ISSN 1024-588X. Вісник Львівського університету. Серія фізична. 2022. Випуск 59. С. 3–14
Visnyk of the Lviv University. Series Physics. 2022. Issue 59. P. 3–14

УДК 538.9
PACS 71.15.Mb
https://doi.org/10.30970/vph.59.2022.3

Pressure effect on the electronic spectra of CdTe crystal calculated by DFT

A. I. Kashuba, I. V. Semkiv, H. A. Ilchuk, R. Yu. Petrus

Lviv Polytechnic National University,
12 S. Bandera Str., Lviv, Ukraine, 79013
e-mail: andrii.i.kashuba@lpnu.ua

The effect of pressure on the electronic band structure of CdTe crystal has been investigated using the density functional theory. In this approach, the generalized gradient approximation (GGA) and the Purdue–Burke–Ernzerhof (PBEsol) parameterization were used for the exchange-correlation potential calculation. The ground-state properties are determined for the bulk materials of CdTe in zinc-blende phase. Structure and electronic properties are studied in the range of hydrostatic pressures between 0 and 50 GPa. The electron band-energy structure and density of states were calculated at different pressures. The equilibrium structural parameters, bulk modules and band gaps are calculated and compared with the available experimental data and other theoretical results. The shift in the energy gap, refractive index, high-frequency dielectric constant, bulk module and lattice parameters of CdTe crystal with pressure is determined and compared with other known data.

Key words: electron band structure, band gap, pressure, volume deformation potential, refractive index, high-frequency dielectric constant.

1. Introduction

Cadmium telluride (CdTe) compound is the representatives of $A^{II}B^{VI}$ crystal group and reveal typical semiconductor behavior. CdTe crystal can exist in either zinc-blende (ZnS) structures under normal conditions [1–3]. This crystal remains an important research field because of their wide application in various fields of optoelectronic devices. From this point of view, the research of structural properties and the dynamics of electronic spectra of CdTe crystal under the action of external pressures is fundamental interest for studying the process of stabilization in compounds.

Some information about pressure effect on the structure and fundamental properties of the CdTe crystal has already been reported in the works [4,5]. In particular, theoretical studies of band gap change under the pressure between 0–10 GPa presented in Ref. [4]. Another works [5] give results of the band gap change under the pressure between 0–30 kbar and optical properties study of CdTe crystal. In both case obtained increases of

value of band gap with increasing pressure. Nonetheless, the properties of this material still need further studying.

In this report, we study the pressure effect (0–50 GPa) on the electronic properties of the CdTe crystal in zinc-blende structure. We have performed the electronic band-energy structure calculations for CdTe crystal to obtain the volume deformation potential, first- and second-order pressure derivatives for G–G transition.

2. Methods of calculation

The theoretical calculations were performed within the framework of the density functional theory (DFT). To calculate the properties of the single-crystalline CdTe, the crystalline lattices with the basal parameters given below were used (see Table 1). The Vanderbilt's ultrasoft pseudopotentials [6] were used for the ionic potentials. To describe the exchange-correlation energy of the electronic subsystem, functional in the approximation of generalized gradient (GGA) and the Purdue–Burke–Ernzerhof (PBEsol) parameterization [7] was used. As a correlation potential, the Ceperlay–Alder and Gell–Mann–Brueckner equations were applied to the high electron-density boundaries.

The charge-density distribution was calculated by the method of special points involving the techniques of charge damping. The relaxation of ions positions was achieved on the basis of calculated atomic forces for each crystal structure, and then the integral stress of the cell was determined.

The value of $E_{cut-off}$= 660 eV for the energy of cutting-off the plane waves was used in our calculations. The electronic configurations $4d^{10}5s^2$ for Cd, $5s^25p^4$ for Te atoms formed the valence electronic states. The integration over the Brillouin zone (BZ) was performed on the 4×4×4 grid of k points using the Monkhorst–Pack scheme [8]. The self-consistent convergence of the total energy was taken as 5.0×10^{-6} eV/atom. Geometry optimization of the lattice parameters and atomic coordinates was performed using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization technique with the maximum ionic Hellmann–Feynman forces within 0.01 eV/Angstrom, the maximum ionic displacement within 5.0×10^{-4} Angstrom, and the maximum stress within 0.02 GPa. These parameters are sufficiently small to lead to a well-converged total energy of the structures studied.

