Optik - International Journal for Light and Electron Optics 170 (2018) 37–42

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

Optical properties and exciton binding energy and related parameters of CdTe: Pressure-induced effects

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ARTICLE INFO

Keywords:
Pressure
Optical properties
Excitons
CdTe
Infrared

ABSTRACT

The present paper reports on the hydrostatic pressure dependence of the direct and indirect energy band-gaps, refractive index, static and high-frequency dielectric constants, exciton banding energy and exciton Bohr radius for CdTe in the zinc-blende structure. The applied pressure is taken in the range 0–30 kbar. The calculations are performed using a pseudopotential approach. At zero pressure, our results show a good accord with experiment for most studied optical properties. Nevertheless, for exciton binding energy and Bohr radius the use of Adachi's expression [S. Adachi, Properties of Group-IV, III–V, and II—VI Semiconductors, Wiley, Chichester, 2005] has given poor results as compared to experiment. In this respect, a modified Adachi's expression formula have been proposed and found to give meaningful accord with experiment. Upon compression up to 30 kbar, the material of interest is found to remain a direct (Γ-Γ) band-gap semiconductor. All optical features being studied here have shown a monotonic behavior under compression. The present study can be useful for infrared applications.

1. Introduction

Cadmium telluride (CdTe) is a direct band-gap semiconductor which belongs to the group II—VI family. It is a stable crystalline compound formed from cadmium and tellurium. The material of interest has considerable application in optoelectronics devices. It is used as an infrared optical material for optical windows and lenses [1]. It has been considered as a suitable candidate that can be used as absorber layer for CdTe/CdS solar cells devices [2–4]. CdTe can be alloyed with either zinc or mercury to make a versatile infrared detector material (CdZnTe or HgCdTe) [5,6]. On the other hand, when CdTe is alloyed with a small amount of zinc it can found useful application in radiation detectors [7–9]. Besides, this material operates at room temperature which allows the construction of compact detectors that have a large range of applications in nuclear spectroscopy [10].

The optical properties of semiconductors have been investigated extensively both experimentally and theoretically in the last years [11–13]. This is because these properties are one of the best tools for studying electron states and band structures. As a matter of fact, the optical spectra in semiconductors exhibit a structure near the fundamental edge. The latter is explained to be due to the formation of a direct exciton [14]. The exciton is a basic optical excitation of any semiconductor system. In fact, in the optical absorption and emission of semiconductors which have a direct band-gap, excitonic effects usually can be observed [12,15–17]. The contribution of excitons in solar cells is very important and is considered to be as the primary effect of the absorption of light and the

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https://doi.org/10.1016/j.ijleo.2018.05.069
Received 28 March 2018; Accepted 17 May 2018

Table 1
Band-gap energies for zinc-blende CdTe fixed in the fits at zero pressure.

$E_{\Gamma\text{-}\Gamma}$ (eV)	$E_{\Gamma\text{-}X}$ (eV)	$E_{\Gamma\text{-}L}$ (eV)
1.5045[a]	3.48[b]	2.47[b]

[a] Experimental value reported in Ref. [31].
[b] Theoretical values reported in Ref. [32].

dissociation of exciton allows the creation of free electrons and holes [18].

At ambient pressure CdTe crystallizes in the zinc-blende structure which transforms under applied pressure to the cinnabar phase [19]. The transition pressure to the first phase is reported to be 35.3 kbar [19] and about 39 kbar [20]. The continuous development of the diamond anvil cell technology over the last years has opened a large field of high pressure science [21]. On the other hand the theoretical understanding of physics of solids under strong compression seems to be more advanced [21–26].

In the present work we report on the effect of hydrostatic pressure on the direct and indirect energy band-gaps, optical properties namely the refractive index and static and high-frequency dielectric constants and the exciton binding energy and related parameters in CdTe compound semiconductor. The calculations are performed using essentially a pseudopotential approach. The aim of the present contribution is to show to what extent the pressure-induced effects affect the investigated properties of the material of interest. Furthermore, accurate knowledge of optical properties of the material in question and their hydrostatic pressure dependence can be very useful for eventual technological applications.

2. Computational details

The calculations presented in this work are essentially based on the empirical pseudopotential method (EPM). For more details about the EPM, we refer the reader to the book by Martin [27]. With this method, the potential is obtained by needing only a small number of parameters, the pseudopotential form factors. This potential is used then in the secular equation which gives the one electron energy levels and wave functions. In order to reproduce the experimental inter-band optical transition energies at selected high-symmetry points in the Brillouin zone, the pseudopotential form factors are adjusted. The non-linear least-squares fit method as described in Refs. [28–30] is used so as to optimize the empirical pseudopotential parameters. The experimental and known data concerning the energy band-gaps for CdTe at Γ, X and L high symmetry points in the Brillouin zone at zero pressure used in the fitting procedure are given in Table 1. The dimension of the present eigenvalue problem is a 136 × 136 matrix.

For pressures greater than zero, taken in the range 0–30 kbar in this study, the first-order pressure coefficients of direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) band-gaps are fitted to those reported in Ref. [33] so as to obtain the pseudopotential form factors. The pressure dependence of the lattice constant has been determined using the Murnaghan equation of state. The equilibrium bulk modulus (B_0) is taken to be 4.24×10^{11} dyn/cm^2 [19], whereas its first pressure derivative ($B_0^{'}$) is taken to be 6.4 [19]. The final adjusted pseudopotential form factors of CdTe at pressures ranging from 0 up to 30 kbar are shown in Table 2.

3. Results and discussion

The variation in the optical transitions that correspond to the direct (Γ-Γ) and indirect (Γ-X) and (Γ-L) energy band-gaps as a function of pressure in the range 0–30 kbar for zinc-blende CdTe is displayed in Fig. 1. Note that both the direct (Γ-Γ) and the indirect (Γ-L) band-gap energies increase monotonically with increasing pressure from 0 up to 30 kbar. This is not the case for the indirect (Γ-X) energy band gap which decreases slightly and monotonically with increasing pressure in the range 0–30 kbar. Such a behavior has also been reported for AlSb binary semiconductor [34]. It is worth noting that there is no crossing between the curves that represent the energy band-gaps (Γ-Γ), (Γ-X) and (Γ-L). This suggests that under hydrostatic compression up to 30 kbar, CdTe remains a direct band-gap semiconductor.

The refractive index (n) is an important optical parameter of a material. It is a dimensionless number which describes the propagation of light through a medium. In this contribution, n has been determined using the revised relation as suggested by

Table 2
Pseudopotential form factors for zinc-blende CdTe at various pressures up to 30 kbar.

Pressure (kbar)	Form factors (Ry)					
	$V_S(3)$	$V_S(8)$	$V_S(11)$	$V_A(3)$	$V_A(4)$	$V_A(11)$
0	−0.396388	0.198275	0.459548	0.1311	0.28	0.708145
5	−0.396388	0.196840	0.463735	0.1311	0.28	0.709870
10	−0.396388	0.196538	0.467002	0.1311	0.28	0.711524
15	−0.396388	0.196773	0.469829	0.1311	0.28	0.713181
20	−0.396388	0.197330	0.472401	0.1311	0.28	0.714861
25	−0.396388	0.198098	0.474800	0.1311	0.28	0.716564
30	−0.396388	0.199018	0.477076	0.1311	0.28	0.718290