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Electron mobility in $Cd_xHg_{1-x}Se$

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Abstract. Electron scattering on the short-range potential caused by interaction with polar and nonpolar optical phonons, piezoelectric and acoustic phonons, static strain, ionized impurities in $Cd_xHg_{1-x}Se$ ($0 \le x \le 0.547$) samples annealled in selenium vapour or in dynamic vacuum are considered. Within the framework of the precise solution of the stationary Boltzmann equation on the base of short-range principle, temperature dependences of the electron mobility within the range 4.2 – 300 K are calculated. A good coordination of the theory to experiment in the investigated temperature range is established.

Keywords: cadmium-mercury-selenium solid solution, charge carrier scattering.

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1. Introduction

The electron scattering in the solid solution $Cd_xHg_{1-x}Se$ was considered in [1-4] in relaxation time approximation. The models of electron scattering by lattice defects used in these works have an essential shortcoming – they are long-range. In these models, it is supposed that either charge carrier interacts with all the crystal (electron-phonon interaction) or it interacts with the defect potential of the impurity, the action radius of which is approximately equal to $50–100a_0$ (a_0 – lattice parameter). However, such an assumption contradicts the special relativity according to which the charge carrier should interact only with the neighbouring crystal region. Besides, for defects with the interaction energy $U \approx \frac{1}{r^n}(n=1,2)$, at the distances $\sim 10a_0$ the potential takes the magnitude of the second order, while all the theories mentioned above are considered in the first (Born) approximation. On the other hand, in [5] the short-range models of electron scattering in $Cd_xHg_{1-x}Te$ were proposed, in which the above mentioned shortcomings were absent. There, it has been supposed that the carrier interacts with the defect potential only within the limits of one elementary cell. The purpose of this work is to use this approach for description of the electron scattering processes by various types of crystal defects in CdHgSe solid solution.

2. Theory

The electron transition probability from a state k to a state k' caused by the interaction with polar optical (PO), nonpolar optical (NPO), piezooptic (POP) and piezoacoustic (PAC), acoustic (AC) phonons, ionized impurity (II) was chosen from [5]:

$$W_{\mathrm{PO}}(\mathbf{k},\mathbf{k}') = \frac{64\,\pi^7 \gamma_{\mathrm{PO}}^{10}\, e^4}{225\,\varepsilon_0{}^2 a_0{}^4 G}\ \frac{M_x + M_{\mathrm{Te}}}{M_x\, M_{\mathrm{Te}}} \times$$
$$\times \left\{ \frac{1}{\omega_{\mathrm{LO}}} \left[N_{\mathrm{LO}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega_{\mathrm{LO}}) + \right.\right.$$
$$\left.\left. + (N_{\mathrm{LO}} + 1)\, \delta(\varepsilon' - \varepsilon + \hbar\omega_{\mathrm{LO}}) \right] + \frac{2}{\omega_{\mathrm{TO}}} \times \right.$$
$$\left. \times \left[N_{\mathrm{TO}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega_{\mathrm{TO}}) + (N_{\mathrm{TO}} + 1)\, \delta(\varepsilon' - \varepsilon + \hbar\omega_{\mathrm{TO}}) \right] \right\}, \quad (1)$$

$$W_{\mathrm{NPO}}(\mathbf{k},\mathbf{k}') = \frac{\pi^3 E_{\mathrm{NPO}}{}^2}{288\, a_0{}^2 G}\ \frac{M_x + M_{\mathrm{Te}}}{M_x\, M_{\mathrm{Te}}} \times$$
$$\times \left\{ \frac{1}{\omega_{\mathrm{LO}}} \left[N_{\mathrm{LO}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega_{\mathrm{LO}}) + (N_{\mathrm{LO}} + 1) \times \right.\right. \quad (2)$$
$$\left.\left. \times\, \delta(\varepsilon' - \varepsilon + \hbar\omega_{\mathrm{LO}}) \right] + \frac{2}{\omega_{\mathrm{TO}}} \left[N_{\mathrm{TO}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega_{\mathrm{TO}}) + \right.\right.$$
$$\left.\left. + (N_{\mathrm{TO}} + 1)\, \delta(\varepsilon' - \varepsilon + \hbar\omega_{\mathrm{TO}}) \right] \right\},$$

