Kinetic Properties of CdSe₀.₄Te₀.₆: Connection of Ab initio Approach with Short-range Principle

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In the presented article a relationship between the structure of defects in $CdSe_xTe_{1-x}$ ($x = 0.4$) and its kinetic properties is established. For the first time, a method for determining the energy spectrum, wave function, and self-consistent crystal potential in $CdSe_{0.4}Te_{0.6}$ at a predetermined temperature is proposed. Within the framework of the supercell method, the structure of defects is studied and the temperature dependences of the ionization energies of various types of defects are determined. The proposed method also makes it possible to determine the temperature dependences of the optical and acoustic deformation potentials, as well as the temperature dependence of electron scattering parameters on different types of crystal defects. Within the framework of the short-range scattering models, the dependences of the electron mobility and electron's Hall factor vs temperature are established.

Keywords: CdSeTe, Electron transport, Point defects, Ab initio calculation, Short-range principle.

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1. INTRODUCTION

The solid solution $CdSe_xTe_{1-x}$ is widely used in the manufacturing of solar energy devices and infrared detectors. This is due to the fact that this material has a required band gap and a large absorption coefficient. Such properties make it suitable for photovoltaic applications in solar energy converters. Therefore, the study of the quality of crystals of this solid solution attracts the attention of many researchers and is an important applied problem. It is known that the main factor determining the optical and electrical properties of the solid solution $CdSe_xTe_{1-x}$ is crystal lattice defects of various types. The structure of crystal defects of this solid solution is systematically studied in works [1-13]. However, these works do not investigate the relationship between the defect structure and the kinetic properties of $CdSe_xTe_{1-x}$. On the other hand, in work [14] an attempt is made to establish such a relationship in the sphalerite n-$CdSe_xTe_{1-x}$ ($0.1 \le x \le 0.5$) crystals by combining two theoretical methods: 1) application of the wave function and self-consistent potential obtained from first principles using the ABINIT code; 2) application of the short-range principle to consider the scattering of a charge carrier on different types of crystal defects [15-17]. However, there are certain shortcomings in this work: 1) the used wave function and self-consistent potential describe the ground state of the crystal ($T = 0$) and therefore cannot be used to describe the crystal state at $T > 0$; 2) the defects structure is described by a donor defect of an unknown nature with the ionization energy $\Delta E_D \approx 10$ meV, which do not depend on temperature. To eliminate the above-mentioned shortcomings, the proposed work, for the first time, suggests a method for calculating the wave function and self-consistent crystal potential of the solid solution $CdSe_xTe_{1-x}$ ($x = 0.4$) with the sphalerite structure

which will be used to describe the crystal state at $T > 0$. In addition, here we consider the method of determining the structure of donor defects in $CdSe_xTe_{1-x}$ ($x = 0.4$), which will allow the temperature dependences of the ionization energies of various types of defects to be defined. These methods are used to describe the kinetic properties of the $CdSe_{0.4}Te_{0.6}$ solid solution.

2. THE METHOD OF CALCULATING THE WAVE FUNCTION AND SELF-CONSISTENT CRYTAL POTENTIAL AT A GIVEN TEMPERATURE

When calculating, a value of the lattice constant for each value of the composition of the solid solution was chosen so as to coincide with the experimental data. These values were used to calculate the wave functions and crystal potentials of CdTe and CdSe unit cells, as well as Cd_8Te_8 and Cd_8Se_8 supercells.

The wave function and self-consistent potential of the ideal $CdSe_{0.4}Te_{0.6}$ solid solution were determined as follows. Initially, these values and the energy spectrum were calculated for the unit cells of the sphalerite CdTe and CdSe (note that Cd atoms are on the cell boundary, and Te or Se atoms are inside the cell). For this purpose, previously selected GGA exchange-correlation potentials of Cd, Se, and Te were used as initial data. Then a certain mixture of these exchange-correlation potentials and the Hartree-Fock exchange-correlation potential was chosen (this mixture is determined by the parameter α)[17]. The value of the parameter α was chosen for the following reasons: at a given temperature, the theoretical value of the band gap should be equal to its experimental value, which was determined from the expression [18, 19]:

$$E_{gCdSeTe} = x\,E_{gCdSe} + (1-x)E_{gCdSe} - 0.9x(1-x) \quad eV, \qquad (1)$$

Using such a method, it is possible to select, for a given solid solution composition, certain values of the parameter α that correspond to the width of the band

gap at 0 K and 300 K. Herewith, the wave functions Ψ_{CdTe}, Ψ_{CdSe} and potentials U_{CdTe}, U_{CdSe} of the spha-lerite CdTe and CdSe unit cells at 0 K and 300 K are calculat-

ed. The calculation results are presented in Table 1.

