

Electron Mobility in Cadmium Sulfide

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The processes of the electron scattering by the short-range potential caused by the interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain centers, ionized and neutral impurities in CdS crystals with impurity concentration of $\sim 5.6 \times 10^{16} - 8.7 \times 10^{17} \text{ cm}^{-3}$ are considered. The temperature dependences of the electron mobility and the Hall factor in the temperature range of 10-400 K are calculated.

Keywords: Transport phenomena, Charge carrier scattering, Cadmium sulfide.

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1. INTRODUCTION

Cadmium sulfide finds wide application in the production of thin-film solar energy converters [1, 2]. Further progress in the optimization of devices based on CdS requires more careful modeling of its physical parameters. The charge carrier mobility is one of the important parameters of this material. Experimental data on the study of the temperature dependence of the electron mobility in CdS are presented in [3]. As a rule, theoretical analysis of these dependences is performed in the relaxation time approximation or by the variational method. The use of the long-range models of carrier scattering for the description of the transport phenomena in this material is a common feature of all these methods. It was assumed in these models that the carrier interacts with the entire crystal (electron-phonon interaction) or the carrier interacts with the charged impurity potential, whose radius of action is $\sim 20-100a_0$ (a_0 is the lattice constant). However, such approximation contains the following contradictions: a) it contradicts the special relativity theory, according to which the carrier interacts only with the adjacent crystal regions; b) it contradicts the atomistic principle, according to which the carrier interacts (returns energy) only with one atom, not with many atoms simultaneously. Moreover, for defects with the interaction potential of $U \approx 1/r^n$ ($n = 1, 2$) at distances of $\sim 10a_0$ potential becomes the second-order infinitesimal, while the above mentioned models are considered in the first (Born) order of the perturbation theory. On the other hand, the authors of [4-7] have proposed the short-range

models of charge carrier scattering in the AIBVI and AIIIBV compounds with the structure of zinc blende and wurtzite, in which the above stated disadvantages were absent. At that, it was assumed that the carrier interacts with the defect potential only within a single unit cell. Along with this, the authors of [7] have taken into account the complex structure of optical vibrations of the crystal lattice when considering the electron scattering in the semiconductor with the wurtzite structure. The aim of the present work is the application of this approach for the description of the electron scattering by different types of defects of the crystal lattice in CdS.

2. THEORY

The wurtzite structure of the CdS crystal lattice contains 4 atoms in the unit cell that leads to the existence of 12 vibrational modes. According to the group theory, atomic vibrations of the unit cell can be represented as a sum of irreducible images [8]: $\Gamma = 2A_1 + 2B_1 + 2E_1 + 2E_2$. One A_1 mode and one couple of the E_1 mode represent the acoustic vibrational branches. Correspondingly, the sum $\Gamma_{opt} = A_1 + 2B_1 + E_1 + 2E_2$ represents the optical vibrational modes. Optical vibrations are classified by the shift of atoms along the c_0 -axis and direction perpendicular to the c_0 -axis. As a result we obtain: A_1 and E_1 modes represent the polar optical vibrations and $B_1^{(1)}$, $B_1^{(2)}$, $E_2^{(1)}$, $E_2^{(2)}$ modes are the nonpolar optical vibrations.

The probability of electron transition from \mathbf{k} state to \mathbf{k}' state, caused by the interaction with a polar optical phonon of the vibrational mode A_1 , has the view of [7]

$$W_{A_1}(\mathbf{k}, \mathbf{k}') = \frac{2\pi^7 \gamma_{PO}^{10} e^4}{675 \varepsilon_0^2 a_0^4 c_0^2 G} \frac{M_{Cd} + M_S}{M_{Cd} M_S} (3a_0^2 + c_0^2) \left\{ \frac{1}{\omega_{LO}} [N_{LO} \delta(\varepsilon' - \varepsilon - \hbar\omega_{LO}) + (N_{LO} + 1) \delta(\varepsilon' - \varepsilon + \hbar\omega_{LO})] + \frac{1}{\omega_{TO} c_0^2} [N_{TO} \delta(\varepsilon' - \varepsilon - \hbar\omega_{TO}) + (N_{TO} + 1) \delta(\varepsilon' - \varepsilon + \hbar\omega_{TO})] \right\}, \quad (1)$$

