PHYSICS AND CHEMISTRY OF SOLID STATE
V. 20, № 4 (2019) p. 338-344

Vasyl Stefanyk Precarpathian National University

DOI: 10.15330/pcss.20.2.338-344

ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 20, № 4 (2019) С. 338-344

PACS 72.20.Dp

ISSN 1729-4428

O.P. Malyk, S.V. Syrotyuk

Electron Mobility in $CdSe_xTe_{1-x}$ (x = 0.25) Solid Solution: *Ab Initio* Calculation

Lviv Polytechnic National University, Lviv, 79013 Ukraine, omalyk@ukr.net

In this paper an assessment of the quality of a solid solution of $CdSe_xTe_{1-x}$ is done by study of its transport properties. The description of the kinetic phenomena is carried on the base of the wave function and self-consistent potential for solid solution $CdSe_xTe_{1-x}$ (x = 0.25) which were determined from the first principles using the projector augmented waves as implemented in the ABINIT code. The scattering processes were considered in the framework of short-range scattering models where the electron interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain centers, neutral and ionized impurities was taken into account. The transition matrix elements were obtained by integration over the unit cell using three-dimensional B-spline interpolation. For crystals with impurity concentration 5.6×10^{15} - 5×10^{18} cm^{-3} the temperature dependences of electron mobility and Hall factor in the range 15 - 1200 K are calculated. The theoretical curves obtained in the short-range approach differ qualitatively and quantitatively from those obtained within the long-range models in relaxation time approximation.

Keywords: electron transfer, point defects, CdSeTe solid solution, ab initio calculation.

Article acted received 23.10.2019; accepted for publication 15.12.2019.

Introduction

At present the main method for increasing the efficiency of solar cells based on cadmium telluride is the using an additional absorbent layer created on the base of triple compounds of cadmium chalcogenides, in particular the solid solution $CdSe_xTe_{1-x}$ [1-4]. This solid solution has the unique photovoltaic parameters necessary for the production of solar cells [5-14]. Therefore, the study of the quality of these absorbing layers is an actual application problem.

In this paper for the first time within the framework of ab initio approach we proposed the description of kinetic properties of solid solution (in particular $CdSe_{0.25}Te_{0.75}$) using the short-range principle. The description of the kinetic properties is carried on the base of the wave function and self-consistent potential for solid solution $CdSe_xTe_{1-x}$ (x = 0.25) which were determined from the first principles using the projector augmented waves as implemented in the ABINIT code [15]. The description of the electron interaction with different types of the point crystal defects is made using the short-range scattering models [16-20].

I. Theory

First we put that the lattice constant corresponding to the composition *x=0.25* of the solid solution equal to a_0 = 6.38 Å. This value was used to calculate the wave functions and self-consistent potentials in CdTe and CdSe crystals. These wave functions and self-consistent potentials were determined from the first principles on the base of projector augmented waves (PAW) [21]. The PAW basis functions have been generated by means of the AtomPAW [22] code for the following valence states: $\{5s^2 5p^0 4d^{10}\}$ for Cd, $\{4s^2 5s^2 4p^2 5p^4\}$ for Te and $\{4s^2 4p^4\}$ for Se, respectively. The exchange-correlation potential was selected in the form of PBE0 [23-26] obtained from the functional of the exchange-correlation energy.

To obtain the wave function of the solid solution $CdSe_xTe_{1-x}$ the following consideration was used – on the base of the obtained wave functions of CdTe and CdSe crystals the wave function of the solid solution was defined:

$$|\psi(\boldsymbol{r})_{CdSeTe}|^2 = x|\psi(\boldsymbol{r})_{CdSe}|^2 + (1-x)|\psi(\boldsymbol{r})_{CdTe}|^2;\ x=0.25. \quad (1)$$

According to the short-range scattering models the carrier transition probability from state $\boldsymbol{k}$ to state $\boldsymbol{k}'$ caused by the interaction with polar optical (PO), nonpolar optical (NPO), acoustic (AC), piezooptic (PAC) and piezoacoustic (POP) phonons, static strain (SS) potential and ionized (II) impurity looks like [16-20]:

$$W_{PO}(\boldsymbol{k},\boldsymbol{k}') = \frac{\pi^5 A_{PO}^2 e^4}{16\,\varepsilon_0^2 a_0^8 G}\,\frac{M_{Cd}+M_x}{M_{Cd}\,M_x}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(E'-E-\hbar\omega_{LO}) + (N_{LO}+1)\times \delta(E'-E+\hbar\omega_{LO})\right] + \frac{2}{\omega_{TO}}\left[N_{TO}\delta(E'-E-\hbar\omega_{TO}) + (N_{TO}+1)\delta(E'-E+\hbar\omega_{TO})\right]\right\}; \quad (2)$$