$$W_{\mathrm{POP}}(\mathbf{k},\mathbf{k}') = \left(\frac{32}{75}\right)^2 \frac{\pi^9 e^2 e_{14}^2\, \gamma_{\mathrm{PZ}}^{10}}{\varepsilon_0{}^2 G} \frac{M_x + M_{\mathrm{Te}}}{M_{\mathrm{x}}\, M_{\mathrm{Te}}} \times$$
$$\times \left\{ \frac{1}{\omega_{\mathrm{LO}}} \left[N_{\mathrm{LO}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega_{\mathrm{LO}}) + \right.\right.$$
$$\left. + (N_{\mathrm{LO}} + 1)\, \delta(\varepsilon' - \varepsilon + \hbar\omega_{\mathrm{LO}}) \right] + \frac{2}{\omega_{\mathrm{TO}}} \times$$
$$\left. \times \left[N_{\mathrm{TO}}\, \delta(\varepsilon' - \varepsilon - \hbar\omega_{\mathrm{TO}}) + (N_{\mathrm{TO}} + 1)\, \delta(\varepsilon' - \varepsilon + \hbar\omega_{\mathrm{TO}}) \right] \right\}, \tag{3}$$

$$W_{\mathrm{PAC}}(\mathbf{k},\mathbf{k}') = \frac{128\,\pi^7\, e^2\, e_{14}^2\, a_0^2\, \gamma_{\mathrm{PZ}}^{10}\, k_{\mathrm{B}} T}{225\,\varepsilon_0^2\, \hbar\, G \left[x\, M_{\mathrm{Cd}} + (1-x) M_{\mathrm{Hg}} + M_{\mathrm{Te}} \right]} \times$$
$$\times \left(\frac{1}{c_{\mathrm{LO}}} + \frac{2}{c_{\mathrm{TO}}} \right)^2 \delta(\varepsilon' - \varepsilon), \tag{4}$$

$$W_{\mathrm{AC}}(\mathbf{k},\mathbf{k}') = \frac{\pi^3 k_{\mathrm{B}} T\; E_{\mathrm{AC}}^2}{144\,\hbar\, G \left[M_x + M_{\mathrm{Te}} \right]} \times$$
$$\times \left(\frac{1}{c_{\mathrm{LO}}} + \frac{2}{c_{\mathrm{TO}}} \right)^2 \delta(\varepsilon' - \varepsilon), \tag{5}$$

$$W_{\mathrm{II}}(\mathbf{k},\mathbf{k}') = \frac{\pi\, e^4 Z_i^2\; N_{\mathrm{II}}\, \gamma_{\mathrm{II}}^4\, a_0^4}{2\,\varepsilon_0^2\, \hbar\, V} \delta(\varepsilon' - \varepsilon), \tag{6}$$

where $M_x = x M_{\mathrm{Cd}} + (1-x) M_{\mathrm{Hg}}$, M_{Hg}, M_{Cd}, M_{Se} are atom masses; G – number of unit cells in the crystal bulk; N_{LO}, N_{TO} – number of longitudinal (LO) and transverse (TO) phonons with frequencies ω_{LO} and ω_{TO}, respectively; e_{14} – non-vanishing component of the piezoelectric tensor; c_{LO}, c_{TO} – respective sound velocities; V – crystal volume; N_{II} – concentration of ionized impurities; Z_i – the impurity charge in electron-charge units; E_{AC}, E_{NPO} – acoustic and optical deformation potentials (E_{AC} = 2.04 eV, E_{NPO} = 29.8 eV), respectively; γ_{PO}, γ_{PZ}, γ_{II} – adjustable parameters determining the action radius of the short-range potential ($R = \gamma\, a_0$, $0 \le \gamma_{\mathrm{PO}}, \gamma_{\mathrm{PZ}} \le 0.86$, $0 \le \gamma_{\mathrm{II}} \le 1$); ε_0 – dielectric constant; e – elementary charge; k_{B} – Boltzmann constant; $\hbar$ – Planck constant; $\delta(\varepsilon)$ – Dirac delta-function; ε – carrier energy.

It should be noted that the strong power dependence of parameters γ_{PO}, γ_{PZ}, γ_{II} sharply limits opportunities to choose their numerical values.

To describe the electron-disorder (DIS) scattering, the respective transition probability defined in [6] was used.

Besides, the above mentioned scattering mechanisms of the so-called static strain (SS) scattering on the short-range potential was considered. According to Fedders [7], the potential caused by the strain field takes the following form:

$$U(\mathbf{r}) = \frac{9\, b_0{}^3 e\, e_{14}}{\varepsilon_0} \frac{1}{r^2}, \tag{7}$$

where b_0 has the length units and is related to the size of defect.

