TRANSPORT PHENOMENA IN COPPER DOPED CADMIUM TELLURIDE: CALCULATION FROM THE FIRST PRINCIPLES

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Abstract: In the presented work, the method of determining the energy spectrum, the wave function of the heavy hole 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 copper impurity in cadmium telluride are calculated. Also the proposed method makes it possible to define the temperature dependence of the optical and acoustic deformation potentials, as well as the temperature dependence of the scattering parameters of heavy holes on ionized impurities, polar optical, piezooptical and piezoacoustic phonons. Within the framework of short-range scattering models, the temperature dependences of the heavy hole mobility and Hall factor are considered.

Key words: transport phenomena, CdTe, acceptor defects, ab initio calculation.

1. 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 a 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 wave function and potential energy in a crystal lattice. The above characteristics are usually assumed to 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 heavy hole 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 copper impurities into cadmium telluride are determined by the supercell method. These ionization energies and charge carrier scattering parameters being known, it is possible to calculate the Fermi level and, in turn, the kinetic coefficients of CdTe. It should be noticed that in the literature there are a number of works on the transport phenomena in semiconductors, in particular in CdTe [8], which are based on ab initio calculations [9-13]. However, these studies do not indicate the connection between the defect structure and kinetic properties.

2. Calculation of temperature dependences of wave function, crystal potential and effective mass of heavy holes

When considering the transport phenomena in p-CdTe, the heavy hole short-range scattering models were used [8,14,15]. To calculate the heavy hole transition probability, it is necessary to determine some scattering constants the finding of which, in turn, requires the determination of the valence band wave function and the crystal potential. Using pre-selected exchange-correlation GGA potentials of Cd and Te (pseudopotentials) and choosing a certain mixture of these usual exchange-correlation GGA potentials and the Hartree-Fock exchange potential (this mixture is determined by the "exchmix" parameter of ABINIT code) one can obtain a set the totality of mathematical solutions of the Schrödinger equation corresponding to the value of the parameter "exchmix" in the range limits from 0 to 1.

To check the accuracy and convergence of calculations, certain values of the parameters "pawecutdg" and "ecut" were selected. The parameter "ecut" strongly affects the quality of calculations: the greater "ecut", the better convergence of calculations. The parameter "pawecutdg" specifies the energy cut-off for the fine FFT grid, usually the parameter "pawecutdg" is chosen

greater than the parameter "ecut". All calculations were performed at the following values of the parameters: "ecut"=48 Ha, "pawecutdg"= 64 Ha. An additional study showed that increasing the value of these parameters causes a change in the position of the energy levels of the electron spectrum by $1,2 \times 10^{-5}$ eV, which is much less than the accuracy of the experiment.

Based on the proposed method, the selection of physical solutions of the Schrödinger equation from the totality of mathematical solutions of the Schrödinger equation was carried out. We formulate the criterion for choosing the physical solutions of the Schrödinger equation as follows: at a given temperature, the experimental value of the width of the band gap, which was determined from the experimental expression for solid solution $Hg_{1-x}Cd_xTe$ [16]:

$$E_g(x,T) = -0,302 + 1,93x - 0,81x^2 + \\ + 0,82x^2 + 5,35 \times 10^{-4}T(1-2x)$$ (1)

must coincide with its theoretical value.

Using this approach, for cadmium telluride (ideal sphalerite unit cell) the theoretical value of the band gap was fitted to the experimental value for temperatures T = 0 K (exchmix=0,397) and T = 300 K (exchmix=0,288). Accordingly, the valence band wave function and the crystal potential at temperatures of 0 K and 300 K were obtained. Based on the short-range scattering models [8,14,15] , as well as using the obtained wave functions and crystal potentials, the following scattering constants can be calculated at 0 K and 300 K, namely:

1. Scattering constants for heavy hole-polar optical (PO) phonon interaction, heavy hole-piezoacoustic (PAC) phonon and heavy hole-piezooptic (POP) phonon interaction

$$A_{PO} = A_{PAC} = A_{POP} = \int \psi^* \left(R^2 - r^2/3\right)\psi \, dr; \\ R = \sqrt{3}\,a_0/2,$$ (2)

(a_0 – lattice constant). The integration is carried out in a volume equal to 1/8 of the unit cell volume, and which contains two atoms of different sort.

