

O. P. Malyk

Transport phenomena in CdTe:Cl and CdTe:Cu - calculation from the first principles

*Semiconductor Electronics Department, Lviv Polytechnic National University, Lviv, 79013, S. Bandera Str., 12, Ukraine.
omalyk@ukr.net*

In the presented article the method of determining the energy spectrum, the wave function of the charge carrier and the crystal potential in CdTe at an arbitrarily given temperature is considered. Using this approach within the framework of the supercell method the temperature dependences of the ionization energies of various types of defects caused by the introduction of chlorine and copper impurities in cadmium telluride are calculated. Also the offered method allows to define the temperature dependence of the optical and acoustic deformation potentials and as well as the dependence on the temperature the charge carrier's scattering parameters on ionized impurities, polar optical, piezooptic and piezoacoustic phonons. Within the framework of short-range scattering models the temperature dependences of the charge carrier's mobility and Hall factor are considered.

Keywords: Transport phenomena, Crystal defects, CdTe, Ab initio calculation.

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Introduction

Cadmium telluride possesses unique physical properties necessary for photovoltaic converters of solar energy, namely, a required band gap width and needed absorption coefficient value. The structure of intrinsic and impurity defects predominantly determines the electrical and optical properties of this material. Therefore, the study of the defects structure of CdTe is an actual applied problem. In literature there is a wide range of works where the ab initio approach is used to calculate the structure of defects in cadmium telluride [1-7]. However, these works do not specify the way to establish the relationship between the structure of point defects and the kinetic properties of CdTe, which directly determine the electrical properties of the material. In the current work, this problem will be solved in two stages.

At the first stage on the basis of density functional theory (DFT) the calculation from the first principles of energy characteristics of a semiconductor is carried out: energy spectrum, electron (or heavy hole) wave function and potential energy in a crystal lattice. Usually it is assumed that the above characteristics describe the state of

the crystal at $T = 0$ K. In the current article, a method for calculating these characteristics of a sphalerite semiconductor at a predetermined temperature will be proposed. Based on this method the charge carrier (electrons and heavy holes) scattering parameters on different point defects of the crystal will be calculated at a given temperature. At the second stage, the ionization energies of various types of defects caused by the introduction of chlorine and copper impurities into cadmium telluride are determined by the supercell method. Knowing these ionization energies and charge carrier scattering parameters it is possible to calculate the Fermi level and, in turn, the kinetic coefficients of CdTe. It should be noticed that there are a series of works in literature devoting to transport phenomena in semiconductors, in particular in CdTe [8], which are based on ab initio calculations [9-13]. However, in these works the connection between defect structure and kinetic properties is not specified.

I. Calculation of temperature dependences of wave function and crystal potential

When considering the transport phenomena in cadmium telluride, the charge carrier short-range scattering models were used [8, 14-16]. These short-range scattering models include several scattering constants as parameters, which, in turn, require the calculation of the conduction and valence band wave function and the self-

consistent crystal potential. To calculate these above-mentioned constants the method of calculating the electron energy spectrum and the crystal potential, presented in [17,18], was used. This allowed to separate the physical solutions of the Schrödinger equation from the set of mathematical solutions of the Schrödinger equation using the following criterion for selecting physical solutions of the Schrödinger equation, namely: at a given temperature, the theoretical width of the band gap must coincide with its experimental value, which was determined from the experimental expression for solid solution $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ [19]:

$$E_g(x, T) = -0.302 + 1.93x - 0.81x^2 + 0.832x^3 + 5.35 \times 10^{-4}T(1 - 2x) \quad (1)$$

Using this approach, the following values of the factor α (this parameter defines the mixture of the conventional GGA exchange correlation potentials for Cd and Te, pseudopotentials [20, 21], and the Hartree Fock exchange potential [22]) were obtained for the ideal unit cell (sphalerite structure) of cadmium telluride: $\alpha = 0.397$ corresponds to $T = 0$ K, $\alpha = 0.288$ corresponds to $T = 300$ K. Herewith, the electron wave functions in the conduction and valence band and the crystal potential at temperatures of 0 K and 300 K were obtained.

Accordingly, the following scattering constants for electrons and heavy holes were determined, namely:

1) Scattering constants for charge carrier-polar optical (PO) phonon interaction, charge carrier-piezoacoustic (PAC) phonon and charge carrier-piezo-optic (POP) phonon interaction

$$A_{PO} = A_{PAC} = A_{POP} = \int \psi^*(R^2 - r^2)\psi \, dr \quad (2)$$

2) d_0 is the optical deformation potential constant which choose equal to the maximum value among three optical deformation potential constants corresponding to one longitudinal and two transverse branches of the lattice optical vibrations:

$$d_{0v} = a_0 \int \psi^* \varepsilon_v \cdot V \psi \, dr, \quad v = 1, 2, 3; \quad (3)$$

where the region of integration is the same as in the case of PO scattering; ε_v – unitary contravariant polarization vector of the optical oscillations; vector V is expressed in terms of the derivatives of the self-consistent electron potential energy over the coordinates of the atoms of the unit cell [15].