where ε_0 is the dielectric constant of vacuum; γ_{PO} is the adjustable parameter determining the radius of action of the short-range potential $R = \gamma_{PO} \frac{1}{2} \sqrt{3a_0^2 + c_0^2}$ ($0 < \gamma_{PO} \leq 1$; a_0, c_0 are the constants of the unit cell of the wurtzite structure);

G is the number of unit cells in the bulk crystal; M_{Cd} , M_S are the masses of atoms; N_q is the number of phonons with the corresponding frequency of the longitudinal ($\omega(\mathbf{q}) = \omega_{LO}$) and the transverse ($\omega(\mathbf{q}) = \omega_{TO}$) vibrations at $\mathbf{q} \rightarrow 0$.

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For the polar optical mode E_1 , the unit polarization vector (in the direction of vibrations of Cd atom) takes

$$W_{E_1}(\mathbf{k}, \mathbf{k}') = \frac{8\pi^7 \gamma_{PO}^{10} e^4}{675 \varepsilon_0^2 a_0^4 c_0^2 G} \frac{M_{Cd} + M_S}{M_{Cd} M_S} (3a_0^2 + c_0^2) \left\{ \frac{1}{\omega_{LO}} [N_{LO} \delta(\varepsilon' - \varepsilon - \hbar\omega_{LO}) + (N_{LO} + 1) \delta(\varepsilon' - \varepsilon + \hbar\omega_{LO})] + \frac{1}{\omega_{TO}} \frac{c_0^2}{a_0^2} [N_{TO} \delta(\varepsilon' - \varepsilon - \hbar\omega_{TO}) + (N_{TO} + 1) \delta(\varepsilon' - \varepsilon + \hbar\omega_{TO})] \right\}, \quad (2)$$

and for the second case

$$W_{E_{12}}(\mathbf{k}, \mathbf{k}') = \frac{4}{3} \frac{2\pi^7 \gamma_{PO}^{10} e^4}{675 \varepsilon_0^2 a_0^4 c_0^2 G} \frac{M_{Cd} + M_S}{M_{Cd} M_S} (3a_0^2 + c_0^2) \frac{1}{\omega_{TO}} \left(1 + \frac{c_0^2}{a_0^2} \right) \times [N_{TO} \delta(\varepsilon' - \varepsilon - \hbar\omega_{TO}) + (N_{TO} + 1) \delta(\varepsilon' - \varepsilon + \hbar\omega_{TO})]. \quad (3)$$

Then, the transition probability for the polar optical mode E_1 is determined from the expression

$$W_{E_1}(\mathbf{k}, \mathbf{k}') = W_{E_{11}}(\mathbf{k}, \mathbf{k}') + W_{E_{12}}(\mathbf{k}, \mathbf{k}'), \quad (4)$$

and the total transition probability at polar optical (PO) vibrations can be written as

$$W_{PO}(\mathbf{k}, \mathbf{k}') = W_{A_1}(\mathbf{k}, \mathbf{k}') + W_{E_{11}}(\mathbf{k}, \mathbf{k}') + W_{E_{12}}(\mathbf{k}, \mathbf{k}'). \quad (5)$$

$$W_{B_1^{(1)}}(\mathbf{k}, \mathbf{k}') = \frac{128\pi^3 A^2 d_0^2 e^4 a_0^4 c_0^2}{6MG\omega_{LO} (3a_0^2 + c_0^2)^4} [N_{LO} \delta(\varepsilon' - \varepsilon - \hbar\omega_{LO}) + (N_{LO} + 1) \delta(\varepsilon' - \varepsilon + \hbar\omega_{LO})], \quad (6)$$

where d_0 is the constant of the optical strain potential; $A = 1.137$; $M = 2M_{Cd} + 2M_S$ is the mass of the unit cell.