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

$$d_{0v} = a_0\int \psi^* \mathbf{e}_v \times \nabla\psi \, dr, \quad v=1,2,3,$$ (3)

where the region of integration is the same as in the case of PO scattering; $\mathbf{e}_v$ – a 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 [15,17].

3) E_{AC} is the acoustic deformation potential constant which was equal to the maximum value among three acoustic deformation potential constants corresponding to one longitudinal and two transverse branches of the lattice acoustic vibrations [8]:

$$E_{AC\parallel} = -\left(\frac{I_1}{4} + \frac{I_2}{2} + \frac{I_3}{2}\right);$$

$$E_{AC1\wedge} = -\left(\frac{I_1}{2} - \frac{I_2}{4} + \frac{I_3}{2}\right),$$ (4)

$$E_{AC2\wedge} = -\left(\frac{I_1}{2} + \frac{I_2}{2} - \frac{I_3}{4}\right)$$

where

$$I_1 = \int \psi^* V_1\psi \, dr, \quad I_2 = \int \psi^* V_2\psi \, dr, \quad I_3 = \int \psi^* V_3\psi \, dr,$$

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 and the region of integration is the same as in the case of PO scattering.

4) The ionized impurity scattering constant

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

where integration is carried out throughout the sphalerite elementary cell.

Formulas (2) - (5) show that the abovementioned 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 [18,8]. 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:

$$A_{PO} = A_{PAC} = A_{POP} = \\ = \left(12,2 + 1,84 \times 10^{-3}T\right) \times 10^{-20};$$ (6a)

$$d_0 = -43,1 - 0,018T \ eV;$$ (6b)

$$E_{AC} = -3,07 - 2,28 \times 10^{-3}T \ eV;$$ (6c)

$$A_{II} = \left(0,442 - 8,90 \times 10^{-6}T\right) \times 10^{10} m^{-1}.$$ (6d)

Expressions (6a)-(6d) allow us to calculate the temperature dependences of the heavy hole transition probabilities and, in turn, the kinetic coefficients of p-type cadmium telluride.

To calculate the heavy hole effective mass, an ab initio calculation of the dependence of the charge carrier energy on the wave vector near the point G was preformed. In this case the vicinity of G point was a cube, the ribs of which were parallel to the Cartesian coordinate axes and for which the magnitude of the wave vector varied from -0.02 to 0.02 (reduced coordinates in p/a_0 units). Each rib of the cube was divided into eight intervals. Based on the obtained dependence $E(k)$ and using three-dimensional B-spline interpolation, the tensor of the inverse effective mass was calculated. This tensor was reduced to the principal axes (for cadmium telluride, one of these axes coincides with the [100] direction). As a result, we obtain the value of the components of the effective mass of heavy holes (at $T=0$ K): $m_1 = m_2 = 0,516 m_0; m_3 = 0,037 m_0$. It should be noted that in the literature there are various numerical values of this parameter [19-22]: $m_h = 0,4 m_0$ [19]; $m_h = 0,41 m_0$ [20]; $m_h = 0,63 m_0$ [21]; $m_h = 0,60 m_0$ [22]. The work [22] deserves special attention where measurements were made for the direction [100]. It can be seen that the obtained experimental value of the effective mass of heavy holes is quite close to the calculated one. Such calculation was performed for temperatures of 0 K and 300 K. This allowed us to determine the temperature dependence of the effective mass of the heavy hole:

$$m_h = \left(0,214 + 9,902 \times 10^{-5} T\right) m_0. \qquad (7)$$

It should be noted 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 [23].