3) E_{AC} is the acoustic deformation potential constant which was choose equal to the maximum value among three acoustic deformation potential constants corresponding to one longitudinal and two transverse branches of the lattice acoustic vibrations:

$$\begin{aligned} E_{AC\parallel} &= -(-I_1/4 + I_2/2 + I_3/2); \\ E_{AC1\perp} &= -(-I_1/4 + I_2/4 + I_3/2); \\ E_{AC2\perp} &= -(-I_1/2 + I_2/2 + I_3/4); \end{aligned} \quad (4)$$

where $I_1 = \int \psi^* V'_1 \psi \, dr'$; $I_2 = \int \psi^* V'_2 \psi \, dr'$; $I_3 = \int \psi^* V'_3 \psi \, dr'$; V'_1 ; V'_2 ; V'_3 ; are the projections of the vector V in an oblique coordinate system created by the primitive vectors of the zinc blende structure;

4) The ionized impurity scattering constant:

$$A_{II} = \int_{\Omega} \psi^* \frac{1}{r} \psi \, dr \quad (5)$$

It should be noticed that in (2)-(5) integration is carried out according to the method proposed in [17].

Formulas (2) - (5) show that the above mentioned scattering constants are expressed in terms of the integrals over the wave function Ψ and crystal potential U . Calculation of these integrals was made on the base of three-dimensional B-spline interpolation and finite displacement method [23]. The dependence of Ψ and U on temperature causes the temperature dependence of scattering constants. Assuming the simplest, linear, temperature dependence, one can calculate the temperature dependences of the scattering constants for heavy holes and electrons:

$$A_{POhh} = (12.2 + 1.84 \times 10^{-3}T) \times 10^{-20} m^2, \quad A_{POe} = (12.24 + 2.088 \times 10^{-4}T) \times 10^{-20} m^2, \quad (6a)$$

$$d_{0hh} = -43.1 - 0.018T \, eV, \quad d_{0e} = -20.93 - 4.053 \times 10^{-3}T \, eV \quad (6b)$$

$$E_{AChh} = -3.07 - 2.28 \times 10^{-3}T \, eV, \quad E_{ACe} = -2.423 - 4.628 \times 10^{-4}T \, eV \quad (6c)$$

$$A_{IIhh} = (0.442 - 8.90 \times 10^{-6}T) \times 10^{10} m^{-1}, \quad A_{IIe} = (0.4794 - 7.405 \times 10^{-6}T) \times 10^{10} m^{-1} \quad (6d)$$

Using these relations, one can calculate the temperature dependences of electron transition probabilities and in turn the kinetic coefficients of

cadmium telluride.

Note that the temperature dependence of the heavy hole effective mass, which was determined in [17], was

used to calculate the mobility of heavy holes. This temperature dependence has a form:

$$m_{hh} = (0.214 + 9.902 \times 10^{-5}T)m_0 \quad (7)$$

It is possible to note the qualitative similarity of expression (7) to analogous expression for $Cd_xHg_{1-x}Te$ ($x \sim 0.2$), obtained by fitting to experimental data [24].

II. Determination of temperature dependences of ionization energy of different types of impurity defects

The proposed study considers the acceptor defects caused by the introduction of copper impurity were investigated, namely: Cu_{Cd} , $V_{Te} - Cu_{Cd}$, $Cu_{Cd} - Te_{Cd}$, $Cu_{Cd} - V_{Cd}$. The study of the energy spectrum of the defects structure of cadmium telluride was carried out within the framework the supercell method on the basis of the ABINIT code: Cu_{Cd} – supercell Cd_7Te_8Cu ($1 \times 1 \times 2$ sphalerite cubic structure); $V_{Te} - Cu_{Cd}$ – supercell Cd_7Te_7Cu ($1 \times 1 \times 2$ sphalerite cubic structure); $Cu_{Cd} - Te_{Cd}$ – supercell $Cd_{14}Te_{17}Cu$ ($2 \times 1 \times 2$ sphalerite cubic structure); $Cu_{Cd} - V_{Cd}$ – supercell $Cd_{14}Te_{16}Cu$ ($2 \times 1 \times 2$ sphalerite