$$W_{NPO}(\boldsymbol{k},\boldsymbol{k}') = \frac{\pi^3 d_0^2}{1152\,a_0^2 G}\,\frac{M_{Cd}+M_x}{M_{Cd}\,M_x}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(E'-E-\hbar\omega_{LO}) + (N_{LO}+1)\times \delta(E'-E+\hbar\omega_{LO})\right] + \frac{2}{\omega_{TO}}\left[N_{TO}\delta(E'-E-\hbar\omega_{TO}) + (N_{TO}+1)\delta(E'-E+\hbar\omega_{TO})\right]\right\}; \quad (3)$$

$$W_{AC}(\boldsymbol{k},\boldsymbol{k}') = \frac{\pi^3 k_B T\, E_{AC}^2}{576\,\hbar\, G\,[M_{Cd}+M_x]}\left(\frac{1}{c_{\parallel}} + \frac{2}{c_{\perp}}\right)^2 \delta(E'-E); \quad (4)$$

$$W_{PAC}(\boldsymbol{k},\boldsymbol{k}') = \frac{\pi^5 e^2 e_{14}^2\, A_{PZ}^2\, k_B T}{128\,\hbar\, G\, e_0^2 a_0^2\,[M_{Cd}+M_x]}\left(\frac{1}{c_{\parallel}} + \frac{2}{c_{\perp}}\right)^2 \delta(E'-E); \quad (5)$$

$$W_{POP}(\boldsymbol{k},\boldsymbol{k}') = \frac{\pi^7 e^2 e_{14}^2 A_{PZ}^2}{400\varepsilon_0^2 a_0^4\, G}\,\frac{M_{Cd}+M_x}{M_{Cd}\,M_x}\left\{\frac{1}{\omega_{LO}}\left[N_{LO}\delta(E'-E-\hbar\omega_{LO}) + (N_{LO}+1)\times \delta(E'-E+\hbar\omega_{LO})\right] + \frac{2}{\omega_{TO}}\left[N_{TO}\delta(E'-E-\hbar\omega_{TO}) + (N_{TO}+1)\delta(E'-E+\hbar\omega_{TO})\right]\right\}; \quad (6)$$

$$W_{SS}(\boldsymbol{k},\boldsymbol{k}') = \frac{2^5 3^4 \pi^3 C^2 a_0^6 e^2\, e_{14}^2 N_{SS}}{V e_0^2 \hbar}\,\frac{1}{q^2}\,\delta(E'-E); \quad (7)$$

$$W_{II}(\mathbf{k},\mathbf{k}') = \frac{Z_i^2 e^4 N_{II}\, A_{II}^2\, a_0^6}{512 e_0^2\,\hbar V}\,\delta(E'-E);\ A_{II} = \int_{\Omega} \psi^* \frac{1}{r} \psi\, d\mathbf{r}, \quad (8)$$

where $M_x = x\,M_{Se} + (1-x)M_{Te}$; M_{Cd}, M_{Se}, M_{Te} – atomic masses; N_{LO} and N_{TO} denote the number of longitudinal (LO) and transverse (TO) phonons with a frequency ω_{LO} and ω_{TO} respectively; G– the number of unit cells in a crystal volume; $c_{\parallel}$ and $c_{\perp}$ – the longitudinal and transverse sound velocity respectively; e_{14} the non-vanishing component of the piezoelectric tensor of zinc blende structure; ψ – electron wave function; N_{II} – the concentration of ionized impurities; Z_i – the multiplicity ionization of impurity; integration in (8) is carried out over the elementary cell and the value A_{II} is equal to: $A_{II} = 0.483\times10^{10}\,m^{-1}$; $C \approx 0.1$; $q = |\boldsymbol{k}'-\boldsymbol{k}|$; N_{SS} – concentration of the static strain centers, the method of calculation of which at present is unknown. Therefore this material characteristic was used as an adjustable parameter to agreement the theory and experiment.