The longitudinal vibrations in the S sublattice are dominant for the nonpolar optical vibrational mode $B_1^{(2)}$. For this mode, the carrier transition probability $W_{B_1^{(2)}}(\mathbf{k}, \mathbf{k}')$ looks similar to the relation (6) with the corresponding values of ω_{LO} and $A = -6.299$.

For the nonpolar optical vibrational mode $E_2^{(1)}$, the following conditions are true:

$$q = q_z; \quad \mathbf{q}_x = q_y = 0 \quad \begin{cases} \xi_x = 1; \quad \xi_y = \xi_z = 0 - \text{TO mode}; \\ \xi_y = 1; \quad \xi_x = \xi_z = 0 - \text{TO mode}. \end{cases} \quad (7)$$

For these two TO-modes, the dominant vibrations are observed in the Cd sublattice. For this mode, the carrier transition probability $W_{E_2^{(1)}}(\mathbf{k}, \mathbf{k}')$ looks similar to (6) with the corresponding values of ω_{LO} and $A = -0.583$.

Vibrations of the $E_2^{(2)}$ mode satisfy the condition (7) with the difference that the dominant vibrations occur in the S sublattice. As in the previous case, the carrier transition probability $W_{E_2^{(2)}}(\mathbf{k}, \mathbf{k}')$ has the view of (6) with the corresponding values of ω_{LO} and $A = 3.41$.

The resulting carrier transition probability at scattering by nonpolar optical (NPO) phonons is determined from the expression

$$W_{NPO}(\mathbf{k}, \mathbf{k}') = W_{B_1^{(1)}}(\mathbf{k}, \mathbf{k}') + W_{B_1^{(2)}}(\mathbf{k}, \mathbf{k}') + W_{E_2^{(1)}}(\mathbf{k}, \mathbf{k}') + W_{E_2^{(2)}}(\mathbf{k}, \mathbf{k}'). \quad (8)$$

two values $\xi_1 = (1, 0, 0)$ and $\xi_1 = (0, 1, 0)$. For the first case, the transition probability has the view of [7]:

Condition $\mathbf{q} = (0, 0, q)$, $\xi = (0, 0, 1)$ holds for the nonpolar optical vibrational mode $B_1^{(1)}$. For this LO-mode, one sublattice (S) is at rest, while in another sublattice (Cd) the neighboring atoms move in the opposite directions. Then, the transition probability for this vibrational type is determined from the expression [7]

The carrier transition probability from \mathbf{k} state to \mathbf{k}' state, caused by the interaction with acoustic vibrations (AV) of the crystal lattice, is defined from relation [7]

$$W_{AV}(\mathbf{k}, \mathbf{k}') = \frac{8}{3} \cdot \frac{a_0^4 c_0^2}{(3a_0^2 + c_0^2)^3} \times \frac{\pi^3 E_{AC}^2 k_B T}{\hbar GM} \left(\frac{1}{c_{\parallel}} + \frac{2}{c_{\perp}} \right)^2 \cdot \delta(\varepsilon' - \varepsilon), \quad (9)$$

where the elastic behavior of the scattering process is taken into account; E_{AC} is the constant of the acoustic strain potential; c_{\parallel} and c_{\perp} are the longitudinal and the transverse velocities of sound, respectively.

When considering the interaction of an electron with piezoelectric vibrations, it is necessary to determine the components of the piezoelectric tensor \mathbf{e} and macroscopic strain tensor \mathbf{S} . For the wurtzite structure, the tensor \mathbf{e} components are the following:

$$\mathbf{e} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{13} & e_{13} & e_{33} & 0 & 0 & 0 \end{pmatrix}, \quad (10)$$

where the Voigt notations are used for the tensor components, in the coordinate notations these components are expressed as follows: $e_{13} = e_{133}$, $e_{33} = e_{333}$, $e_{15} = e_{113}$, and the rest $-e_{\alpha\beta\gamma} = 0$.