cubic structure). Next donor defects caused by the introduction of chlorine impurity were considered, namely: Cl_{Te} , $Cl_{Te} - Cd_{Te}$. The energy spectrum of these defect structures was calculated using the supercell method ($1 \times 1 \times 2$ sphalerite cubic structure) based on the ABINIT code: for Cl_{Te} – supercell Cd_8ClTe_7 ; $Cl_{Te} - Cd_{Te}$ – supercell Cd_9ClTe_6 . Analogous calculations were performed for the ideal supercell Cd_8Te_8 ($1 \times 1 \times 2$ sphalerite cubic structure) and $Cd_{16}Te_{16}$ ($2 \times 1 \times 2$ sphalerite cubic structure). At the same time, the following values of the α parameter were obtained for the ideal supercells: Cd_8Te_8 – $\alpha = 0.09$ corresponds to $T=0$ K, $\alpha = 0.0182$ corresponds to $T = 300$ K; $Cd_{16}Te_{16}$ – $\alpha = 0.076$ corresponds to $T=0$ K, $\alpha = 0.00571$ corresponds to $T=300$ K The calculated energy spectra of the above-indicated supercells are presented in Table I.

The next stage of the calculations consists in establishing the temperature dependence of the ionization energy of various types of defects. For this purpose, the method presented in [17] was used. After that, assuming a linear relationship, we obtain the temperature dependences of the defect ionization energy:

$$Cu_{Cd}: \Delta E_A = 1.405 - 5.567 \times 10^{-4} T, \quad (8a)$$

$$V_{Te} - Cu_{Cd}: \Delta E_A = 1.476 - 3.533 \times 10^{-4} T, \quad (8b)$$

Table 1.

Energy spectrum of ideal and defect supercell.

1×1×2 sphalerite cubic structure					
T=0, $E_g=1.65$ eV, exchmix=0.09			T=300 K, $E_g=1.48$ eV, exchmix=0.0182		
Energy levels of ideal Cd_8Te_8 , eV	Energy levels of defect, eV	Ionization energy, eV	Energy levels of ideal Cd_8Te_8 , eV	Energy levels of defect, eV	Ionization energy, eV
E_c - 1×(4.194) (0) E_v - 2× (2.541) (2)*	Cu_{Cd} 1×(3.946) (0) 1×(2.344) (1) 1×(2.344) (2)	At T=0 p- type. At $T \geq 0$ $\Delta E_A=1.405$	E_c - 1× (4.108) (0) E_v - 2× (2.620) (2)	Cu_{Cd} 1×(3.858) (0) 1×(2.463) (1) 1×(2.463) (2)	$\Delta E_A = 1.238$
E_c - 1×(4.194) (0) E_v - 2×(2.541) (2)	$V_{Te} - Cu_{Cd}$ 1×(4.017) (0) 1×(2.226) (1) 1×(1.910) (2)	At T=0 p- type. At $T \geq 0$ $\Delta E_A=1.476$	E_c - 1×(4.108) (0) E_v - 2× (2.620) (2)	$V_{Te} - Cu_{Cd}$ 1×(3.990) (0) 1×(2.214) (1) 1×(2.054) (2)	$\Delta E_A = 1.370$
E_c - 1×(4.194) (0) E_v - 2×(2.541) (2)	Cl_{Te} 1×(5.073) (0) 1×(3.637) (1) 2×(2.394) (2)	$\Delta E_D=0.557$	E_c - 1×(4.108) (0) E_v - 2×(2.620) (2)	Cl_{Te} 1×(5.070) (0) 1×(3.569) (1) 2×(2.459) (2)	$\Delta E_D = 0.539$
E_c -1×(4.194) (0) E_v -2×(2.541) (2)	$Cl_{Te}-Cd_{Te}$ 1×(4.219) (0) 1×(4.177) (1) 1×(4.177) (2)	$\Delta E_D=0.017$	E_c - 1×(4.108) (0) E_v - 2×(2.620) (2)	$Cl_{Te}-Cd_{Te}$ 1×(4.211) (0) 1×(4.148) (1) 1×(4.148) (2)	$\Delta E_D = -0.040$
2×1×2 sphalerite cubic structure					
T=0, $E_g=1.65$ eV, exchmix=0.076			T=300 K, $E_g=1.48$ eV, exchmix=0.00571		
Energy levels of ideal $Cd_{16}Te_{16}$, eV	Energy levels of defect, eV	Ionization energy, eV	Energy levels of ideal $Cd_{16}Te_{16}$, eV	Energy levels of defect, eV	Ionization energy, eV
E_c -1×(4.130) (0) E_v -2× (2.478) (2)	$Cu_{Cd} - V_{Cd}$ 1× (2.967) (0) 1× (2.360) (1) 1× (1.752) (2)	At T=0 p- type. At $T \geq 0$ $\Delta E_A = 0.489$	E_c -1×(4.046) (0) E_v -2×(2.558) (2)	$Cu_{Cd} - V_{Cd}$ 1× (2.881) (0) 1× (2.323) (1) 1× (1.722) (2)	$\Delta E_A = 0.323$
E_c -1×(4.130) (0) E_v -2× (2.478) (2)	$Cu_{Cd} - Te_{Cd}$ 1× (3.085) (0) 1× (3.077) (0) 1× (1.845) (2)	$\Delta E_A = 0.599$	E_c -1×(4.046) (0) E_v -2×(2.558) (2)	$Cu_{Cd} - Te_{Cd}$ 1× (3.012) (0) 1× (3.005) (0) 1× (1.855) (2)	$\Delta E_A = 0.447$