In equation (2) the value A_{PO} is defined as follows:

$$A_{PO} = \int \psi^* (R^2 - r^2/3)\,\psi\, d\mathbf{r};\ R = \sqrt{3}\,a_0/2; \quad (9)$$

integration is carried out over the part of the elementary cell volume, where two atoms of different sort are located, using three-dimensional B-spline interpolation [27]. The size of this volume is determined by the condition:

$$\partial U_0(\boldsymbol{r},\boldsymbol{R})/\partial x = \partial U_0(\boldsymbol{r},\boldsymbol{R})/\partial y = \partial U_0(\boldsymbol{r},\boldsymbol{R})/\partial z = 0,$$

where $U_0(\boldsymbol{r},\boldsymbol{R})$ – the self-consistent electron potential energy $U_0(\boldsymbol{r},\boldsymbol{R})$; $\boldsymbol{r}$ and $\boldsymbol{R}$ – electron and atom coordinates respectively. Method of calculation and error estimation of magnitude A_{PO} is described in detail in [19]. Then one can obtain $A_{PO} = 8.32\times10^{-20}\,m^2$.

In (3)–(4) d_0 and E_{AC} are the optical and acoustic deformation potential constants, which are expressed through the integrals over the volume of elementary cell [19]. The region of integration is the same as in the case of PO scattering. As a result we have $d_0 = -18.3\,eV$, $E_{AC} = -2.16\,eV$.

In (5) - (6) the value $A_{PZ} = A_{PO}$ because the coordinate dependence of the potential energy is the same as in the case of PO scattering therefore the integration over the unit cell is carried out by the method mentioned above.

The electron scattering on the neutral impurity was described on the base of Erginsoy model [28]. Using the short-range principle yields to the next formula for the transition probability [19]:

$$W\left(\boldsymbol{k},\boldsymbol{k}^{'}\right)=\frac{100\,p^{\,2}a_B\,\mathbf{h}^3\,N_{NI}}{V\,m^{*2}\,k(E)}d\,\left(E'-E\right), \qquad (10)$$

where N_{NI} – the neutral impurity concentration; $m^* = \mathbf{h}^2 k(E)\,d\,k(E)/dE$; a_B –Bohr radius.

II. Temperature dependences of electron mobility and Hall factor

For the composition values x<0.5 the $CdSe_xTe_{1-x}$ solid solution has the sphalerite structure. Therefore its point defect structure must be similar to the point defect structure of cadmium telluride. It is well known that in undoped CdTe there exist the intrinsic donor defects with ionization energy $E_D \approx 10\,meV$ which compensate the intrinsic acceptor defects [29]. Following such assumption the electroneutrality equation for calculation the Fermi level was considered:

$$n-p=N_D/\{1+2\exp[(F-E_D)/(k_BT)]\}-N_A, \qquad (11)$$

where N_D, N_A – the donors and acceptors concentration respectively.

Searching of the Fermi energy was made for certain levels of defect concentration the numerical values of which are presented in Table 1. The parameters of the solid solution $CdSe_xTe_{1-x}$ $(x = 0.25)$ used in calculations are presented in Table 2.

To calculate the theoretical temperature dependences of the electron mobility two approaches were used: a) the description of the electron scattering on the base of short-range models and exact solution of the stationary kinetic Boltzmann equation [45]; b) the description of the electron scattering on the base of long-range models and relaxation time approximation for the solution of kinetic equation. The theoretical curves corresponding to the first approach are presented in figure 1(a)-(d). The presented curves are related to the different values of the static strain centers concentration N_{SS}. The possible values of these concentrations were chosen similar to CdTe samples [29] with corresponding concentrations of the intrinsic point defects – donors and acceptors (see Table I). Comparison of two abovementioned theoretical approaches (short-range and long-range scattering models) are depicted in figure 2 (a)-(d). Solid curves 1 were obtained using the short-range scattering models within the framework of the exact solution of the Boltzmann's kinetic equation. Dashed curves 2 and 3 were obtained within the framework of the long-range scattering models and using the relaxation time approximation: curve 2 relates to the case of low temperature region $\mathbf{h}w >> k_BT$ whereas curve 3 relates to the case of high temperature region $\mathbf{h}w << k_BT$. The determining of the temperature dependence of electron mobility is presented elsewhere (see Appendix B in [19]). As it can be seen, these curves demonstrate the significant qualitative and quantitative difference between the temperature dependences of the charge carrier's mobility (calculated by two approaches) over the investigated range of defect concentrations and