Table 1 – Energy spectrum of CdTe and CdSe elementary cell

$T = 0, E_g = 1.512\ eV, \Delta = 1.545^*\ eV$		
Energy levels of CdTe cell, eV	E_c–1 × (5.854) (0) E_v–3 × (4.342) (2)**	$\alpha = 0.08866$
Energy levels of CdSe cell, eV	E_c–1 × (4.309) (0) E_v–3 × (2.797) (2)	$\alpha = 1.1941$
$T = 300, E_g = 1.380\ eV, \Delta = 1.503\ eV$		
Energy levels of CdTe cell, eV	E_c–1 × (5.798) (0) E_v–3 × (4.418) (2)	$\alpha = 0.0309$
Energy levels of CdSe cell, eV	E_c–1 × (4.295) (0) E_v–3 × (2.915) (2)	$\alpha = 1.17045$

*Δ – a shift between the energy levels of ideal CdTe and CdSe elementary cells.

** Recording 3 × (4.342) (2) means that there is exist 3-fold degenerate energy level with an occupation number equal 2.

As can be seen from Table I, at a given temperature, the energy levels E_c and E_v in CdTe and CdSe cells do not match, i.e., there exist energy barriers in the transition between cells of different types. However, it is known from experiment that a solid solution CdSe$_{0.4}$Te$_{0.6}$ at a given temperature has the same band gap width in all parts of the crystal. To eliminate this contradiction between experiment and theory, we shall use the following technique: the energy levels of the CdSe cell is shifted up by the value Δ, which is equal to the difference in the levels of the bottom of the conduction band E_c (or the top of the valence band E_v) in two different unit cells. Then we obtain a crystal that has the same band gap width in each of its parts (see Fig. 1). It should be noted that a similar result is obtained if the energy levels of the CdTe cell are shifted down by the value Δ.
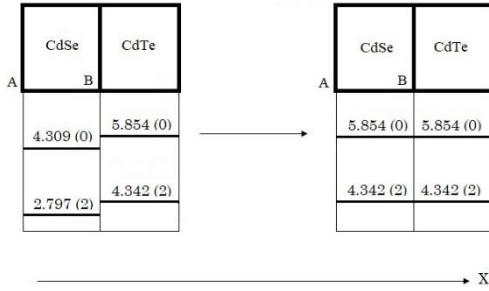

Fig. 1 – The location along the X axis of ideal CdTe and CdSe elementary cells and the corresponding positions of the energy levels for ideal elementary cells at T = 0 K for CdSe$_{0.4}$Te$_{0.6}$.

The above theoretical approach can be justified as follows: a) in the experiment, the width of the band gap E_g is measured, i.e., the difference in the energy levels, but not their absolute values. Therefore, the reference point of the energy in each cell can be chosen arbitrarily; b) the coordinate systems in the cells of CdTe and CdSe are not related to each other. This means that in Fig. 1 point A is the reference point of the coordinate system ($x = 0$, $y = 0$, $z = 0$) in the CdSe cell, and point B is the reference point of the coordinate system ($x' = 0$, $y' = 0$, $z' = 0$) in the CdTe cells.

Based on the wave functions and crystal potentials of the unit cells, the wave functions and derivatives of the crystal potential with respect to the coordinates of the

cell atoms can be calculated for the ideal CdSe$_x$Te$_{1-x}$ solid solution [14]. Using these characteristics of the ideal CdSe$_x$Te$_{1-x}$ solid solution and short-range scattering models [15-17], it is possible to calculate the electron scattering constants on crystal lattice defects [20]. These scattering constants are represented as integrals over the wave function $\psi(\mathbf{r})_{CdSeTe}$ and the crystal potential $U(\mathbf{r})_{CdSeTe}$. Since the functions $\psi(\mathbf{r})_{CdSeTe}$ and $U(\mathbf{r})_{CdSeTe}$ are different at 0 K and 300 K, then, accordingly, the scattering constants are different, i.e., these scattering parameters depend on temperature. Assuming the simplest, linear, temperature dependence, it is possible to obtain these dependences of the above-mentioned constants:

$$A_{PO} = (10.07 + 2 \times 10^{-4}\ T) \times 10^{-20}\ m^2, \quad (2a)$$

$$d_0 = -7.3 - 2 \times 10^{-3}\ T\ eV, \quad (2b)$$

$$E_{AC} = -2.06 - 2.33 \times 10^{-4}\ T\ eV, \quad (2c)$$

$$A_{II} = (0.498 - 3.33 \times 10^{-6}\ T) \times 10^{10}\ m^{-1}, \quad (2d)$$

The obtained temperature dependences of the scattering constants make it possible to calculate the electron scattering probability on different types of crystal defects and, in turn, the kinetic coefficients of the CdSe$_{0.4}$Te$_{0.6}$ solid solution.

3. CALCULATION OF THE TEMPERATURE DEPENDENCE OF THE IONIZATION ENERGY OF CRYSTAL DEFECTS

This article considers the following intrinsic donor defects: Cd$_{Te}$, Cd$_{Se}$, V$_{Se}$-Cd$_{Se}$. The energy spectrum of the defect structure was calculated using the supercell method [20]: for Cd$_{Te}$ – supercell Cd$_9$Te$_7$; Cd$_{Se}$ – supercell Cd$_9$Se$_7$; V$_{Se}$–Cd$_{Se}$ – supercell Cd$_9$Se$_6$. In addition, the energy spectrum of the ideal Cd$_8$Te$_8$ and Cd$_8$Se$_8$ supercell were calculated.

To calculate the energy spectrum of ideal and defective supercells, it is necessary to have pseudopotentials of Cd, Se and Te atoms. The pseudopotentials for these atoms were obtained by means of the AtomPAW (Atompaw v3.0.1.9 and AtomPAW$_2$Abinit v3.3.1) code. The PAW functions have been generated for the following valence basis states: $5s^25p^04d^{10}$ for Cd, $4s^24p^4$ for Se and $4s^24p^65s^25p^4$ for Te. The radii of the augmentation spheres r_{PAW} have the following values: 2.2, 1.8 and 2.4 for Cd, Se and Te respectively. The exchange and correlation effects have been taken into account within density-functional theory (DFT), namely in generalized gradient approximation (GGA) formalism. The output files of the AtomPAW code contain a full set of data which are input parameters for initiation of the ABINIT code. The result of calculations of energy spectra of ideal supercells for the CdSe$_{0.35}$Te$_{0.65}$ solid solutions is presented in Table 2.

As can be seen from Table 2, the energy levels of the spectra of the ideal Cd$_8$Te$_8$ and Cd$_8$Se$_8$ supercells do not coincide, i.e., there are energy barriers between the Cd$_8$Te$_8$ and Cd$_8$Se$_8$ supercells. Therefore, as in the case of CdTe and CdSe unit cells, it is necessary to shift the energy levels of the Cd$_8$Se$_8$ supercell up (or the energy levels of the Cd$_8$Te$_8$ supercell down) by the value Δ equal to the difference in the levels of the bottom of the

conduction band (or the top of the valence band) in two different supercells. As a result, we will get an ideal solid solution in which the ideal Cd$_8$Te$_8$ and Cd$_8$Se$_8$ supercells are located in a certain way, for which the lattice constant and the theoretical value of the band gap coincide with the experiment.

Table 2 – Energy spectrum of ideal Cd$_8$Te$_8$ and Cd$_8$Se$_8$ supercells

$T = 0, E_g = 1.512\ eV, \Delta = 1.23\ eV$		
Energy levels of ideal Cd$_8$Te$_8$ supercell, eV	$E_{c-}1 \times (5.021)\ (0)$ $E_{v-}2 \times (3.509)\ (2)$	$\alpha = -0.08165$
Energy levels of ideal Cd$_8$Se$_8$ supercell, eV	$E_{c-}1 \times (3.791)\ (0)$ $E_{v-}2 \times (2.279)\ (2)$	$\alpha = 0.93$
$T = 300, E_g = 1.380\ eV, \Delta = 1.216\ eV$		
Energy levels of ideal Cd$_8$Te$_8$ supercell, eV	$E_{c-}1 \times (4.963)\ (0)$ $E_{v-}2 \times (3.583)\ (2)$	$\alpha = -0.1243$
Energy levels of ideal Cd$_8$Se$_8$ supercell, eV	$E_{c-}1 \times (3.747)\ (0)$ $E_{v-}2 \times (2.367)\ (2)$	$\alpha = 0.7871$