*Recording 2×(2.541) (2) means that there is exist 2-fold degenerate energy level with an occupation number equal 2.

$$Cu_{Cd} - Te_{Cd}: \Delta E_A = 0.599 - 5.067 \times 10^{-4} T, \quad (8c)$$

$$Cu_{Cd} - V_{Cd}: \Delta E_A = 0.489 - 5.533 \times 10^{-4} T, \quad (8d)$$

$$Cl_{Te}: \Delta E_D = 0.557 - 6 \times 10^{-5} T, \quad (8e)$$

$$Cl_{Te} - Cd_{Te}: \Delta E_D = 0.017 - 1.9 \times 10^{-4} T, \quad (8f)$$

It should be noted that only for one type of defects studied, the discrete level of the defect merges with the conduction band, namely: $Cl_{Te} - Cd_{Te}$ at $T = 89$ K. For other types of defects, with the temperature increasing, there is only a decrease in ionization energy without merging with the conduction band.

III. Discussion

Only defects with the lowest ionization energy were taken into account in the calculations of transport properties, as they make the dominant contribution to the transport phenomena. As can be seen from the equations (8a) - (8f) that for copper-doped CdTe such a defect is $Cu_{Cd} - V_{Cd}$, while for chlorine-doped CdTe, it is a defect complex $Cl_{Te} - Cd_{Te}$.

Comparison of theoretical temperature dependences

of heavy holes mobility was made with experimental data presented in [25]. Cadmium telluride parameters used for calculation are presented elsewhere [17]. Therefore, for copper-doped cadmium telluride the Fermi level is determined by the electroneutrality equation, which has the form:

$$p - n = N_A / \{1 + 2 \exp[(E_A - F)/(k_B T)]\}, \quad (9)$$

where N_A – copper impurity concentration and the defect level E_A at a given temperature is choose according to (8d).

The calculation of the temperature dependences of the heavy hole mobility was performed on the basis of short-range scattering models [14,15,17] within the framework of the exact solution of the Boltzmann's kinetic equation [26].

The temperature dependences of the heavy holes mobility in cadmium telluride crystals with a copper impurity concentration of $1 \times 10^{14} \div 1 \times 10^{18} \text{ cm}^{-3}$ were calculated. The results of the calculation are presented in Fig.1. For each value of the concentration of copper atoms N_A , such values of the concentration of the static strain centers N_{SS} were chosen, which would allow to cover all possible values of the heavy holes mobility at low