In (7) we neglected the angular dependence of $U(\mathbf{r})$. Following the short-range principle, we put $b_0 = a_0$. To calculate the transition matrix element, we shall use the electron plain wave function normalized over the crystal volume:

$$\left\langle \mathbf{k}' \middle| U(\mathbf{r}) \middle| \mathbf{k} \right\rangle = \frac{9 a_0{}^3 e\, e_{14}}{V \varepsilon_0} \frac{4\pi}{q} Si(qR), \tag{8}$$

where $q = \left| \mathbf{k}' - \mathbf{k} \right|$, $Si(x)$ is the sine integral.

Our calculations show that the electron wave vector (and q together with it) varies within the limits from 0 up to 10^9 m^{-1} when the energy changes from 0 up to 10 $k_{\mathrm{B}}T$ within the temperature range 4.2-300 K. For $R \sim 10^{-10}$ m, this gives the estimation of $Si(x) = C \approx 0.1$. Then the transition probability looks like:

$$W_{\mathrm{SS}}(\mathbf{k},\mathbf{k}') = \frac{2^5 3^4 \pi^3 C^2 a_0{}^6 e^2\; e_{14}{}^2 N_{\mathrm{SS}}}{V \varepsilon_0{}^2 \hbar} \frac{1}{q^2} \delta(\varepsilon' - \varepsilon), \tag{9}$$

where N_{SS} is the concentration of strain centers.

Using the formalism of a precise solution for the stationary Boltzmann equation [8], one can obtain the logarithmic divergence of the integral over angular variable θ. To eliminate this divergence, let's specialize the lower limit of the integral in a manner providing coordination of the theory and experiment for using this integral as an adjustable parameter:

$$\gamma_{\mathrm{SS}} = \int_{\theta_0}^{\pi} \frac{\sin\theta}{1 - \cos\theta} d\theta, \tag{10}$$

where θ_0 is the angle that corresponds to an adjustable parameter γ_{SS}.

Let's note that the similar way to choose the lower limit of the integral is used in the Conwell-Weisskopf method [9], when considering the electron-ionized impurity scattering. However, the values received using this method are too large (for the impurity concentration ~10^{15} cm^{-3} the action radius of the potential is approximately 160a_0).

After that, the values $K_{\beta\alpha}^{nm}$ from a precise solution of the stationary Boltzmann equation for this scattering mechanism can be now obtained:

$$K_{\beta\alpha}^{nm} = \frac{2V}{(2\pi)^3} \frac{2^3 3^3 \pi^2 a_0{}^6 C^2 \hbar\, e^2 e_{14}^2 N_{\mathrm{SS}}\, \gamma_{\mathrm{SS}}}{\varepsilon_0^2\, k_{\mathrm{B}} T} \times$$
$$\times \delta_{\alpha\beta} \left(\frac{2 m_{hh}}{\hbar^2} \right)^3 \int f_{0p}(\varepsilon) \left[1 - f_{0p}(\varepsilon) \right] \left(-\varepsilon - \varepsilon_g \right) \varepsilon^{n+m} d\varepsilon, \tag{11}$$

where $f_{0p}(\varepsilon)$ is the Fermi-Dirac function for electrons; $\delta_{\alpha\beta}$ – Kronecker delta symbol and zero of the energy is at the bottom of the conduction band.

It should be noted that in (11) the product $N_{\mathrm{SS}}\gamma_{\mathrm{SS}}$ is used as an adjustable parameter.