Components of the tensor \mathbf{S} are determined from the relation

$$S_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial Q_{\alpha}}{\partial x^{\beta}} + \frac{\partial Q_{\beta}}{\partial x^{\alpha}} \right), \quad (11)$$

where Q is the vector of displacement of atoms in the unit cell, which is a function of the discrete variables $Q = Q_i(n_1, n_2, n_3)$.

Using the technique for calculation of the derivatives $\frac{\partial Q_\alpha}{\partial x^\beta}$ described in [7], we will obtain the following expression:

$$B_{13} = \frac{1}{2} i \left[q_x \left(2\xi_{z,\nu} + \xi_{x,\nu} \frac{a_0}{c_0} \right) + q_z \left(2\xi_{z,\nu} \frac{c_0}{a_0} + \xi_{x,\nu} \right) \right]; \quad B_{33} = i \xi_{z,\nu} \left(q_x \frac{a_0}{c_0} + q_z \right). \quad (13)$$

Polarization of the crystal is determined from the expression $\mathbf{P} = \mathbf{e} \cdot \mathbf{S}$, correspondingly, we have

$$P_1 = e_{1ik} S_{ik} = e_{133} S_{33} + 2 e_{113} S_{13}; \quad P_2 = e_{2ik} S_{ik} = 0; \quad P_3 = e_{3ik} S_{ik} = e_{333} S_{33}, \quad (14)$$

i.e. it is necessary to know only two components of the macroscopic strain tensor (S_{13} and S_{33}).

Firstly, we consider propagation of the longitudinal

$$S_{\alpha\beta} = \sum_{\mathbf{q},\nu} \left[\frac{\hbar}{2MG\omega_\nu} \right]^{1/2} B_{\alpha\beta} \left[b_{\mathbf{q},\nu} e^{i\mathbf{q}\mathbf{a}} - b_{\mathbf{q},\nu}^* e^{-i\mathbf{q}\mathbf{a}} \right], \quad (12)$$

where $b_{\mathbf{q},\nu}$ and $b_{\mathbf{q},\nu}^*$ are the phonon annihilation and production operators, respectively; $B_{\alpha\beta}$ are some quantities, among which, as it will be shown below, B_{13} and B_{33} are essential ones.

acoustic wave along the c_0 crystal axis: $\mathbf{q} = (0, 0, q)$ and $\xi = (1, 0, 0)$. In this case, components of the tensor \mathbf{S} can be written as

$$\mathbf{S} = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & 0 & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}; \quad S_{13} = \sum_{\mathbf{q}} \left[\frac{\hbar}{2MG\omega_{|1}} \right]^{1/2} \left[b_{\mathbf{q}} e^{i\mathbf{q}\mathbf{a}} - b_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{a}} \right] i q \frac{c_0}{a_0};$$

$$S_{33} = \sum_{\mathbf{q}} \left[\frac{\hbar}{2MG\omega_{|1}} \right]^{1/2} \left[b_{\mathbf{q}} e^{i\mathbf{q}\mathbf{a}} - b_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{a}} \right] i q.$$

Using the calculation technique presented in [4], we obtain the expression for the carrier transition probabi-

lity in the case of propagation of the longitudinal acoustic wave along the c_0 crystal axis

$$W_{|1} \Pi_{\text{IAK}}(\mathbf{k}, \mathbf{k}') = \frac{e^2 \pi^7 \gamma_{PZ}^{10} (3a_0^2 + c_0^2) k_B T}{450 \varepsilon_0^2 \hbar c_{|1}^2 GM} E_{PZ|1}^2 \delta(\varepsilon' - \varepsilon), \quad (15)$$

where γ_{PZ} is the adjustable parameter which determines

the radius of action of the short-range potential.

$$R = \gamma_{PZ} \frac{1}{2} \sqrt{3 a_0^2 + c_0^2} \quad (0 < \gamma_{PO} \leq 1), \quad E_{PZ|1} = 2 \frac{c_0}{a_0} \left(e_{13} + 2e_{15} \frac{c_0}{a_0} \right) + e_{33}.$$