3. Determination of temperature dependences of acceptor ionization energy of different types of crystal defects

In the proposed study, 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 defect structure of cadmium telluride was carried out within the framework the supercell method on the basis of the ABINIT code: for Cu_{Cd} – supercell Cd_7Te_8Cu ($1'1'2$ sphalerite cubic structure); for $V_{Te} - Cu_{Cd}$ – supercell Cd_7Te_7Cu ($1'1'2$ sphalerite cubic structure); $Cu_{Cd} - Te_{Cd}$ – supercell $Cd_{14}Te_{17}Cu$ ($2'1'2$ sphalerite cubic structure); $Cu_{Cd} - V_{Cd}$ – supercell $Cd_{14}Te_{16}Cu$ ($2'1'2$ sphalerite cubic structure). Analogous calculations were performed for the ideal supercell Cd_8Te_8 ($1'1'2$ sphalerite cubic structure) and $Cd_{16}Te_{16}$ ($2'1'2$ sphalerite cubic structure). The calculated energy spectra of the above-indicated supercells are presented in Table I.

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		
Energy levels of ideal Cd_8Te_8, eV	Energy levels of defect, eV	Acceptor 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 ³ 0 ΔE_A = 1.405
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 ³ 0 ΔE_A = 1.476
T=300 K, E_g=1.48 eV, exchmix=0.0182		
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)	ΔE_A = 1.238
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)	ΔE_A = 1.370
2´1´2 sphalerite cubic structure		
T=0, E_g=1.65 eV, exchmix=0.076		
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 ³ 0 ΔE_A =0.489
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)	ΔE_A =0.599
T=300 K, E_g=1.48 eV, exchmix=0.00571		
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)	ΔE_A =0.323
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)	ΔE_A =0.447

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

Consider as an example the calculation of the ionization energy of the $Cu_{Cd} - V_{Cd}$ defect. As can be seen at T = 0 K, the electrons of the valence band from the level 2´ (2.478) (2) will pass to the lower level 1´ (2.360) (1) of copper atom (thus forming a hole in the valence band), i.e. there is a complete ionization of the acceptor impurity. Therefore, at T = 0, cadmium telluride will have a p-type conductivity. As the temperature increases, the electron of the valence band will pass to the unfilled level 1´ (2.967) (0) of the copper atom, forming a hole in the valence band.

Other electron transitions (for example transition from defect level 1´ (2.360) (2) to conduction band

level $1'$ (4.130) (0)) are unlikely due to high ionization energy. A similar situation occurs at 300 K. The valence band electron fills the defect level $1'$ (2.323) (1), forming a hole in the valence band. Henceforward the transition of the electron from the valence band to the defect level $1'$ (2.881) (0) becomes the most probable. Based on the assumption that the temperature dependence of the ionization energy of the defect is linear, this dependence can be obtained.

A similar approach can be applied to other types of acceptor defects. As a result of calculations one can obtain the following temperature dependences of ionization energies:

$$Cu_{Cd}: \quad DE_A = 1,405 - 5,567 \times 10^{-4}T, \quad (8a)$$

$$V_{Te} - Cu_{Cd}: DE_A = 1,476 - 3,533 \times 10^{-4}T, \quad (8b)$$

$$Cu_{Cd} - Te_{Cd}: DE_A = 0,599 - 5,067 \times 10^{-4}T, (8c)$$

$$Cu_{Cd} - V_{Cd}: DE_A = 0,489 - 5,533 \times 10^{-4}T. \quad (8d)$$

4. Dicussion

Comparison of theoretical temperature dependences of heavy holes mobility was made with experimental data presented in [21]. It is known that defects with minimal ionization energy make the largest contribution to the transport phenomena in semiconductors. Accordingly, it follows from equations (8a) - (8d) that the defect that makes the largest contribution is $Cu_{Cd} - V_{Cd}$. From Table I it follows that this defect is ionized at T = 0 K, and further ionization occurs during the transition of the electron from the valence band to a higher energy level. Thus, the electroneutrality equation for the Fermi level takes the form:

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

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

To calculate the mobility of heavy holes the short-range scattering models were used on the base of the exact solution of the Boltzmann kinetic equation [24]. CdTe parameters used for calculation are presented elsewhere [8].