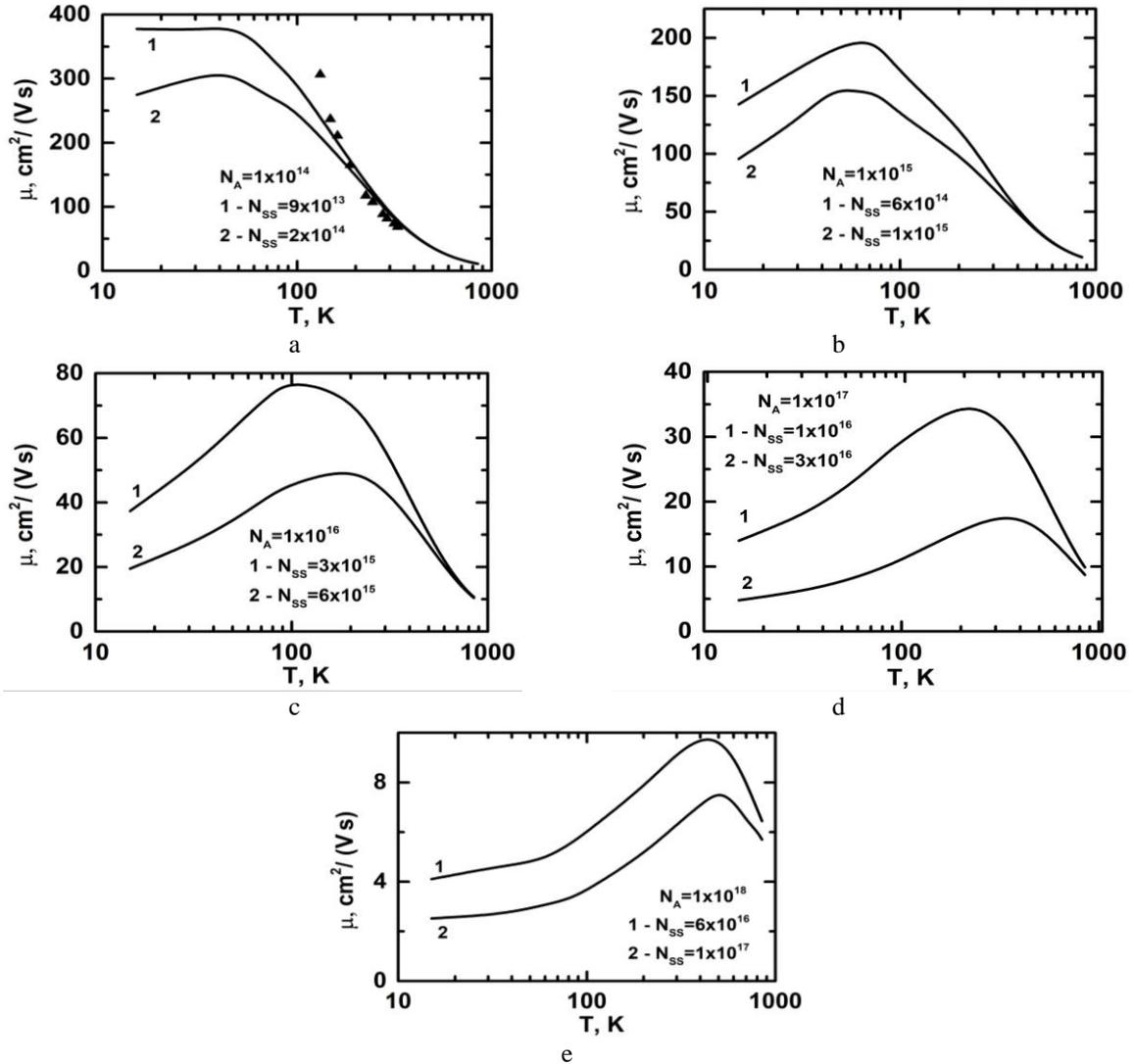


Fig. 1. – The temperature dependences of heavy hole mobility in cadmium telluride crystals with different defect concentration. a – $N_A=1 \times 10^{14} \text{ cm}^{-3}$; b – $N_A=1 \times 10^{15} \text{ cm}^{-3}$; c – $N_A=1 \times 10^{16} \text{ cm}^{-3}$; d – $N_A=1 \times 10^{17} \text{ cm}^{-3}$; e – $N_A=1 \times 10^{18} \text{ cm}^{-3}$.

temperatures. Comparison of theoretical curves with experimental data was performed only for the concentration of acceptor defects $1 \times 10^{14} \text{ cm}^{-3}$ (see Fig. 1a). It can be seen that the theoretical curve agrees well enough with the experimental data. Unfortunately, there are no experimental data in the literature for other values of copper impurity concentrations.

For heavy holes, the theoretical curves obtained by two competing approaches were compared: short-range scattering models and long-range scattering models. The results of the calculation are presented in Fig. 2. The dashed lines 1 and 2 represent the results of the calculation of the dependence $\mu(T)$ obtained in the relaxation time approximation using long-range scattering models: curve 2 describes the high-temperature region ($\hbar\omega \ll k_B T$, ω – optical oscillation frequency), curve 1 describes the low-temperature region ($\hbar\omega \gg k_B T$). Regarding curves 1 and 2, the following remark should be made. For cadmium telluride the Debye temperature is $\theta_D = 239 \text{ K}$. Therefore, according to the above inequalities,

the low-temperature region will be determined by the condition $T < 24 \text{ K}$, and the high-temperature region will be determined by the condition $T > 2400 \text{ K}$. As can be seen from Fig. 2(a), the experimental points fall into the region where $T \sim \theta_D$, i.e., where the application of the relaxation time approximation (elastic scattering) is incorrect. On the other hand, the heavy hole short-range scattering models allow to describe inelastic scattering, so their application in this temperature range is correct. In addition, curve 3 differs significantly qualitatively and quantitatively from curves 1 and 2. Given the coincidence of curve 3 with the experiment, it can be argued that the short-range scattering models give a more adequate description of physical reality than long-range models.

Calculated on the basis of the proposed method the dependences of heavy hole's Hall factor on temperature are presented in Fig. 3. It is seen that these dependencies have minimums, which are situated as follows - the higher the concentration of copper impurities, the higher the temperature of minimum.