The energy band diagram was constructed using the points of the BZ in the inverse space, which were as follows: X(0.5, 0, 0.5), R(0.5, 0.5, 0.5), M(0.5, 0.5, 0) and G(0, 0, 0).

3. Results and Discussion

In Table 1, the experimental and theoretical values for equilibrium lattice parameters (at zero pressure) in the crystals unit cells, as well as the ground state parameters $E_{g,0}$, V_0 and B_0, are tabulated. Certain excess in theoretically obtained values for lattice parameters a was induced by neglecting the zero vibrations and overestimating the binding energy values in the GGA formalism.

In Fig. 1, the full-energy band diagrams of the CdTe crystal is shown along the highly-symmetric lines of the BZ at high pressures (10 GPa) (electron band energy structure at normal conditions can be found in Ref. [1]). The energy in this case is counted from the

Fermi level (ΔE= E-E_F). In our case, position Fermi level corresponding to zero energy on figure 1.

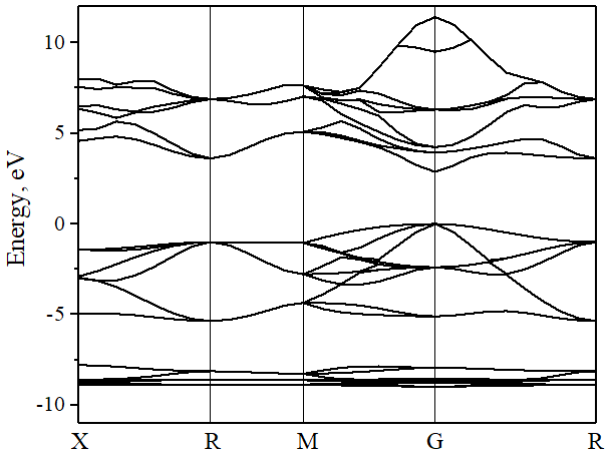

Fig. 1: Band structure of CdTe crystal at 10 GPa.

Analysis of the results of theoretical calculations of the energy band spectra shows that the smallest band gaps are localized in the center of the BZ (the point G). This means that the crystals are characterized by a direct energy band gap. Applied pressures don't change type of the band gap, execution of value witch are increases with increasing pressure (see Fig. 2). At higher pressures there is an increase in band gap, indicating a lower electrical conductivity at higher pressures (below 30 GPa). This behavior is normal and observed in other research works [4, 5, 9, 10]. But, above 30 GPa we can see decreases band gap with increasing pressure. Such behavior can be connected with effect of metallization sample. The same behavior was observed in CdS crystal [11]. Pressure of metallization in CdS crystal is 6.9133 Mbar (691.33 GPa) [11]. In our case, if extrapolation data to zero value of band gap is obtained pressure of metallization. This pressure is near 114 GPa.

Comparing the theoretical results with the experimental data (see Table 1), one can see that the calculations in the GGA-PBEsol approximation for the crystals give rise to underestimated values of the band gap. However, the precision values of band gaps are not the subject of this work. We desire to observe the dependence of basic energetic parameters on applied pressures. We can determine the pressure coefficients by fitting the calculated band gap $E_{g,p}$ to a function (for data below 30 GPa):

$$E_{g,p} = E_g^0 + Ap + Cp^2, \tag{1}$$

where E_g^0 is the energy in eV, p the pressure in GPa, A and C are the first- and second-order pressure derivatives, respectively. The calculated values of A and C for the G–G transitions for the compounds under study are given in Table 1.

The volume deformation potential (α) is given by the expression [14]:

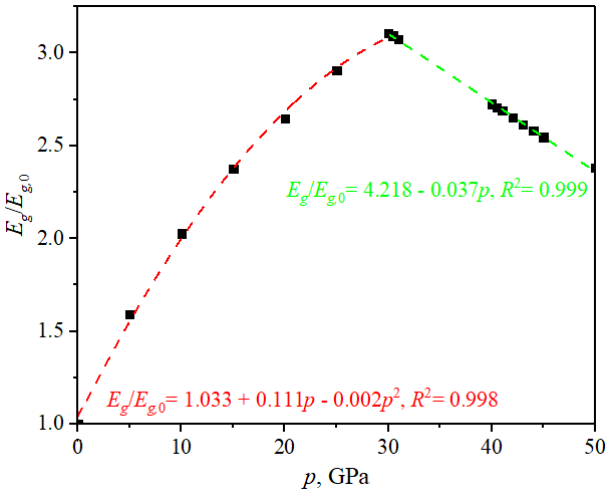

Fig. 2: Calculated ratio of energy gaps to equilibrium value of band gap for CdTe crystal as function of pressure.