A comparison of the energy spectra of the ideal (the energy levels of which are shifted by the appropriate value Δ) and defect (the origin energy levels of which are also shifted by the appropriate value Δ) supercells is presented in Table 3. Based on these data and using the method proposed in [20], it is possible to determine the ionization energies of various defects in the crystal lattice of CdSe$_{0.4}$Te$_{0.6}$ solid solution. The results of the calculations take the form.

It should be noted that the above method for describing an ideal CdSe$_{0.4}$Te$_{0.6}$ crystal and the structure of its defects is a combination of the short-range principle (exchange of energy (electrons) occurs only between neighbouring crystal regions) and the first principles approach (calculation of the energy spectra of different regions of the crystal).

Table 3 – Energy spectrum of ideal and defect supercell

$T = 0, E_g = 1.512\ eV$		
Energy levels of ideal Cd$_8$Te$_8$ (Cd$_8$Se$_8$), eV	Energy levels of defect, eV	Ionization energy, eV
$E_{c-}1 \times (5.021)\ (0)$ $E_{v-}2 \times (3.509)\ (2)$	Cd$_{Te}$ $2 \times (5.200)\ (0)$ $1 \times (4.957)\ (2)$	$\Delta E_D = 0.064$
$E_{c-}1 \times (5.021)\ (0)$ $E_{v-}2 \times (3.509)\ (2)$	Cd$_{Se}$ $2 \times (5.917)\ (0)$ $1 \times (5.555)\ (2)$	$\Delta E_D = -0.534$
$E_{c-}1 \times (5.021)\ (0)$ $E_{v-}2 \times (3.509)\ (2)$	V$_{Se}$ –Cd$_{Se}$ $2 \times (5.027)\ (0)$ $1 \times (4.964)\ (2)$	$\Delta E_D = 0.057$
$T = 300, E_g = 1.380\ eV$		
$E_{c-}1 \times (4.963)\ (0)$ $E_{v-}2 \times (3.583)\ (2)$	Cd$_{Te}$ $2 \times (5.211)\ (0)$ $1 \times (4.973)\ (2)$	$\Delta E_D = -0.010$
$E_{c-}1 \times (4.963)\ (0)$ $E_{v-}2 \times (3.583)\ (2)$	Cd$_{Se}$ $2 \times (5.930)\ (0)$ $1 \times (5.562)\ (2)$	$\Delta E_D = -0.599$
$E_{c-}1 \times (4.963)\ (0)$ $E_{v-}2 \times (3.583)\ (2)$	V$_{Se}$ –Cd$_{Se}$ $2 \times (5.035)\ (0)$ $1 \times (4.933)\ (2)$	$\Delta E_D = 0.030$

$$Cd_{Te}: \Delta E_D = 0.064 - 2.47 \times 10^{-4}\ T, \qquad (3a)$$

$$V_{Se} - Cd_{Se}: \Delta E = 0.057 - 9 \times 10^{-5}\ T, \qquad (3b)$$

4. DISCUSSION

Based on the theoretical assumptions presented in the two previous sections, the article considers the transport phenomena in the CdSe$_{0.4}$Te$_{0.6}$ solid solution in the temperature range of $10 \div 400$ K and defects concentration $N_D = 5 \times 10^{14} \div 5 \times 10^{18}$ cm^{-3}. When solving the neutrality equation, the transition of defects Cd$_{Te}$ and V$_{Se}$–Cd$_{Se}$ into a fully ionized state, as well as complete ionization of the defect Cd$_{Se}$, was taken into account:

$$T < 224.9\ \text{K},$$

$$n - p = (1 - x)N_D / \{1 + 2 \exp\left[\frac{F - \Delta E_{Cd_{Te}}}{k_B T}\right]\} + \frac{xN_D}{2} + \frac{1}{2}xN_D / \{1 + 2exp\left[\frac{F - \Delta E_{V_{Se} - Cd_{Se}}}{k_B T}\right]\},$$

$$224.9\ \text{K} < T,$$

$$n - p = (1 - x)N_D + \frac{1}{2}xN_D + \frac{1}{2}xN_D / [1 + 2exp\left[\frac{F - \Delta E_{V_{Se}Cd_{Se}}}{k_B T}\right]],$$

The theoretical dependences of the electron mobility on temperature for different defects concentrations (donors and static strain (SS) centers) are shown in Fig.3. The electron mobility was calculated on the basis of short-range scattering models [14-17] using the exact solution of the Boltzmann kinetic equation.