Table 1

Parameters of the defect structure of the $CdSe_{0.25}Te_{0.75}$ samples

Sample	N_D (cm^{-3})	N_A (cm^{-3})	N_D+ N_A (cm^{-3})	N_{SS} (cm^{-3})
A	3.2×10^{15}	2.4×10^{15}	5.6×10^{15}	$(2 \div 4)\times10^{15}$
B	3.0×10^{16}	2.0×10^{16}	5.0×10^{16}	$(1 \div 2)\times10^{16}$
C	3.0×10^{17}	2.0×10^{17}	5.0×10^{17}	$(4 \div 5)\times10^{16}$
D	3.0×10^{18}	2.0×10^{18}	5.0×10^{18}	$(6 \div 8)\times10^{16}$

Table 2

Parameters of $CdSe_xTe_{1-x}$ (x=0.25) used in calculations

Material parameter	Value
Lattice constant, a_0 (m)	$6.38´10^{-10}$ [a]
Energy gap, E_g (eV)	$E_g=x\,E_{gCdSe}+(1-x)\,E_{gCdTe} — 0.9\,x\,(1-x)$ [b,c,d]
Energy equivalent of the matrix element, E_p (eV)	$21 – x$ [e]
Density, r (kg m^{-3})	$5.75\times10^3 – 95\,x$ [f]
Spin-orbit splitting, D (eV)	$0.92 – 0.51\,x$ [g]
Optical deformation potential, d_0 (eV)	-18.3 [h]
Acoustic deformation potential, E_{AC} (eV)	-2.16 [h]
Transverse optical phonon frequency, ω_{TO} (rad s^{-1})	$2.63´10^{13} + 4.8´10^{12}$ [i, j]
Lattice dielectric constant, e_L	$10.5 – 1.1\,x$ [j, k]
High frequency dielectric constant, $e_{¥}$	$7.4 – 1.3\,x$ [j, k]
Elastic constants (×10^{-10}, N m^{-2}): C_l	$6.32 + 1.04\,x$ [l, m, n]
C_t	$1.538 – 0.188\,x$ [l, m, n]
Piezoelectric tensor component, e_{14} (C m^{-2})	$(1 – x)\,0.03457 – 1.39\times10^{-5}\,T + 0.347\,x$ [o, p]

[a] [30]. [b] [31]. [c] [32]. [d] [33]. [e] [34]. [f] [35]. [g] [36]. [h] Present article. [i] [37]. [j] [38]. [k] [39]. [l] [40]. [m] [41]. [n] [42]. [o] [43]. [p] [44].

temperatures.

However, only an experiment must determine which of the theoretical models can describe better the experimental data. From the literature authors know only one source, which presents experimental data on the study of transport phenomena in $CdSe_xTe_{1-x}$ [46]. Analysis of these data shows that the investigated