For propagation of the transverse acoustic wave along the c_0 crystal axis, we have two cases:

1)

$$\mathbf{q} = (0, 0, q); \quad \xi = (1, 0, 0); \quad \mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & 0 & 0 \\ S_{31} & 0 & 0 \end{pmatrix}; \quad S_{13} = \frac{1}{2} \sum_{\mathbf{q}} \left[\frac{\hbar}{2MG\omega_{|1}} \right]^{1/2} \left[b_{\mathbf{q}} e^{i\mathbf{q}\mathbf{a}} - b_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{a}} \right] i q;$$

$$S_{33} = 0; \quad P_1 = 2 e_{15} S_{13}; \quad P_2 = P_3 = 0;$$

$$\frac{\partial P_1}{\partial x} = 2e_{15} \frac{\partial S_{13}}{\partial x} = - \sum_{\mathbf{q}} \left[\frac{\hbar}{2MG\omega_{|1}} \right]^{1/2} \left[b_{\mathbf{q}} e^{i\mathbf{q}\mathbf{a}} + b_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{a}} \right] q^2 2e_{15} \frac{c_0}{a_0}.$$

2)

$$\mathbf{q} = (0, 0, q); \quad \xi = (0, 1, 0); \quad \mathbf{S} = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & S_{22} & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix}; \quad S_{13} = 0; \quad S_{33} = 0; \quad P_1 = P_2 = P_3 = 0.$$

Calculation of the electron transition probability is similar to the previous case and gives

$$W_{\perp \text{PAC}}(\mathbf{k}, \mathbf{k}') = \frac{e^2 \pi^7 \gamma_{PZ}^{10} (3 a_0^2 + c_0^2) k_B T}{450 \varepsilon_0^2 \hbar c_{\perp}^2 GM} E_{PZ\perp}^2 \delta(\varepsilon' - \varepsilon), \quad (16)$$

where $E_{PZ\perp} = 2e_{15}(c_0/a_0)$.

Let us consider propagation of the longitudinal optical wave along the c_0 crystal axis: $\mathbf{q} = (0, 0, q)$, $\xi = (1, 0, 0)$.

A_1 vibrations of the PO mode and $B_1^{(1)}$, $B_1^{(2)}$ NPO modes satisfy these conditions. As a result, one can obtain the carrier transition probabilities when interacting with these vibrational branches

$$A_1 \text{ mode: } W_{|POP}(\mathbf{k}, \mathbf{k}') = \frac{32}{75^2} \frac{e^2 \pi^9 \gamma_{PZ}^{10} E_{PZ\perp}^2}{\varepsilon_0^2 G \omega_{LO}} \frac{M_{Zn} + M_O}{M_{Zn} M_O} [N_{LO} \delta(\varepsilon' - \varepsilon - \hbar \omega_{LO}) + (N_{LO} + 1) \delta(\varepsilon' - \varepsilon + \hbar \omega_{LO})]; \quad (17)$$

$$B_1^{(1)} \text{ and } B_1^{(2)} \text{ modes: } W_{|POP}(\mathbf{k}, \mathbf{k}') = \frac{64}{75^2} \frac{e^2 \pi^9 \gamma_{PZ}^{10} E_{PZ\perp}^2 A^2}{\varepsilon_0^2 G M \omega_{LO}} [N_{LO} \delta(\varepsilon' - \varepsilon - \hbar \omega_{LO}) + (N_{LO} + 1) \delta(\varepsilon' - \varepsilon + \hbar \omega_{LO})]. \quad (18)$$

Propagation of the transverse optical wave along the c_0 crystal axis is similar to the previous case. Here, E_1 vibrations of the PO mode and $E_2^{(1)}, E_2^{(2)}$ vibrations of the