$$\alpha = \frac{dE_{g,p}}{dlnV_p}. \tag{2}$$

As can see the sign of volume deformation potential is changed from minus to plus with change pressure region from 0–30 GPa to 30–50 GPa. Also, we was obtained much higher value of volume deformation potential (absolute value) for CdTe crystal if comparisons with other materials of $A^{II}B^{VI}$ group [9].

The analysis of partial contributions of individual levels to the function of the total density of states (Fig. 3) and the partial contributions of individual bands to the electronic density allows us to find genesis of the valence bands (VBs) and conduction bands (CBs) for the CdTe crystal at 10 GPa. The lowest bands near –9 eV are formed by the d states of Cd. The peak of the VB complex is formed by the p states of Te, with 'contamination' of the p states of Cd, and the CB bottom is mainly formed by the p states of Cd and Te, as well as by the s states of Cd. Taking into account the selection rules, the results of calculations of the energy band spectra and the densities of states, we can assume that the direct s–p transitions form the smallest energy band gap. It is possible that the direct-band transitions (localized at the G point of the BZ) can be formed by the Te-Cd link, and this behavior is realized when applying pressure [1].

Refractive index represents a fundamental optical parameter closely related to the band structure and the electronic properties of optoelectronic materials. A number of empirical relationships that link the refractive index n with the band gap E_g are known from the literature, the most notorious of which are those suggested by Moss [15], Ravindra [16], Herve and Vandamme [17], and Tripathy [18]. According to these models, a refractive index of a semiconductor (with the band gap being usually in the range $0 < E_g < 5$ eV) can be calculated as [19]:

Table 1: Experimental and theoretical equilibrium structural parameters of CdTe crystal in the zinc-blende structure.

Parameters	This work	Value from literature
a, nm	0.6564376	0.64765(19) [1]
V_0, nm^3	0.276	–
$E_{g,0}$, eV	1.418	1.44 [12]
B_0, GPa	54.69437	39 [13]
E_g^0, eV	1.465	–
A, eV GPa^{-1}	0.157	–
C, eV GPa^{-2}	0.003	–
α, eV (p= 0-30 GPa)	-3.29	–
α, eV (p= 30-50 GPa)	3.53	–

$$n_M^4 E_g = C, n_R = a - bE_g, n_{HV}^2 = 1 + [A/(E_g + B)]^2, n_T = n_0[1 + \alpha \exp(-\beta E_g)], \quad (3)$$

where the normal conditions are assumed, the band gap units are eV, and the n's subscripts abbreviate the authors mentioned above. In Eqs. (3), C= 95 eV, a= 4.084 eV, b= 0.62 eV^{-1}, A= 13.6 eV is the hydrogen ionization energy, B= 3.47 eV the constant equal to the difference between the ultraviolet resonance energy and the band gap E_g, n_0= 1.73, α= 1.9017 and β= 0.539 eV^{-1} [15–19]. In spite of a wide variety of empirical relationships, sometimes there can arise some problems with interpreting quantitatively the refractive index in terms of Eqs. (3) and preferring one formula over the other (see Refs. [19]).

Using different models given by Eqs. (3), we have calculated the n values for the CdTe crystal, which correspond to the photon energies $\hbar\nu$ exactly equal to the band gaps. Fig. 4 displays the appropriate pressure dependencies n. The experimental data for CdTe (n= 2.865 at the wavelength 861 nm [20]) and compare it with the data of Fig. 4 shows better correlation with Moss relation. It turns out that the refractive index calculated with the Moss equation is only < 0.15 % different from the experimental one. The relative accuracy of the Herve-Vandamme formula remains high enough (3.2 %), whereas the Ravindra and Tripathy equations provide poorer results (11.9 % and 13.9 %, respectively). As a conclusion, the canonical Moss relationship between the refractive index and the band gap works extremely well in case of the CdTe crystal.