The temperature dependences of the heavy holes mobility in cadmium telluride crystals with a copper impurity concentration of $1'10^{14}$, $1'10^{18}$ 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 us to cover all possible values of the heavy holes mobility at low temperatures.

Comparison of theoretical curves with experimental data was performed only for the concentration of acceptor defects $1'10^{14}$ cm^{-3} (see Fig. 1a). It can be seen that the theoretical curve agrees quite well with the ex- perimental data. Unfortunately, experimental data for other values of acceptor concentrations are not available in the literature.
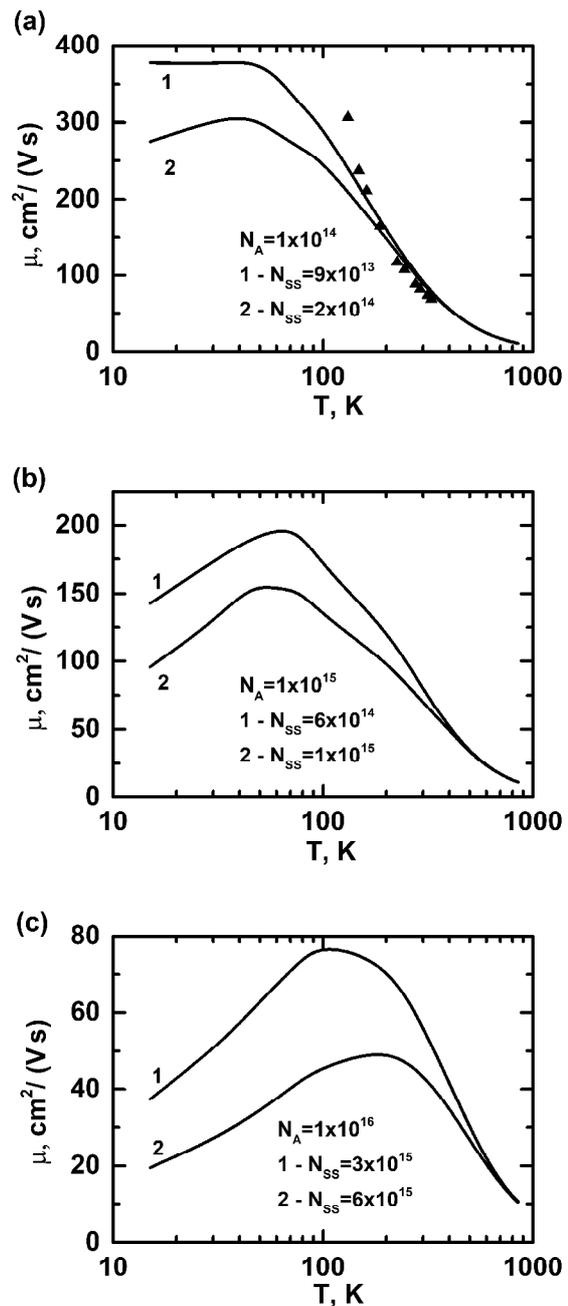