NPO mode give the corresponding contribution. And the corresponding expressions for the carrier transition probability can be written as follows:

$$E_1 \text{ mode: } W_{\perp POP}(\mathbf{k}, \mathbf{k}') = \frac{32}{75^2} \frac{e^2 \pi^9 \gamma_{PZ}^{10} E_{PZ\perp}^2}{\varepsilon_0^2 G \omega_{TO}} \frac{M_{Zn} + M_O}{M_{Zn} M_O} [N_{TO} \delta(\varepsilon' - \varepsilon - \hbar \omega_{TO}) + (N_{TO} + 1) \delta(\varepsilon' - \varepsilon + \hbar \omega_{TO})]; \quad (19)$$

$$E_1^{(1)} \text{ and } E_1^{(2)} \text{ modes: } W_{\perp POP}(\mathbf{k}, \mathbf{k}') = \frac{64}{75^2} \frac{e^2 \pi^9 \gamma_{PZ}^{10} E_{PZ\perp}^2 A^2}{\varepsilon_0^2 G M \omega_{TO}} [N_{TO} \delta(\varepsilon' - \varepsilon - \hbar \omega_{TO}) + (N_{TO} + 1) \delta(\varepsilon' - \varepsilon + \hbar \omega_{TO})]. \quad (20)$$

According to the short-range scattering models in semiconductors with the wurtzite structure, the carrier transition probabilities from \mathbf{k} state to \mathbf{k}' state, caused by the interaction with the static strain (SS) potential, ionized (II) and neutral (NI) impurity, have view of [7]

$$W_{SS}(\mathbf{k}, \mathbf{k}') = \frac{2^5 3^4 \pi^3 R_1^6 C^2 e^2 E_{PZ}^2 N_{SS}}{V \varepsilon_0^2 \hbar} \frac{1}{q^2} \delta(\varepsilon' - \varepsilon); \quad (21)$$

$$W_{II}(\mathbf{k}, \mathbf{k}') = \frac{\pi e^4 Z_i^2 R_1^4 N_{II} \gamma_{II}^4}{2 \varepsilon_0^2 \hbar V} \delta(\varepsilon' - \varepsilon); \quad (22)$$

$$W_{NI}(\mathbf{k}, \mathbf{k}') = \frac{\gamma_{II} R_1}{2} \frac{20 \pi^2 N_{NI} \hbar^3}{V m^{*2} k'} \delta(\varepsilon' - \varepsilon), \quad (23)$$

where N_{SS} , N_{II} , N_{NI} are the concentrations of the static strain centers, ionized and neutral impurities, respectively; Z_i is the degree of ionization of defects; m^* is the effective carrier mass; $q = |\mathbf{k}' - \mathbf{k}|$; $C \approx 0.1$; γ_{II} is the adjustable parameter determining the radius of action of the short-range potential of the ionized impurity

$R_1 = \frac{1}{2} \sqrt{3 a_0^2 + c_0^2}$, $0 < \gamma_{II} \leq 1$; E_{PZ} is the piezoelectric constant, which has the form of $E_{PZ\parallel}$ and $E_{PZ\perp}$. We note that it was assumed in (23) that the radius of action of the short-range potential of the neutral impurity is equal to a half of the radius of action of the short-range potential of the ionized impurity (multiplier $\gamma_{II} R_1/2$).

3. COMPARISON OF THE THEORY AND THE EXPERIMENT

Calculation of the conductivity tensor components is performed based on the exact solution formalism of the stationary Boltzmann equation [9]. Using this formalism, we obtain an additional adjustable parameter $\gamma_{SS} N_{SS}$ (it was assumed that $\gamma_{SS} = 1$) for the SS-scattering mechanism. The material parameters used for the calculation are presented in Table 1.

Comparison of the theoretical temperature dependences of the electron mobility was carried out with the experimental data shown in the work [3] for three samples (samples 2, 9, 10) of cadmium sulfide. Fermi level was determined from the equation of electroneutrality for the wide-band-gap semiconductor with n -type conductivity (intrinsic conductivity was neglected) with donors and compensated acceptors

$$n + N_A = \frac{N_D}{1 + 2 \exp\left(\frac{F - E_D}{k_B T}\right)}, \quad (24)$$

where N_D , N_A , E_D are the concentrations of donors and acceptors and donor ionization energy, respectively, whose values were chosen according to the results of [3].