Theoretical calculations were compared with

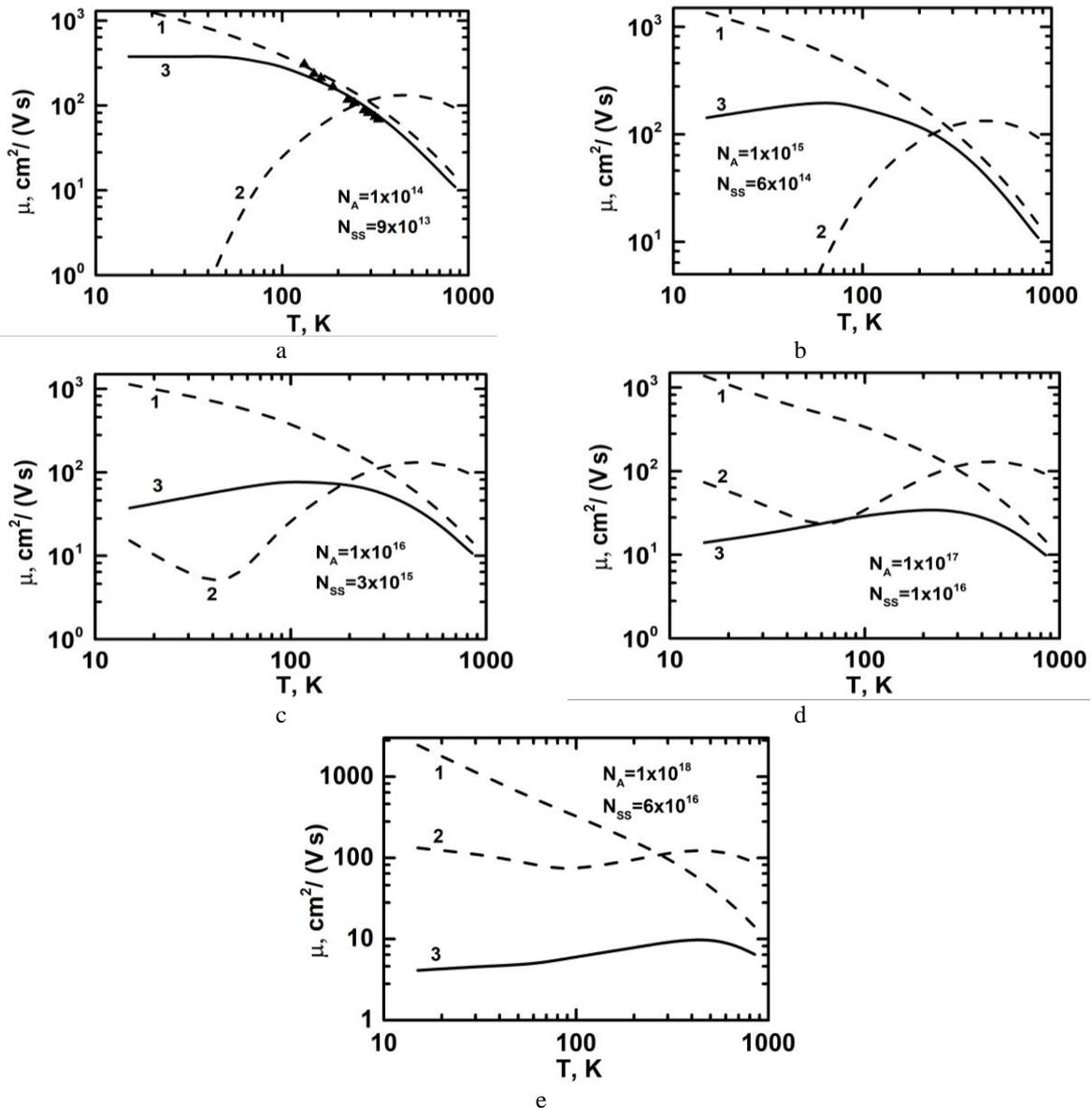


Fig. 2. – Dependencies $\mu(T)$ corresponding to different theoretical approaches. 1, 2 – long-range scattering models (relaxation time approximation); 3– short-range scattering models.

experimental data for chlorine-doped CdTe [27]. As can be seen from (8e)-(8f), the defect with minimum ionization energy is a defect complex $\text{Cl}_{\text{Te}} - \text{Cd}_{\text{Te}}$. Given

$$n - p = N_D / \left[1 + 2 \exp\left(\frac{F - F_D}{k_B T}\right) \right] \text{ - before the merger of the defect level;} \quad (9a)$$

$$n - p = N_D \text{ - after the merger of the defect level,} \quad (9b)$$

where N_D is the chlorine concentration and the defect level E_D at a given temperature is selected according to (8f).

Similar to the case of heavy holes the temperature dependences of the electron mobility were calculated on the basis of short-range scattering models [14,15,17] within the framework of the exact solution of the Boltzmann kinetic equation [26].