A comparison of two competing approaches (short-range and long-range scattering models) in the description of transport phenomena in CdSe$_{0.4}$Te$_{0.6}$ is considered in Fig. 3a – 3e. Solid curves 1 correspond to short-range scattering models and are obtained within the framework of the exact solution of the Boltzmann kinetic equation Dashed curves 2 and 3 correspond to long-range scattering models (relaxation time approximation): curve 2 describes the region of low temperature ($\hbar\omega \gg k_B T$), curve 3 describes the region of high temperatures ($\hbar\omega \ll k_B T$). As it can be seen, these

curves demonstrate significant qualitative and quantitative differences of the temperature dependences of the electron mobility throughout the studied range of defect concentrations and temperatures. Regarding the approximation of the relaxation time, the following remark should be made. It is known that for CdSe$_{0.4}$Te$_{0.6}$ the Debye temperature is equal to $\theta_D = 261$ K. It means that the low-temperature region will be determined by the condition $T < 26.1$ K, and the high- temperature region will be determined by the condition $T > 2610$ K. From this point of view, the application of the relaxation time approximation (elastic scattering) in the range of $26.1\ \text{K} < T < 2610$ K is incorrect because in this temperature range the inelastic scattering occur. At the same time, the short-range scattering models allow a description of inelastic scattering. Thus, it can be argued that the short-range

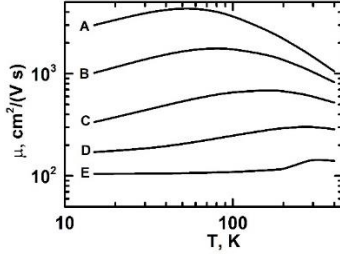models give a more adequate description of the physical reality than the long-range models.

Fig. 2 – Electron mobility versus temperature in $CdSe_{0.4}Te_{0.5}$ with a different defects concentration. $A - N_D = 5 \times 10^{14}$ cm^{-3}, $N_{SS} = 1 \times 10^{15}$ cm^{-3}; $B - N_D = 5 \times 10^{15}$ cm^{-3}, $N_{SS} = 3 \times 10^{15}$ cm^{-3}; $C - N_D = 5 \times 10^{16}$ cm^{-3}, $N_{SS} = 1 \times 10^{16}$ cm^{-3}; $D - N_D = 5 \times 10^{17}$ cm^{-3}, $N_{SS} = 3 \times 10^{16}$ cm^{-3}; $E - N_D = 5 \times 10^{18}$ cm^{-3}, $N_{SS} = 8 \times 10^{18}$ cm^{-3}
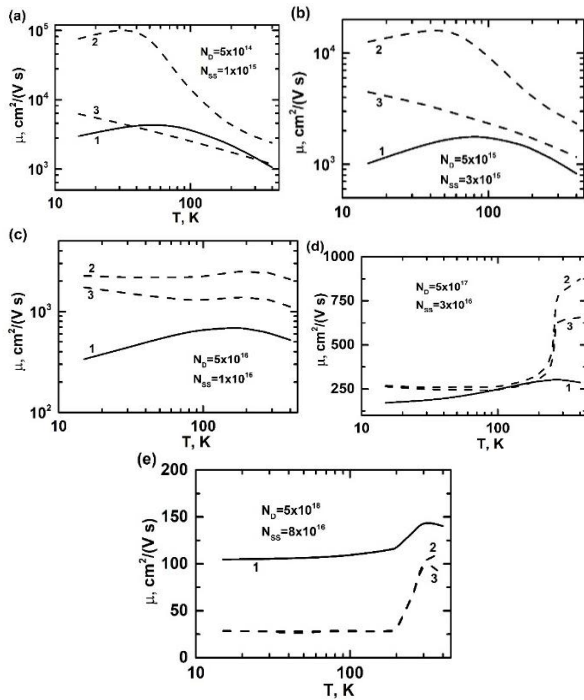