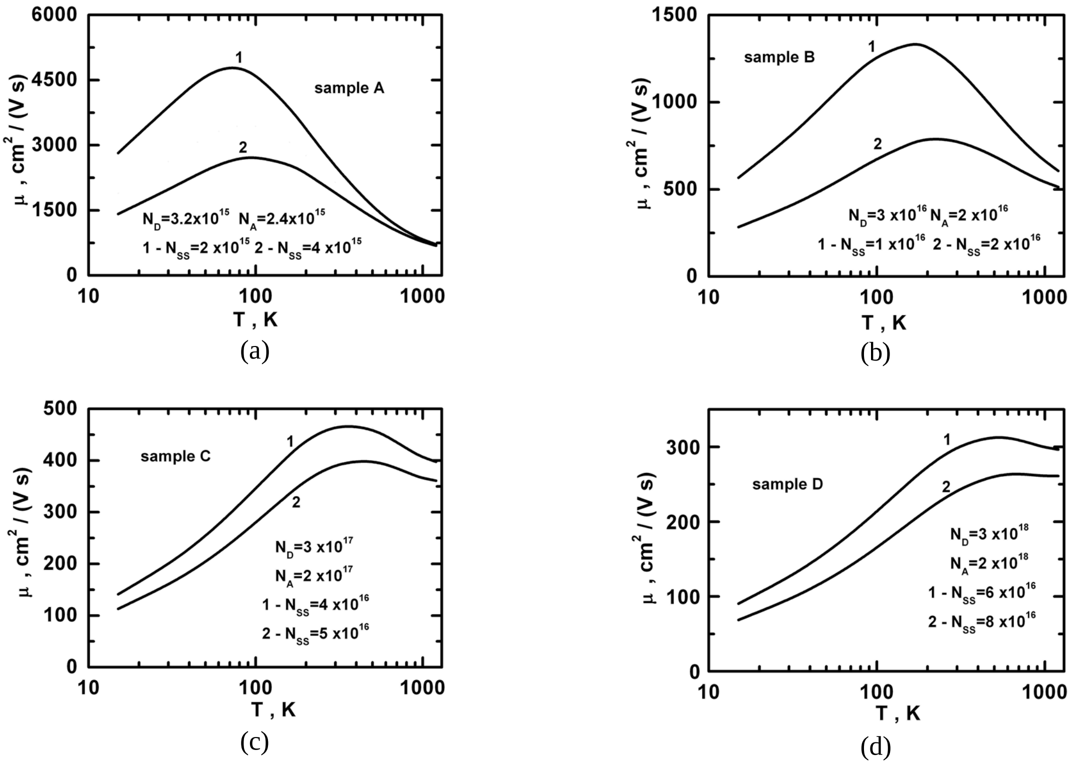

Fig. 1. Temperature dependence of the electron mobility in $CdSe_xTe_{1-x}$ (x = 0.25) crystals with different defect concentration.

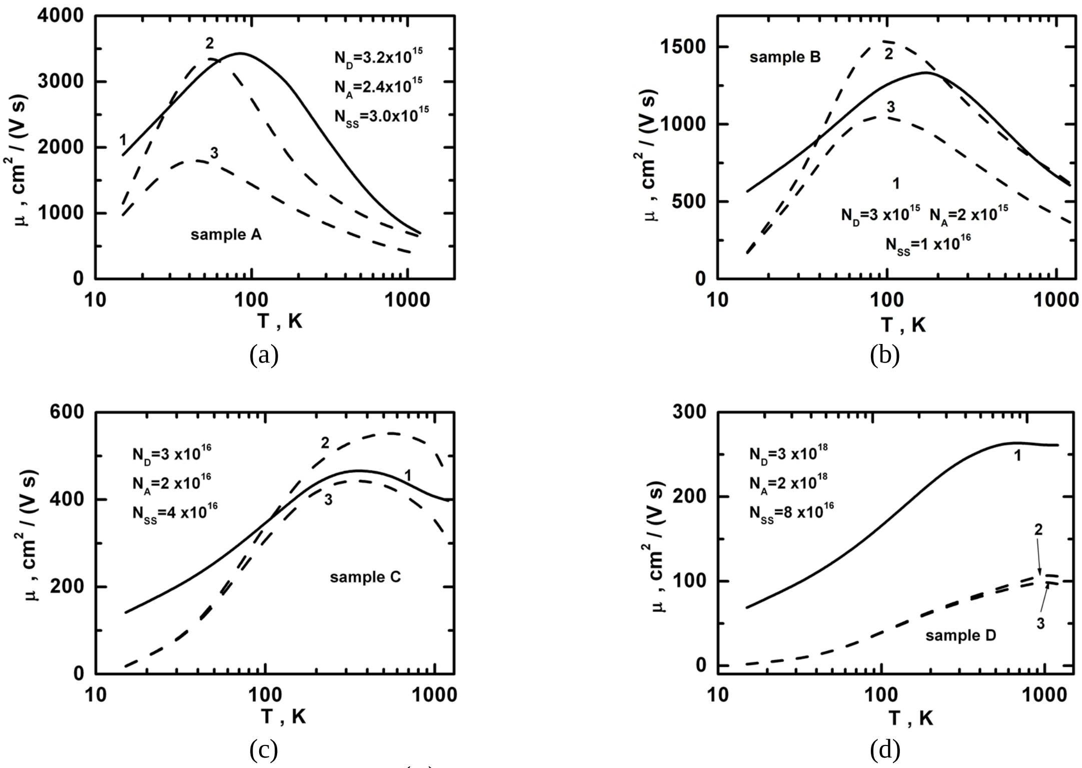

Fig. 2. Dependences $m(T)$ corresponding to different theoretical approaches.

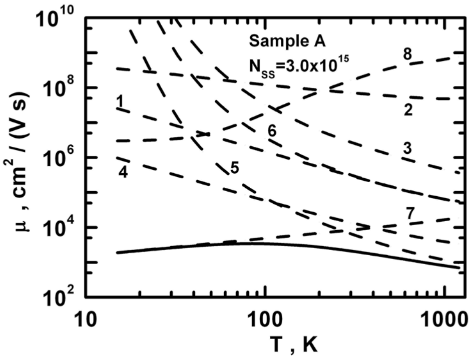

Fig. 3. Contribution of different scattering modes into electron mobility. Solid line – mixed scattering mode; 1, 2, 3, 4, 5, 6, 7, 8 – AC-, II-, NPO-, PAC-, PO-, POP-, SS-, NI- scattering mode respectively.