Another important fundamental property of semiconductors is the dielectric constant which gives information about the ability of a substance to insulate charges from each other [5]. Based on the values of n calculated from the different relations, the pressure behavior of high-frequency dielectric constant $\varepsilon_\infty = n^2$ have been determined for CdTe crystal (see Fig. 5). At normal condition (zero pressure) our results yielded values of ε_∞= 8.19 (Moss relation used for calculation n). The data for CdTe (ε_∞= 8.47 [5]) and compare it with the data of Fig. 5 shows better correlation with Herve-Vandamme relation. It turns out that the high-frequency dielectric constant calculated based on

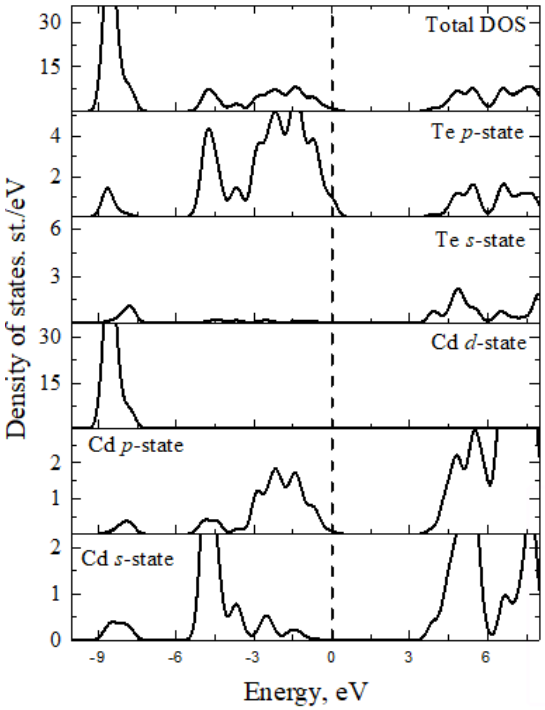

Fig. 3: Total density of states for CdTe crystal at 10 GPa.

refractive index with the Moss and Herve-Vandamme formula for are 3.36 % and 3.20 % different from the other data, respectively.

Fig. 6 shows the effect of hydrostatic pressure on the normalized volume and lattice constants of CdTe crystal. It reveals the volume reduction under pressure. In both cases we can see parabolic behavior of pressure effect on structure parameters (details see on Fig. 6). Also, we were calculated pressure dependence of bulk module B_0 (see Fig. 7). Pressure dependence of bulk module shows parabolic behavior, too (details of fitting analysis see on figures).

4. Conclusion

Based on the application of a number of modern theoretical approaches, in this work we elucidate a set of results that solve an important scientific and applied problem. The main results reported in the present work can be summarized as follows:

First-principle theoretical studies of the electronic energy spectrum for the CdTe crystal have been carried out using the reliable techniques of density functional theory and known approximations. It has been established that the smallest band gap is localized at the center of the BZ (point G) and does not shift with pressure appliance. Therefore, our substances should reveal direct optical transitions. We obtained a good agreement of obtained theoretical values of band gaps with the known experimental results. We also

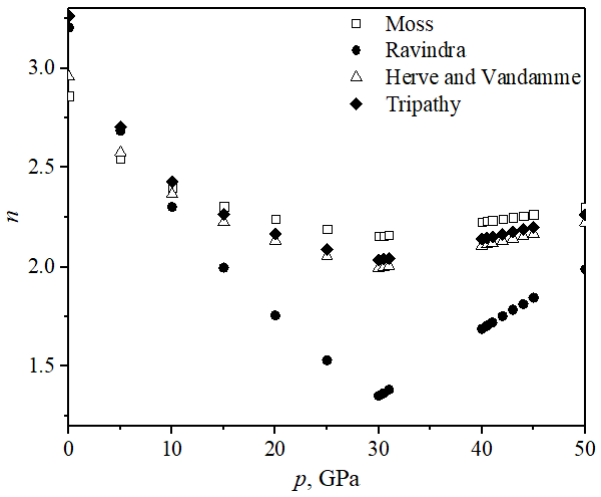

Fig. 4: Calculated of refractive index n for CdTe crystal as function of pressure.

calculated the volume deformation potential, first- and second-order pressure derivatives for G–G transition and dynamics of band gap value change. We obtained that near 114 GPa in CdTe crystal can be metallization effect (transition from semiconductor to metal). Finally, the refractive index calculated from the band gap using the Moss formula agrees very well with the available experimental data.