Fig. 3 – Comparison of two theoretical approaches in $CdSe_{0.4}Te_{0.6}$ samples: 1– short-range scattering models; 2 and 3 – relaxation time approximation

The proposed method of calculation allows the temperature dependence of the electron's Hall factor for $CdSe_{0.4}Te_{0.6}$ to be obtained (see. Fig. 4). As can be seen, at low temperatures in sample D the electron gas is in a degenerate state, while in samples A, B, C and D the electron gas is non-degenerate or in an intermediate (between degenerate and non-degenerate) state. At high temperatures, the minima of the curves are observed in the region where the transition from the dominance of one scattering mechanism to another takes place. The higher defect concentration in the crystal determines the higher temperature where the minimum of dependence r_H(T) is observed.
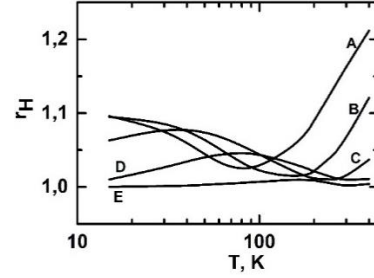

Fig. 4 – Electron's Hall factor versus temperature in $CdSe_{0.4}Te_{0.6}$ samples with a different defects concentration. The notation of the samples is the same as on Fig. 2

It should be noted that the proposed above calculation method can be applied to ternary, quaternary and higher multicomponent solid solutions with sphalerite structure. Indeed, if in the case of the binary solid solution $CdSe_xTe_{1-x}$, it was necessary to apply the supercell method to two supercells Cd_8Te_8 and Cd_8Se_8, then, for example, in the case of the ternary solid solution CdSeSTe one more supercell Cd8S8 should be added. Further, by carrying out the calculation proposed above, it is possible to determine the type of defects, as well as the temperature dependence of their ionization energies. By modifying electroneutrality equations, it is possible to determine the Fermi level and, accordingly, calculate the kinetic coefficients of the CdSeSTe solid solution. The same can be done in the case of higher multicomponent solid solutions.

5. CONCLUSION

In the presented paper, for the first time, a method for calculating the energy spectrum of electrons, wave function, and self-consistent potential of the $CdSe_xTe_{1-x}$ ($x = 0.4$) solid solution for a predetermined temperature is proposed. The application of this method to an ideal unit cell made it possible to determine the temperature dependences of the electron scattering constants on crystal defects. This made it possible to calculate the probability of electron scattering on crystal defects and, accordingly, to identify the kinetic coefficients of $CdSe_{0.4}Te_{0.6}$. The application of the same method for Cd_8Te_8 and Cd_8Se_8 supercells made it possible to define the structure of defects, as well as to calculate the temperature dependence of the ionization energies of crystal defects. Within the framework of the short-range scattering models, the dependences of electron mobility and electron's Hall factor on temperature were established. A comparison of the theoretical curves $\mu(T)$ obtained within the framework of two competing approaches was made: a) short-range scattering models; b) long-range scattering models (approximation of the relaxation time). It was established that the short-range scattering models more adequately describe the transport phenomena in the solid solution $CdSe_xTe_{1-x}$. The possibility of applying the proposed calculation method not only for other binary solid solutions, but also for ternary, quaternary and higher multicomponent solid solutions with the sphalerite structure is substantiated.

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Кінетичні властивості CdSe$_{0.4}$Te$_{0.6}$: зв'язок ab initio підходу з принципом близькодії

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У статті встановлено зв'язок між структурою дефектів у CdSe$_x$Te$_{1-x}$ ($x = 0,4$) та його кінетичними властивостями. Вперше запропоновано метод визначення енергетичного спектру, хвильової функції та самоузгодженого кристалічного потенціалу в CdSe$_{0.4}$Te$_{0.6}$ при заданій температурі. У рамках методу суперкомірки досліджено структуру дефектів і визначено температурні залежності енергій іонізації різних типів дефектів. Запропонований метод також дає змогу визначити температурні залежності оптичного та акустичного потенціалів деформації, а також температурну залежність параметрів розсіювання електронів на різних типах дефектів кристала. В рамках близькодіючих моделей розсіяння встановлено залежності рухливості електронів і фактора Холла електронів від температури.

Ключові слова: CdSeTe, Перенесення електронів, Точкові дефекти, Ab initio розрахунок, Принцип близькодії.