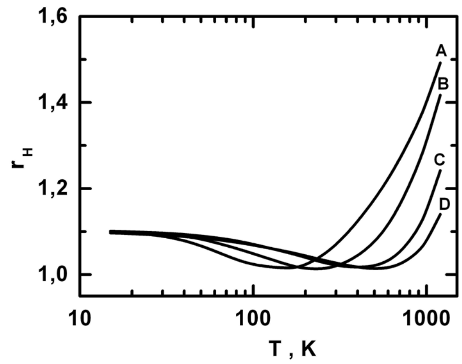

Fig. 4. Temperature dependence of electron's Hall-factor in $CdSe_xTe_{1-x}$ (x = 0.25) crystals.

samples are polycrystalline (the grain size $\sim 566 \div$ 755 Å). Therefore, they have anomalously low values of the electron's mobility which indicates the low quality of the crystals.

It should be noted that the authors assert that an approach based on the short-range principle more accurately describes the kinetic properties of $CdSe_xTe_{1-x}$ solid solution compared with the long-range approach. This statement is based on the fact that for cadmium telluride the short-range models give better agreement with the experiment [19]. Since the solid solution $CdSe_xTe_{1-x}$ ($x \leq 0.5$) has a similar crystalline structure, one should expect a similar situation for this case.

On figure 3 for the sample with minimum defects concentration the description of the role of different scattering mechanisms is presented by dashed lines. As it seen the static strain scattering (curve 7) dominate at low temperatures (T < 180 K). At the temperature interval T> 180 K the polar optical phonon scattering becomes predominant (curve 5). In this temperature interval the piezoacoustic phonon scattering (curve 4) play the significant role too. Other scattering mechanisms give weak contribution to the electron mobility.

Such distribution of the influence of various scattering mechanisms causes the temperature dependences of the electron's Hall factor for the samples with different defects concentration (see figure 4). These temperature dependences demonstrate the minimums in the temperature region where the transition from one scattering mechanism to another occurs. It is seen that the higher defects concentration corresponds to the higher temperature where the minimum of dependence $r_H(T)$ is observed.

Conclusion

In the present paper the problem of quality evaluation of crystals of a $CdSe_xTe_{1-x}$ (*x = 0.25*) solid solution is considered. The idea of the proposed approach consists in analyze of the temperature dependence of the charge carrier mobility which, in turn, is determined by the point defects structure of the crystal. To calculate the abovementioned characteristic of the solid solution $CdSe_xTe_{1-x}$ (*x = 0.25*) two approximations were used: a) short-range scattering models on the base of calculated wave function and self-consistent potential energy within the framework of exact solution of Boltzmann equation; b) long-range scattering models within the framework of relaxation time approximation. It was established that both approximations give substantially different theoretical curves. The question which approximation is preferred should be solved by experiment.

Malyk O.P. **-** Doctor of Physical and Mathematical Sciences, Associate Professor, Associate Professor;
Syrotyuk S.V. – PhD (Physical and Mathematical Sciences), Associate Professor, Associate Professor.

[1] A. Kathalingam, M. R. Kim, Y. S. Chae, J. K. Rhee, S. Thanikaikarasan, T. Mahalingam, J. Alloys Compd. 505, 758 (2010) (https://doi.org/10.1016/j.jallcom.2010.06.136).

[2] Q. Zeng, Z. Chen, Y. Zhao, X. Du, F. Liu, G. Jin, F. Dong, H. Zhang, B. Yang, ACS Appl. Mater. Interfaces 7, 23223 (2015) (https://pubs.acs.org/doi/abs/10.1021/acsami.5b07197).

[3] D.E. Swanson, J.R. Sites, W.S. Sampath, Sol. Energ. Mat. Sol. C. 159, 389 (2017) (https://doi.org/10.1016/j.solmat.2016.09.025).

[4] A.H. Munshi, J. Kephart, A. Abbas, J. Raguse, J.-N. Beaudry, K. Barth, J. Sites, J. Walls, W. Sampath, IEEE J. Photovolt. 8, 310 (2018) (https://doi.org/10.1109/JPHOTOV.2017.2775139).