Acknowledgements

The work was supported by the Project 0121U108649 of Ministry of Education and Science of Ukraine.

1. Ilchuk H.A. Optical-energy properties of the bulk and thin-film cadmium telluride (CdTe) / H. A. Ilchuk, R. Yu. Petrus, A. I. Kashuba, I. V. Semkiv, E. O. Zmiiovska // Nanosistemi, Nanomateriali, Nanotehnologii. – 2018. – Vol. 16(3). – P. 519–533. doi: 10.15407/nnn.16.03.519.
2. Yavorskyi R. Structural and optical properties of cadmium telluride obtained by physical vapor deposition technique / R. Yavorskyi, L. Nykyruy, G. Wisz, P. Potera, S. Adamiak, Sz. Gorny // Applied Nanoscience. – 2019. – Vol. 9. – P. 715–724. doi: 10.1007/s13204-018-0872-z.
3. Saliy Y. P. The surface morphology of CdTe thin films obtained by open evaporation in vacuum / Y. P. Saliy, L. I. Nykyruy, R. S. Yavorskyi, S. Adamiak // Journal of Nano - and Electronic Physics. – 2017. – Vol. 9(5). – P. 05016(5). doi: 10.21272/jnep.9(5).05016.

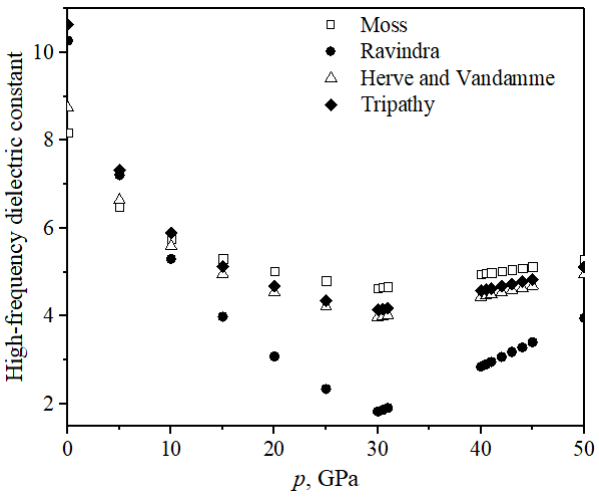

Fig. 5: Calculated of high-frequency dielectric constant ε_∞ for CdTe crystal as function of pressure.

4. Ouendadji S. Theoretical study of structural, electronic, and thermal properties of CdS, CdSe and CdTe compounds / S. Ouendadji, S. Ghemid, H. Meradji, F. El Haj Hassan // Computational Materials Science. – 2011. – Vol. 50. – P. 1460. doi: 10.1016/j.commatsci.2010.11.035.
5. Bouarissa N. Optical properties and exciton binding energy and related parameters of CdTe: Pressure-induced effects/ N. Bouarissa, H. Algarni, O. A. Al-Hagan, M. Ajmal Khan, T. F. Alhuwaymel // Optik. – 2018. – Vol. 170. – P. 37. doi: 10.1016/j.ijleo.2018.05.069.
6. Vanderbilt D. Soft self-consistent pseudopotentials in a generalized eigenvalue formalism / D. Vanderbilt, Physical Review B. – 1990. – Vol. 41. – P. 7892(R). doi: 10.1103/PhysRevB.41.7892.
7. Perdew J. P. Restoring the Density-Gradient Expansion for Exchange in Solids and Surfaces / J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, K. Burke // Physical Review Letter. – 2008. – Vol. 100. – P. 136406. doi: 10.1103/PhysRevLett.100.136406.
8. Monkhorst H. J. Special points for Brillouin-zone integrations / H. J. Monkhorst, J. D. Pack // Physical Review B. – 1976. – Vol. 13. – P. 5188. doi: 10.1103/PhysRevB.13.5188.
9. Kashuba A. I. Influence of pressure on the electronic energy structure of cadmium sulphide crystal with zinc-blende structure / A. I. Kashuba, B. Andriyevsky, I. V. Semkiv, H. A. Ilchuk, M. Ya. Rudysh, P. A. Shchepanskyi, M. S. Karkulovska, R. Y. Petrus // Journal of Physical Studies. – 2022. – Vol. 26(1). – P. 1701(6p). doi: 10.30970/jps.26.1701.
10. Shan W. Pressure dependence of the fundamental band-gap energy of CdSe / W. Shan, W. Walukiewicz, J. W. Ager III, K. M. Yu, J. Wu, E. E. Haller // Applied Physics Letters. – 2004. – Vol. 84. – P. 67. doi: 10.1063/1.1638879.