Fig. 1. The temperature dependences of heavy hole mobility in CdTe with different defect concentration
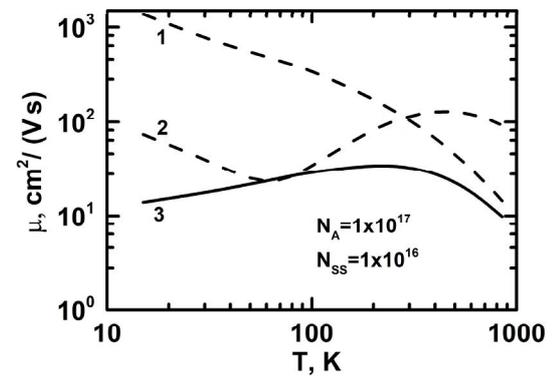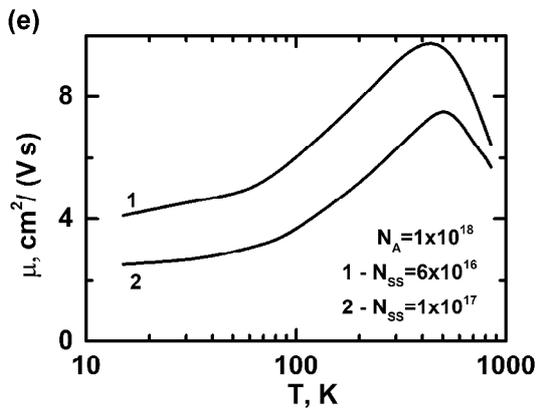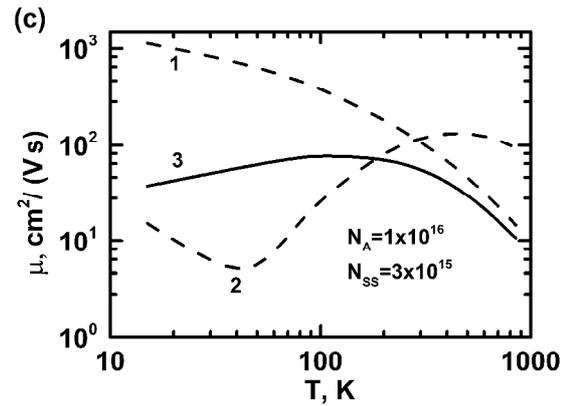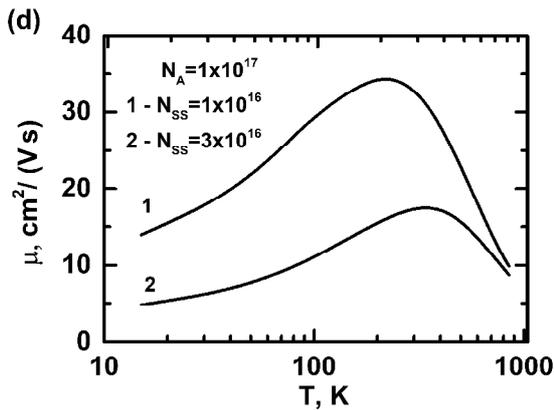
(d)

(e)

Fig. 2. The temperature dependences of heavy hole mobility in CdTe with different defect concentration (cont.)

(a)
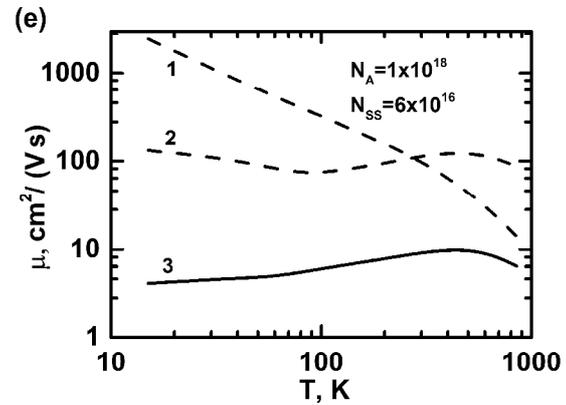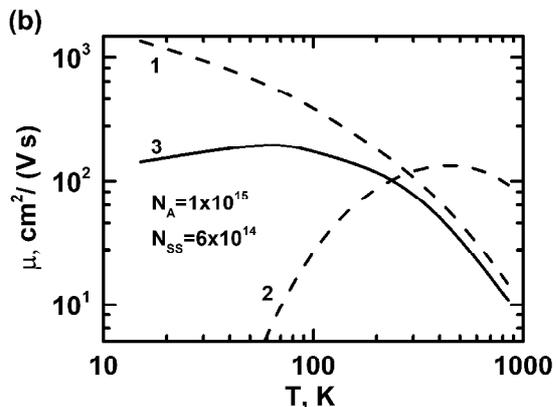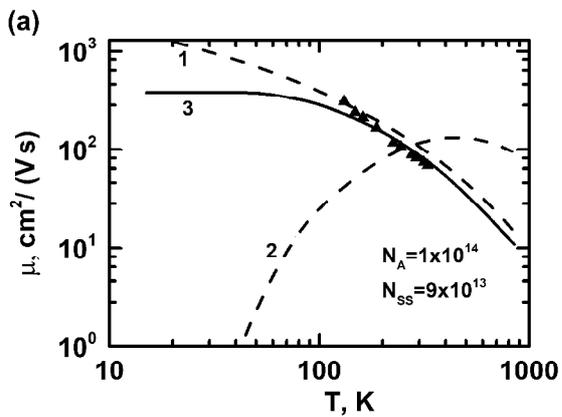