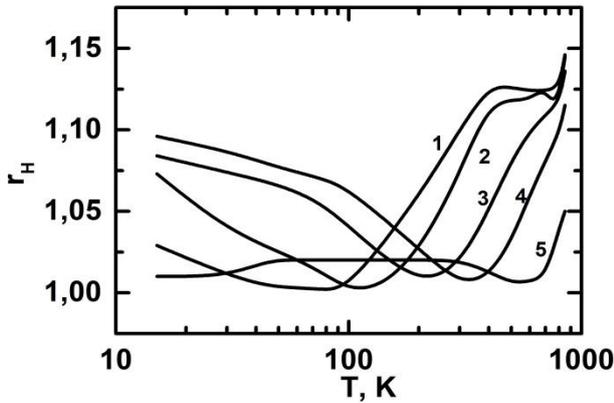


Fig.3. – Heavy hole Hall factor versus temperature in cadmium telluride crystals with different copper concentration. 1 – $N_A=1 \times 10^{14} \text{ cm}^{-3}$; 2 – $N_A=1 \times 10^{15} \text{ cm}^{-3}$; 3 – $N_A=1 \times 10^{16} \text{ cm}^{-3}$; 4 – $N_A=1 \times 10^{17} \text{ cm}^{-3}$; 5 – $N_A=1 \times 10^{18} \text{ cm}^{-3}$.

For chlorine doped samples, theoretical temperature dependences of electron mobility were calculated for the following defect concentrations (see Fig.4):

- sample A – $N_D=5 \times 10^{14} \text{ cm}^{-3}$, $N_{SS}=1.2 \times 10^{15} \text{ cm}^{-3}$;
- sample B – $N_D=5 \times 10^{15} \text{ cm}^{-3}$, $N_{SS}=6 \times 10^{15} \text{ cm}^{-3}$;
- sample C – $N_D=5 \times 10^{16} \text{ cm}^{-3}$, $N_{SS}=8 \times 10^{16} \text{ cm}^{-3}$;
- sample D – $N_D=5 \times 10^{17} \text{ cm}^{-3}$, $N_{SS}=1.8 \times 10^{17} \text{ cm}^{-3}$.

As it is seen, the theoretical curves C and D agree quite well with experimental data at high temperature and high defect concentration. Unfortunately, there are no experimental data in the literature for this type of samples at low defect concentrations.

The abovementioned method of calculation allows the temperature dependence of the electron's Hall factor for chlorine doped samples to be obtained (see Fig. 5). These dependences have minimums that correspond to the temperature at which the transition from the SS-scattering mechanism to the PO-scattering mechanism occurs. From Fig.5 it is seen that the higher the concentration of defects, the higher the transition temperature.

the merger of this defect level with the conduction band, an electroneutrality equation for the Fermi level can be written in the form:

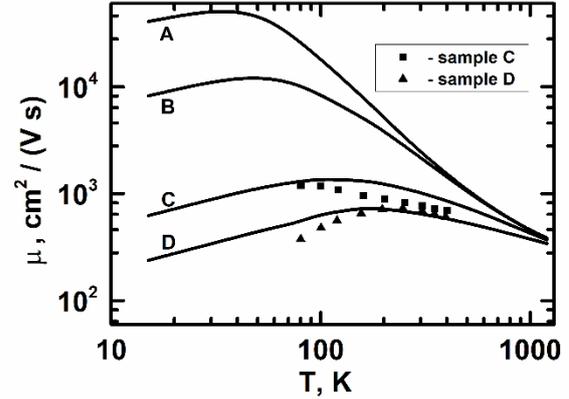


Fig.4. – The temperature dependences of electron mobility in chlorine-doped CdTe. Experimental data – [27].

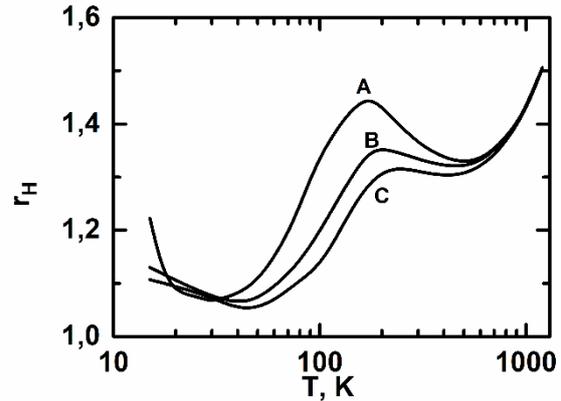


Fig.5. – The temperature dependence of electron's Hall factor in n-CdTe.

If to compare the theoretical curves obtained by the above method with the theoretical curves obtained in the relaxation time approximation (see Fig. 6a-d), one can see that the relaxation time approximation gives theoretical curves that are much less consistent with the experiment (curve 1 corresponds to low temperatures and curve 2 corresponds to high temperatures in the relaxation time approximation) especially in the region of high defects concentrations. This indicates that the method proposed in this article more adequately describes the defect structure of crystals and their kinetic properties.