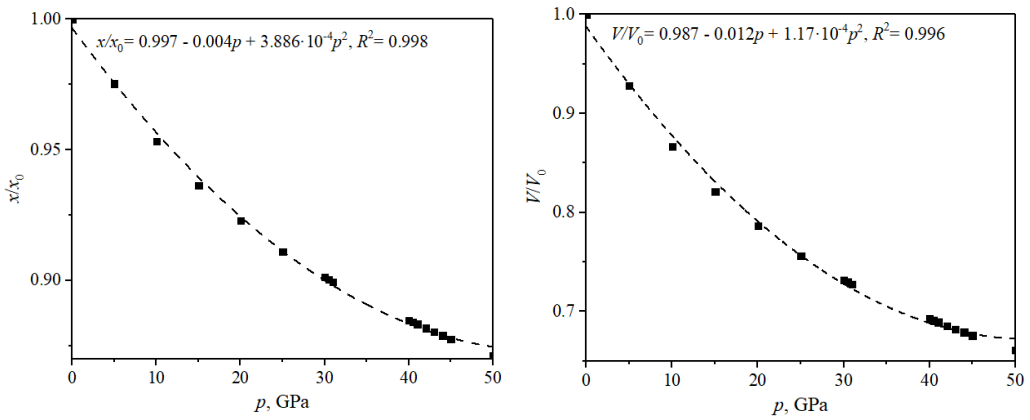

Fig. 6: Dependence of the relative lattice parameters of CdTe crystal on the pressure.

11. Jesse Pius J. High pressure band structure, density of states, structural phase transition and metallization in CdS / J. Jesse Pius, A. Lekshmi, C. Nirmala Louis // Chemical and Materials Engineering. – 2017. – Vol. 5(1). – P. 8. doi: 10.13189/cme.2017.050102.
12. Petrus R. Optical Properties of CdTe Thin Films Obtained by the Method of High-Frequency Magnetron Sputtering / R. Petrus, H. Ilchuk, A. Kashuba, I. Semkiv, E. Zmiiovska // Functional Materials. – 2020. – Vol. 27. – P. 342–347. doi: 10.15407/fm27.02.342.
13. Madelung O., Schlz M., Weiss H. (Eds.), Numerical Data and Functional Relationships in Science and Technology, Landolt-Borstein, Vol. 17, Springer, Berlin, 1982.
14. Okoye C. M. I. Investigation of the pressure dependence of band gaps for silver halides within a first-principles method / C. M. I. Okoye // Solid State Communications. – 2004. – Vol. 129. – P. 69. doi: 10.1016/j.ssc.2003.09.014.
15. Moss T. A. Relationship Between the Refractive Index and the Infra-Red Threshold of Sensitivity for Photoconductors / T. A. Moss // Proceedings of the Physical Society. Section B. – 1950. – Vol. 63.– P. 167–176. doi: 10.1088/0370-1301/63/3/302.
16. Ravindra N. M. On the Penn Gap in Semiconductors / N. M. Ravindra, S. Auluck, V. K. Srivastava // Physica status solidi (b). – 1979. – Vol. 93. – P. K155-K160. doi: 10.1002/pssb.222093025710.1002/pssb.2220930257.
17. Herve P. J. L. Empirical Temperature Dependence of the Refractive Index of Semiconductors / P. J. L. Herve, L. K. J. Vandamme // Journal of Applied Physics. – 1995. – Vol. 77. – P. 5476–5477. doi:10.1063/1.359248.
18. Tripathy S. K. Refractive Indices of Semiconductors from Energy Gaps / S. K. Tripathy // Optical Materials. – 2015. – Vol. 46. – P. 240–246. doi: 10.1016/j.optmat.2015.04.026.
19. Ilchuk H. A. Electronic band structure of cubic solid-state $CdTe_{1-x}Se_x$ solutions / H. A. Ilchuk, B. Andriyevsky, O. S. Kushnir, A. I. Kashuba, I. V. Semkiv, R. Yu. Petrus // Ukr. J. Phys. Opt. – 2021. – Vol. 22(2). – P. 101. doi: 10.3116/16091833/22/2/101/2021.
20. Treharne R. E. Optical Design and Fabrication of Fully Sputtered CdTe/CdS Solar