[5] S.M. Babu, T. Rajalakshmi, R. Dhanasekaran, P. Ramasamy, J. Cryst. Growth 110, 423 (1991) (https://doi.org/10.1016/0022-0248(91)90278-D).

[6] Z. Loizos, A. Mitsis, N. Spyrellis, M. Froment, G. Maurin, Thin Solid Films 235, 51 (1993) (https://doi.org/10.1016/0040-6090(93)90242-H).

[7] S. Benyettou, S. Saib, N. Bouarissa, Chem. Phys. 457,147 (2015) (https://doi.org/10.1016/j.chemphys.2015.06.004).
[8] [8] G. Brill, Y. Chen, P. M. Amirtharaj, W. Sarney, D. Chandler-Horowitz, N. K. Dhar, J. Electron. Mater. 34, 655 (2005) (https://doi.org/10.1007/s11664-005-0080-y).
[9] S. Velumani, X. Mathew, P.J. Sebastian, Sol. Energ. Mat. Sol. C. 76, 359 (2003) (https://doi.org/10.1016/S0927-0248(02)00288-X).
[10] K.R. Murali, B. Jayasutha, Chalcogenide Lett. 6, 1 (2009).
[11] B.I. MacDonald, A. Martucci, S. Rubanov, S.E. Watkins, P. Mulvaney, J.J. Jasieniak, ACS Nano 6, 5995 (2012) (https://doi.org/10.1021/nn3009189).
[12] E. Benamar, M. Rami, M. Fahoume, F. Chraibi, A. Ennaoui, Solid State Sci. 1, 301 (1999) (https://doi.org/10.1016/S1293-2558(00)80084-9).
[13] N. Muthukumarasamy, S. Jayakumar, M.D. Kannan, R. Balasundaraprabhu, Sol. Energy 83, 522 (2009) (https://doi.org/10.1016/j.solener.2008.10.004).
[14] T.C.M. Santhosh, K.V. Bangera, G.K. Shivakumar, Sol. Energy. 153, 343 (2017) (https://doi.org/10.1016/j.solener.2017.05.079).
[15] X. Gonze, et al., Comput. Phys. Commun. 205, 106 (2016) (https://doi.org/10.1016/j.cpc.2016.04.003).
[16] O.P. Malyk, Comput. Mater. Sci. 33, 153 (2005) (https://doi.org/10.1016/j.commatsci.2004.12.052).
[17] O.P. Malyk, Phys. Status Solidi C 6, S86 (2009) (https://doi.org/10.1002/pssc.200881315).
[18] O.P. Malyk, Can. J. Phys. 92, 1372 (2014) (https://doi.org/10.1139/cjp-2013-0075).
[19] O.P. Malyk, S.V. Syrotyuk, Comput. Mater. Sci. 139, 387(2017) (https://doi.org/10.1016/j.commatsci.2017.07.039).
[20] O.P. Malyk, S.V. Syrotyuk, J. Electron. Mater. 47, 4212 (2018)(https://doi.org/10.1007/s11664-018-6068-1).
[21] P.E. Blöchl, Phys. Rev. B. 50, 17953 (1994) (https://doi.org/10.1103/PhysRevB.50.17953).
[22] N.A.W. Holzwarth, A.R. Tackett, G.E. Matthews, Comput. Phys. Commun. 135, 329 (2001) (https://doi.org/10.1016/S0010-4655(00)00244-7).
[23] M. Ernzerhof, G.E. Scuseria, J. Chem. Phys. 110, 5029 (1999) (https://doi.org/10.1063/1.478401).
[24] P .Novák, J. Kunes, L. Chaput, W.E. Pickett, Phys. Status Solidi B 243, 563 (2006) (https://doi.org/10.1002/pssb.200541371).
[25] E. Tran, P. Blaha, K. Schwarz, P. Novák, Phys. Rev. B 74, 155108(10) (2006) (https://doi.org/10.1103/PhysRevB. 74.155108).
[26] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Letters 77, 3865 (1996) (https://doi.org/10.1103/PhysRevLett. 77.3865).
[27] C. de Boor, A Practical Guide to Splines, (Springer-Verlag, New York, 1978).
[28] C. Erginsoy, Phys.Rev. 79, 1013 (1950) (https://doi.org/10.1103/PhysRev.79.1013).
[29] B. Segall, M.R. Lorenz, R.E. Halsted, Phys. Rev. 129, 2471 (1963) (https://doi.org/10.1103/PhysRev.129.2471).
[30] J. Litwin, Phys. Status Solidi 5, 551 (1964) (https://doi.org/10.1002/pssb.19640050311).
[31] G.L. Hansen, J.L. Schmit, T.N. Casselman, J. Appl. Phys. 53, 7099 (1982) (https://doi.org/10.1063/1.330018).
[32] R. Passler, Phys. Status Solidi B 216, 975 (1999) (https://doi.org/10.1002/(SICI) 1521-3951(199912)216:2<975::AID-PSSB975>3.0.CO;2-N).
[33] H.C. Poon, Z.C. Feng, Y. P. Feng, M.F. Li, J. Phys.:Condens. Matter 7, 2783 (1995) (https://doi.org/10.1088/0953-8984/7/14/017).
[34] C. Hermann, C. Weisbuch. Phys. Rev. B, 15, 823 (1977) (https://doi.org/10.1103/PhysRevB.15.823).
[35] J. Brice, P. Capper (ed.), EMIS Datareviews Series No 3, (INSPEC, London, 1987).
[36] W.Gebhardt, G. Schotz, R. Bhargava, (ed.), EMIS Datareviews Series No 17, (INSPEC/IEE London, 1997).
[37] M. Gorska, W. Nazarewicz, Phys. Status Solidi B 65, 193 (1974) (https://doi.org/10.1002/pssb.2220650117).
[38] J. Baars, F. Sorger, Solid State Comm. 10, 875 (1972) (https://doi.org/10.1016/0038-1098(72)90211-6).
[39] R.K. Willardson, A.C. Beer (ed.), Semiconductors and Semimetals, (Academic Press, New York, San Francisco, London, 1975).
[40] Ju.H. Velikov, A.P. Rusakov, Fiz. Tverd. Tela 13, 1157 (1971).
[41] D.L. Rode, J.D. Wiley, Phys. Status Solidi B 56, 699 (1973) (https://doi.org/10.1002/pssb.2220560234).
[42] B. Bonello, B. Fernandez, J. Phys. Chem. Solids 54, 209 (1993) (https://doi.org/10.1016/0022-3697(93)90310-N).
[43] D. Berlincourt, H. Jaffe, L.R. Shiozawa, Phys. Rev. 129, 1009 (1963) (https://doi.org/10.1103/PhysRev.129.1009).
[44] Landolt- Bornstein Numerical Data and Functional Relationship in Science and Technology. New Series, (Springer Verlag, Berlin, 1984).
[45] O.P. Malyk, J. Alloys Compd. 371, 146 (2004) (https://doi.org/10.1016/j.jallcom.2003.07.033).

