
CALCULATED ENERGY COEFFICIENTS OF PRESSURE  
DEPENDENCE FOR CDTE

	$E_0$ (eV)	$b$ ( $10^{-2}$ eV GPa $^{-1}$ )	$c$ ( $10^{-4}$ eV GPa $^{-2}$ )
This work	1.59	7.2	-32.9
EPM	1.59	2.8	-
LMTO	0.583	6.45	-
Experiment	1.606	7.59	-39.9

### B. Transverse effective charge

The transverse or dynamic effective charge  $e^*_{\perp}$  is the fundamental quantity that specifies the leading coupling between lattice displacements and electrostatic fields in insulators [23]. So it is more interesting to study how this quantity changes when the pressure is applied. In the BOM approach, we express  $e^*_{\perp}$  as a function of the pressure by :

$$e^*_{\perp}(P) = 4a_p(P) - \Delta Z + 4ga_p(P)(1 - a_p^2(P)) \quad (5)$$

where  $\Delta Z = \gamma^2 = 2$ . Our calculated value  $e^*_{\perp}$  at  $P = 0$  is in good agreement with the experimental one which is 2.35 [10]. The pressure dependence of the transverse effective charge is illustrated in Fig. 3.

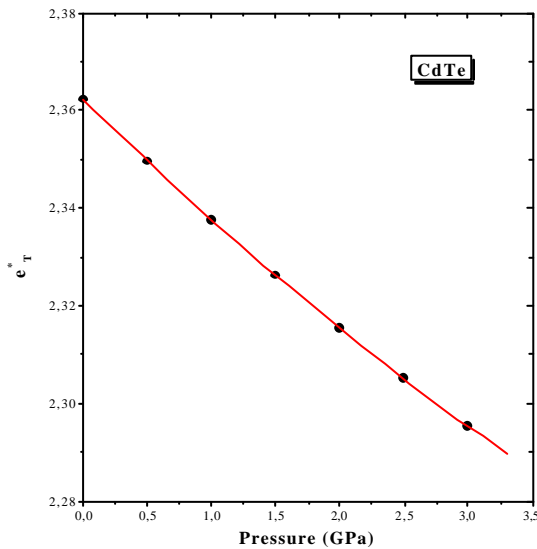


Fig. 3 : Pressure dependence of  $e^*_{\perp}$  for CdTe

We notice that  $e^*_{\perp}$  decreases with increasing pressure. We find the following dependence :

$$e^*_{\perp}(P) = 2.367 - 2.57 \cdot 10^{-2} P + 11.4 \cdot 10^{-4} P^2 \quad (6)$$

### C. Refractive index

The refractive index  $n$  is a very important physical parameter related to the microscopic atomic interactions. Using the Hervé and Vandamme model [11], we have calculated the pressure dependence of the refractive index. The result is displayed in Fig. 6.

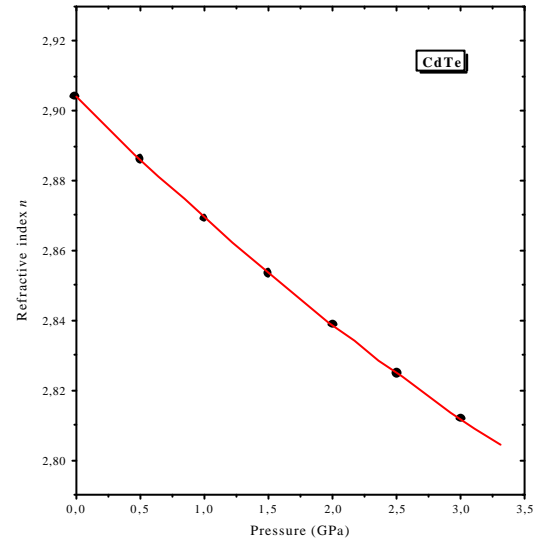


Fig. 4 : Pressure dependence of the refractive index for CdTe

Our best fit yields :

$$n(P) = 2.9 - 3.67 \cdot 10^{-2} P + 20.2 \cdot 10^{-4} P^2 \quad (7)$$

We observe a strong nonlinear decrease of the refractive index with the pressure.

## II. CONCLUSION

Using an  $sp^3s^*$  semi-empirical TB method with the scaling law and Murnaghan's EOS, we have investigated the hydrostatic pressure dependence of the energy band gap  $E_0$ , transverse effective charge  $e^*_{\perp}$  and refractive index  $n$  for CdTe. The obtained  $dE_0/dP$  was in good agreement with the

results for bulk crystals and the refractive index  $n(P)$  was deduced. A good agreement with the experimental data was obtained the transverse effective charge  $e^*_T$ .

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