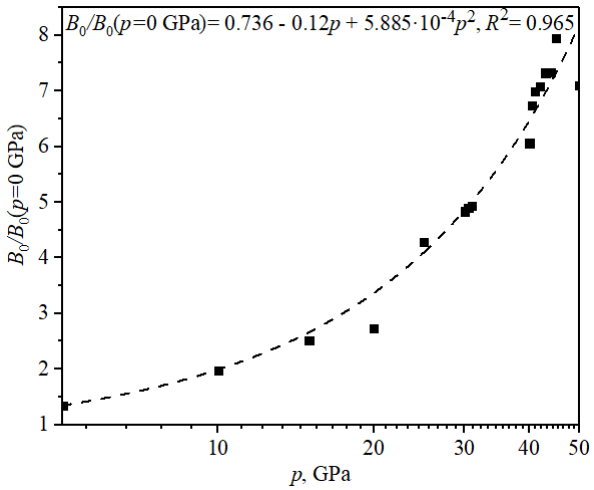

Fig. 7: Dependence of the bulk module B_0 of CdTe crystal on the pressure.

Cells / R. E. Treharne, A. Seymour-Pierce, K. Durose, K. Hutchings, S. Roncallo, D. Lane // J. Phys.: Conf. Ser. – 2011. – Vol. 286. – P. 012038. doi: 10.1088/1742-6596/286/1/012038.

References

1. H. A. Ilchuk, R. Yu. Petrus, A. I. Kashuba, I. V. Semkiv, E. O. Zmiiovska, Nanosistemi, Nanomateriali, Nanotehnologii. **16**(3), 519–533 (2018). doi: 10.15407/nnn.16.03.519.
2. R. Yavorskyi, L. Nykyruy, G. Wisz, P. Potera, S. Adamiak, Sz. Gorny, Applied Nanoscience. **9**, 715–724 (2019). doi: 10.1007/s13204-018-0872-z.
3. Y. P. Saliy, L. I. Nykyruy, R. S. Yavorskyi, S. Adamiak, Journal of Nano - and Electronic Physics. **9**(5), 05016(5) (2017). doi: 10.21272/jnep.9(5).05016.
4. S. Ouendadji, S. Ghemid, H. Meradji, F. El Haj Hassan, Computational Materials Science. **50**, 1460 (2011). doi: 10.1016/j.commatsci.2010.11.035.
5. N. Bouarissa, H. Algarni, O. A. Al-Hagan, M. Ajmal Khan, T. F. Alhuwaymel, Optik. **170**, 37 (2018). doi: 10.1016/j.ijleo.2018.05.069.
6. D. Vanderbilt, Physical Review B. **41**, 7892(R) (1990). doi: 10.1103/PhysRevB.41.7892.
7. J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, K. Burke, Physical Review Letter. **100**, 136406 (2008). doi: 10.1103/PhysRevLett.100.136406.
8. H. J. Monkhorst, J.D. Pack, Physical Review B. **13**, 5188 (1976). doi: 10.1103/PhysRevB.13.5188.
9. A. I. Kashuba, B. Andriyevsky, I. V. Semkiv, H. A. Ilchuk, M. Ya. Rudysh, P. A. Shchepanskyi, M. S. Karkulovska, R. Y. Petrus, Journal of Physical Studies. **26**(1), 1701(6p) (2022). doi: 10.30970/jps.26.1701.