Theoretical curves $\mu(T)$ for CdS are shown in Fig. 1. The solid lines represent the curves calculated based on the short-range models in the context of the exact solution of the Boltzmann equation. In Table 2 we present the obtained values of the scattering parameter γ for different scattering mechanisms. The dashed lines denote the curves calculated based on the long-range scattering models in the relaxation time approximation. We note that the same scattering mechanisms of charge carriers were used when calculating these curves. As seen, in the whole considered temperature range the short-range scattering models give a good enough agreement between the theory and the experiment, while the relaxation time approximation gives both the qualitative (samples 2 and 10) and the quantitative 2-5-fold deviation of the theory from the experiment. This indicates that the short-range models describe more adequately the electron scattering processes in cadmium sulfide compared with the relaxation time approximation.

In order to estimate the roles of different scattering mechanisms, in Fig. 2 we illustrate the corresponding dependences by the dashed lines. It is seen that at low temperatures ($T < 150$ K), the electron scattering by the static strain potential (curve 7) is the main scattering mechanism. At higher temperatures ($T > 150$ K), the scattering by polar optical (curve 5) and piezo-optical (curve 6) phonons becomes the dominant one. Other scattering mechanisms, such as scattering by nonpolar optical phonons, scattering by acoustic and piezo-acoustic phonons, neutral and ionized impurities, give a negligible contribution.

The temperature dependence of the Hall factor of electrons, shown in Fig. 3, was calculated based on the obtained scattering parameters. As seen, the minima on these curves correspond to the transition from one scattering mechanism at low temperatures (SS-scattering) to another mechanism at higher temperatures (PO and POP-scattering). This transition is observed under the following condition: the higher temperature, the larger concentration of the static strain centers.

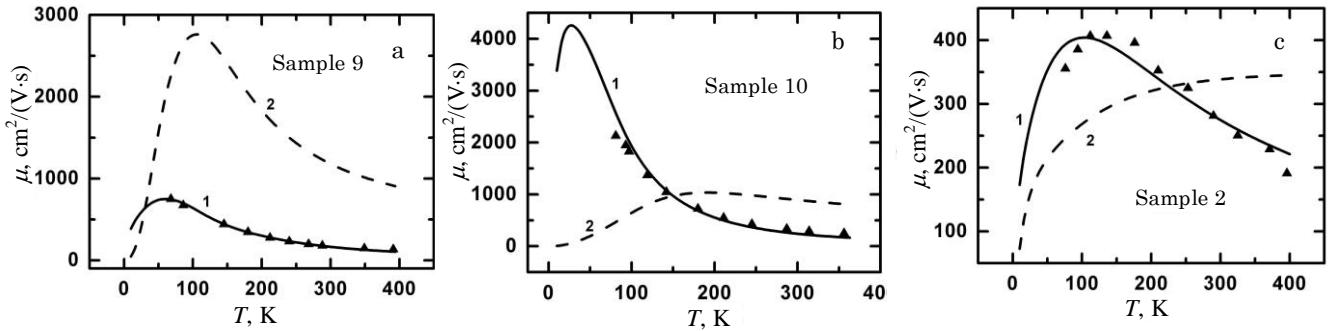
Table 1 – CdS parameters used in the calculation