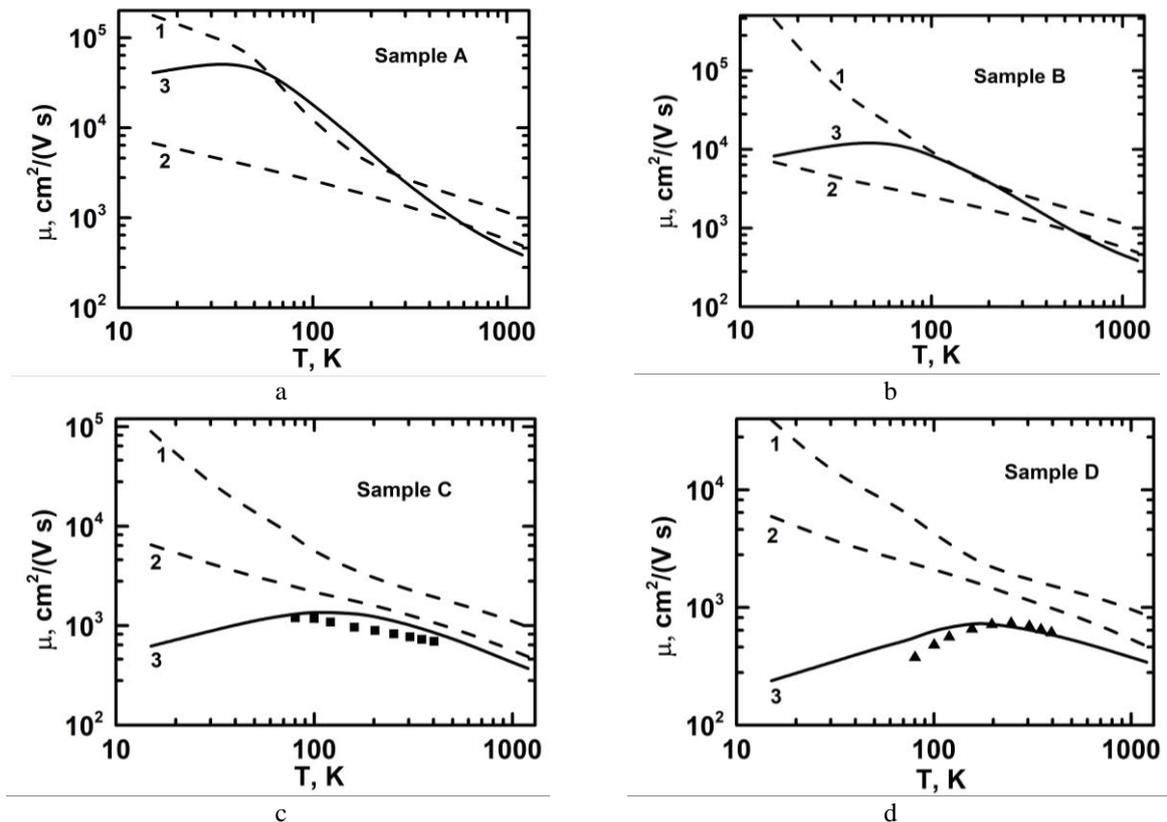


Fig. 6. – Comparing the theoretical curves obtained in the framework of long-range (curves 1 and 2) and short-range (curve 3) scattering models for chlorine doped samples.

Conclusion

The author considers a new scheme for calculating the energy spectrum, wave function and potential energy of an electron in a crystal at a given temperature. Based on this, the temperature dependences of the ionization energies of impurity (Cu and Cl) defects of different types, as well as

the temperature dependences of the kinetic coefficients are determined. It should be noted that the proposed calculation method can be applied to all impurity doped semiconductors with a sphalerite structure.

Malyk O.P. – Doctor of Physical and Mathematical Sciences, Professor, Professor.

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О.П. Малик

Явища переносу в CdTe:Cl і CdTe:Cu – розрахунок з перших принципів

Кафедра напівпровідникової електроніки, Національний університет «Львівська політехніка», Львів, Україна;
omalyk@ukr.net

У представленій статті розглянуто метод визначення енергетичного спектра, хвильової функції носія заряду та кристалічного потенціалу в CdTe при довільно заданій температурі. За допомогою цього підходу в рамках методу суперкомірки розраховано температурні залежності енергій іонізації різних типів дефектів, спричинених введенням домішок хлору та міді в телурид кадмію. Також запропонований метод дозволяє визначити температурну залежність оптичного та акустичного потенціалів деформації, а також залежність від температури параметрів розсіяння носія заряду на іонізованих домішках, полярних оптичних, п'єзооптичних та п'єзоакустичних фонах. У рамках близькодючих моделей розсіяння розглянуто температурні залежності рухливості носія заряду та фактора Холла.

Ключові слова: явища переносу, кристалічні дефекти, CdTe, розрахунок з перших принципів.