10. W. Shan, W. Walukiewicz, J. W. Ager III, K. M. Yu, J. Wu, E. E. Haller, Applied Physics Letters. **84**, 67 (2004). doi: 10.1063/1.1638879.
11. J. Jesse Pius, A. Lekshmi, C. Nirmala Louis, Chemical and Materials Engineering. **5**(1), 8 (2017). doi: 10.13189/cme.2017.050102.
12. R. Petrus, H. Ilchuk, A. Kashuba, I. Semkiv, E. Zmiiovska, Functional Materials. **27**, 342–347 (2020). doi: 10.15407/fm27.02.342.
13. O. Madelung, M. Schlz, H. Weiss (Eds.), Numerical Data and Functional Relationships in Science and Technology, Landolt-Borstein, vol. **17**, Springer, Berlin, 1982.
14. C. M. I. Okoye, Solid State Communications. **129**, 69 (2004). doi: 10.1016/j.ssc.2003.09.014.
15. T. A. Moss, Proceedings of the Physical Society. Section B. **63**, 167–176 (1950). doi: 10.1088/0370-1301/63/3/302.
16. N. M. Ravindra, S. Auluck, V. K. Srivastava, Physica status solidi (b). **93**, K155-K160 (1979). doi: 10.1002/pssb.222093025710.1002/pssb.2220930257.
17. P. J. L. Herve, L. K. J. Vandamme, Journal of Applied Physics. **77**, 5476–5477 (1995). doi: 10.1063/1.359248.
18. S. K. Tripathy, Optical Materials. **46**, 240–246 (2015). doi: 10.1016/j.optmat.2015.04.026.
19. H. A. Ilchuk, B. Andriyevsky, O. S. Kushnir, A. I. Kashuba, I. V. Semkiv, R. Yu. Petrus, Ukr. J. Phys. Opt. **22**(2), 101 (2021). doi: 10.3116/16091833/22/2/101/2021.
20. R. E. Treharne, A. Seymour-Pierce, K. Durose, K. Hutchings, S. Roncallo, D. Lane, J. Phys.: Conf. Ser. **286**, 012038 (2011). doi: 10.1088/1742-6596/286/1/012038.

Стаття надійшла до редколегії: 20.03.2022
Прийнята до друку: 04.04.2022

Вплив тиску на електронний енергетичний спектр кристалу CdTe розрахований методом функціонала густин

А. І. Кашуба, І. В. Семків, Г. А. Ільчук, Р. Ю. Петрусь

Національний університет «Львівська політехніка»,
вул. С. Бандери, 12, Львів, Україна, 79013
e-mail: andrii.i.kashuba@lpnu.ua

Телурид кадмію (CdTe) є представником кристалічної групи $A^{II}B^{VI}$ та кристалізується в структурі сфалерит за нормальних умов. Кристали, тонкі плівки та нанокомпозитні структури на основі CdTe залишаються широко використовуваними матеріалами в оптоелектронних пристроях. З цього погляду вивчення структурних властивостей і динаміки електронного спектра кристалу CdTe під дією зовнішніх тисків становить значний фундаментальний інтерес. За допомогою теорії функціоналу густини досліджено вплив тиску на електронний енергетичний спектр кристала CdTe, який кристалізується в структурі сфалерит (ZnS). Для розрахунку обмінно-кореляційного потенціалу використовувалось узагальнене наближення градієнта (GGA) та параметризація Пердью–Берк–Ернцергофа (PBEsol) для твердих тіл. Розраховано основні рівноважні фізичні параметри кристалу CdTe зі структурою сфалерит. Досліджено структурні та електронні властивості в діапазоні гідростатичного тиску від 0 до 50 ГПа. Розраховано електронну енергетичну структуру і щільність станів при різних тисках. Проведено кореляційний аналіз рівноважних структурних параметрів, модуля об'ємного стиску, найменшої ширини забороненої щілини, показника заломлення та високочастотної діелектричної проникності з наявними літературними відомостями. Встановлено, що за дії на кристал гідростатичного тиску менше 30 ГПа ширина забороненої зони зростає з ростом тиску в параболічній залежності, а за тисків більше 30 ГПа, ширина забороненої зони лінійно спадає. Оцінено величину можливого тиску металізації кристалу CdTe, методом екстраполяції отриманих результатів. Розраховано залежність від тиску показника заломлення з використанням основних емпіричних співвідношень. На основі встановлених значень величини показника заломлення розраховано залежність від тиску величини високочастотної діелектричної проникності. Залежність структурних параметрів та модуля об'ємного стиснення залежно від тиску описується параболічною залежністю.

Ключові слова: електронна енергетична структура, ширина забороненої зони, тиск, потенціал об'ємної деформації, показник заломлення, високочастотна діелектрична проникність.