Semiconductor parameter	Value
Lattice constant, a_0 (m)	4.1365×10^{-10} a
c_0 (m)	6.716×10^{-10} a
Band gap, E_g (eV)	$2.579-4.7 \times 10^{-4} T^2/(T+230)$ b
Density, ρ_0 (kg/m ³)	4.82×10^3 c,d
Velocity of sound, (m/s)	
v_{\perp}	1.76×10^3 e
v_{\parallel}	4.25×10^3 e
Optical strain potential, d_0 (eV)	6.9 f
Acoustic strain potential, E_{AC} (eV)	3.3 g
Energy equivalent of the matrix element, E_P (eVB)	21 h
Spin-orbit splitting, Δ (eV)	0.062 i
Frequency of optical vibrations (rad/s):	
vibrations along the c_0 axis	
A_1 (LO), ω_{LO}	5.71×10^{13} j
A_1 (TO), ω_{TO}	4.37×10^{13} j
$B_1^{(1)}$ (LO), ω_{LO}	2.46×10^{13} j
$B_1^{(2)}$ (LO), ω_{LO}	5.51×10^{13} j
Vibrations perpendicular to the c_0 axis	
E_1 (LO), ω_{LO}	5.77×10^{13} j
E_1 (TO), ω_{TO}	4.56×10^{13} j
$E_2^{(1)}$ (TO), ω_{TO}	7.33×10^{12} j
$E_2^{(2)}$ (TO), ω_{LO}	4.77×10^{13} j
piezoelectric tensor components, (C/m ²)	
e_{13}	-0.262 k
e_{33}	0.385 k
e_{15}	-0.183 k

a – [10]; b – [11]; c – [12]; d – [13]; e – [14]; f – [15]; g – [16]; h – [17]; i – [18]; j – [19]; k – [20];

Table 2 – Parameters γ for different scattering mechanisms

Sample	γ PO	γ PZ	γ II	γ SS, $\times 10^{-14}$ cm ⁻³
2	0.58	0.50	1.0	27.0
9	0.72	0.52	1.0	12.0
10	0.70	0.53	1.0	1.3

**Fig. 1** – Temperature dependences of the electron mobility in CdS with different impurity concentrations. 1 – the short-range scattering models; 2 – the long-range scattering models (relaxation time approximation)

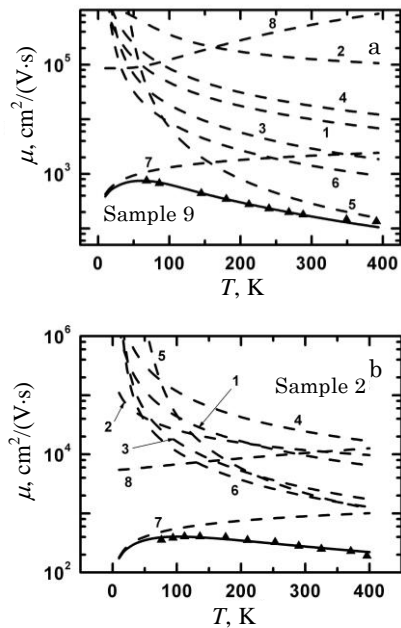


Fig. 2 – Contribution of different scattering mechanisms to the electron mobility in CdS. Solid curve – mixed scattering mechanism, 1, 2, 3, 4, 5, 6, 7, 8 – AC, II, NPO, PAC, PO, POP, SS, NI scattering mechanisms, respectively

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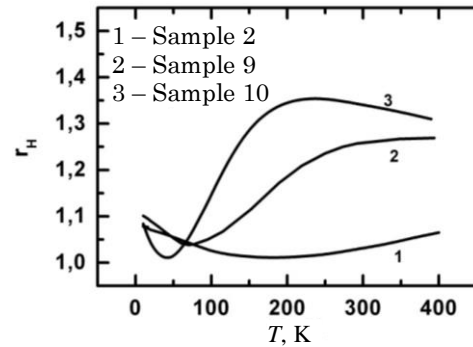


Fig. 3 – Temperature dependence of the Hall factor of electrons in CdS

4. CONCLUSIONS

The processes of electron scattering by different types of lattice defects in cadmium sulfide crystals are considered based on the short-range principle. A sufficiently good agreement between the theory and the experimental data in the studied temperature range is established. It is shown that the short-range models describe more adequately the electron scattering processes in cadmium sulfide compared with the long-range models.

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