(b)

(c)

(e)

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

The theoretical curves obtained using two competing approaches were compared: short-range scattering models and long-range scattering models. The results of the calculation are presented in Fig. 2. Dashed lines 1 and 2 represent the results of the calculation of the dependence $\mu(T)$ obtained in the relaxation time approximation (see Appendix B in [8]) using long-range scattering models:curve 1 describes the high-temperature region ($\hbar w \ll k_B T$, w–optical oscillation frequency), curve 2 describes the low-temperature region $(\hbar w \gg k_B T)$.

Regarding curves 1 and 2, the following remark should be made. For CdTe, the Debye temperature is $q_D = 239$ K. Therefore, according to the above inequalities, the low-temperature region will be determined by the condition $T < 24$ K, and the high-temperature region will be determined by the condition $T > 2400$ K. As can be seen from Fig. 2a, the experimental points fall into the region where $T \sim q_D$, i.e., where the application of the relaxation time approximation (elastic scattering) is incorrect. On the other hand, short-range scattering models allow us 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 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 Hall factor on temperature are presented in Fig. 3. It is seen that these dependencies have minimums, which are located as follows - the higher the concentration of copper impurities, the higher the temperature of minimum.
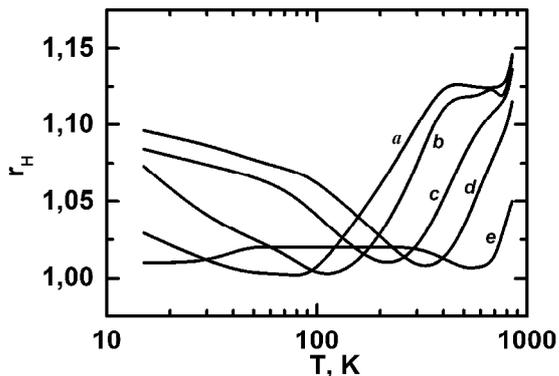

Fig. 4. Heavy hole Hall factor versus temperature in CdTe crystals with different defects concentration

4. Conclusions

A new method for calculating the energy spectrum and potential of a crystal at a beforehand predetermined temperature is proposed. Based on this, the temperature dependences of the ionization energies of defects of different types, as well as the temperature dependences of the kinetic coefficients are determined. Note that the abovementioned method can be used to study the transport phenomena in all semiconductors with the sphalerite structure.

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ЯВИЩА ПЕРЕНОСУ В ТЕЛУРИДІ КАДМІЮ ЛЕГОВАНОМУ МІДДЮ: РОЗРАХУНОК З ПЕРШИХ ПРИНЦИПІВ

Орест Малик, Ігор Петрович, Галина Кеньо

У представленій роботі розглянуто метод визначення енергетичного спектру, хвильової функції важкої дірки та кристалічного потенціалу в CdTe за довільно заданої температури. За допомогою цього підходу в рамках методу суперкомірки розраховано температурні залежності енергій іонізації різних типів дефектів, викликаних впровадженням домішки міді в телурид кадмію.

Також запропонований метод дозволяє визначити температурну залежність оптичного та акустичного потенціалів деформації, а також залежність від температури параметрів розсіювання важких дірок на іонізованих домішках, полярних оптичних, п'єзооптичних та п'єзоакустичних фононах. У рамках близькодіючих моделей розсіяння розглянуто температурні залежності рухливості важких дірок і коефіцієнта Холла.

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