[46] N. Muthukumarasamy, R. Balasundaraprabhu, S. Jayakumar, and M.D. Kannan, Sol. Energ. Mat. Sol. C. 92, 851 (2008) (https://doi.org/10.1016/j.solmat.2008.02.005).

О.П. Малик, С.В. Сиротюк

Рухливість електронів у твердому розчині $CdSe_xTe_{1-x}$ (x = 0,25): *ab initio* розрахунок

Національний університет "Львівська політехніка", Львів, 79013Україна. omalyk@ukr.net, svsnpe@gmail.com

У цій роботі проводиться оцінка якості твердого розчину $CdSe_{0.25}Te_{0.75}$ шляхом дослідження його властивостей перенесення. Опис кінетичних явищ проводиться на основі хвильової функції та самоузгодженого потенціалу твердого розчину $CdSe_xTe_{1-x}$ (x = 0,2), які визначалися з перших принципів, з використанням проекційних приєднаних хвиль, що реалізовано в програмі ABINIT. Процеси розсіяння були розглянуті в рамках близькодіючих моделей розсіяння, де враховувалась взаємодія електронів з полярними та неполярними оптичними фононами, п’єзоелектричними та акустичними фононами, центрами статичної деформації, нейтральними та іонізованими домішками. Елементи матриці переходу були отримані шляхом інтегрування по елементарній комірці з використанням тривимірної B-сплайн інтерполяції. Для кристалів із концентрацією домішок $5.6\times10^{15} \div 5\times10^{18}$ см$^{-3}$ розраховано температурні залежності рухливості електронів та фактора Холла в діапазоні 15 ÷ 1200 К. Теоретичні криві, отримані в близькодіючому підході, якісно і кількісно відрізняються від тих, що отримані в рамках далекодіючих моделей в наближенні часу релаксації.

Ключові слова: перенесення електронів, точкові дефекти, твердий розчин CdSeTe, ab initio розрахунок.