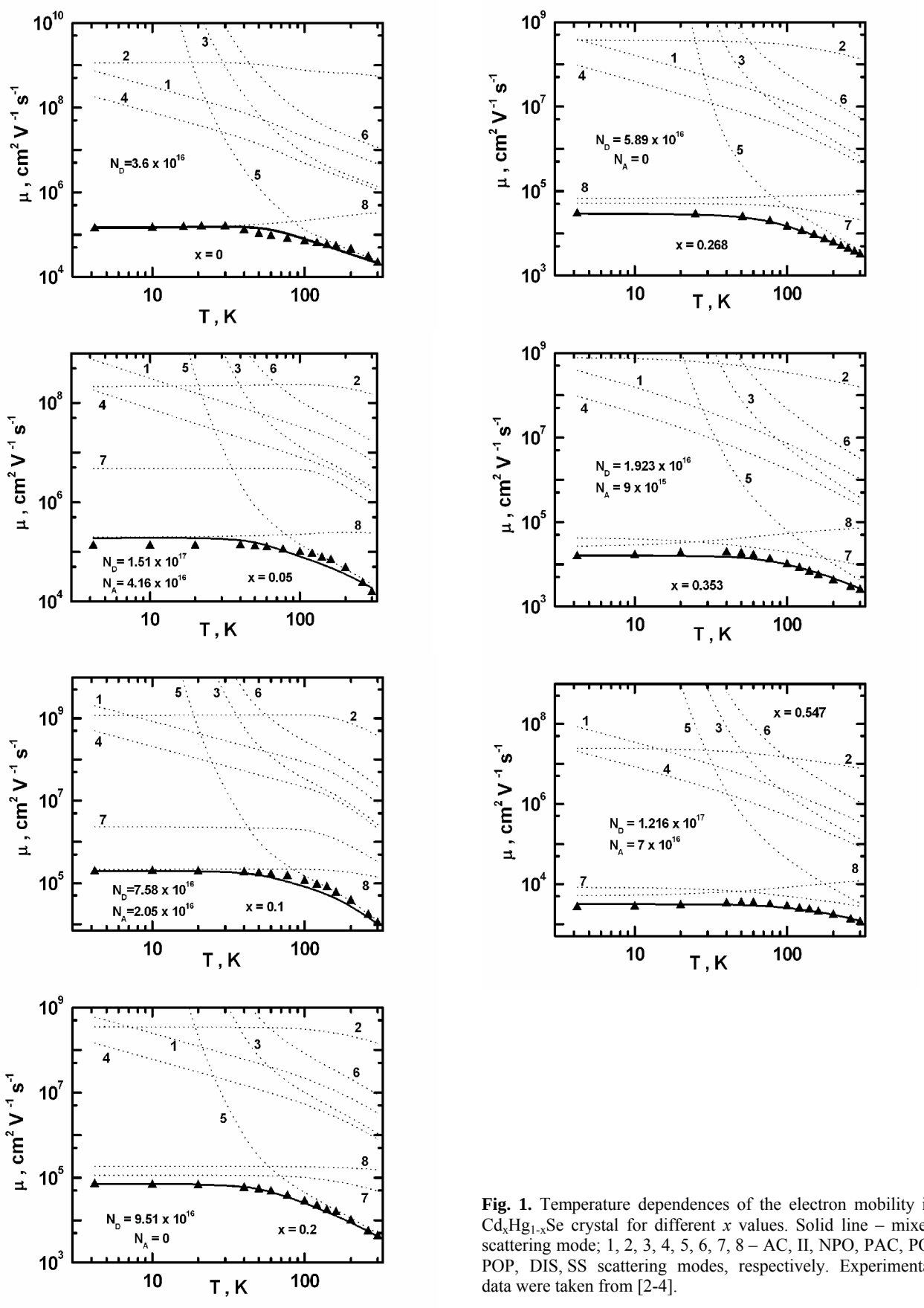

Fig. 1. Temperature dependences of the electron mobility in $Cd_xHg_{1-x}Se$ crystal for different x values. Solid line – mixed scattering mode; 1, 2, 3, 4, 5, 6, 7, 8 – AC, II, NPO, PAC, PO, POP, DIS, SS scattering modes, respectively. Experimental data were taken from [2-4].

3. Comparison of the theory and experiment

The theoretical temperature dependences of the electron mobility $\mu(T)$ were compared to the experimental data presented in [2-4] for $Cd_xHg_{1-x}Se$ crystals with compositions $x = 0$; 0.05 (sample A1); 0.1 (sample B1); 0.2 (sample C1); 0.268 (sample 26BB2); 0.353 (sample 24AA1-1); 0.547 (sample 40EB2). All the samples were obtained by the annealing in selenium vapour or in dynamic vacuum. The Fermi level was obtained from the electroneutrality equation:

$$n - p = N_D - N_A \ , \qquad (12)$$

where N_A, N_D are the ionized acceptor and donor concentrations taken from [2-4].

The material parameters used for calculation were the same as in [2, 3, 10]. The theoretical $\mu(T)$ curves are presented in Figs 1a-g. The solid lines represent the curves calculated on the basis of the short-range models within the framework of the precise solution of the Boltzmann equation. The obtained scattering parameters for different scattering modes are listed in Table. It is seen that the theoretical curves well agree with experimental data in all the investigated temperature range. To estimate the role of different scattering mechanisms in Figs. 1a-1g, the dotted lines represent the appropriate dependences. It is seen that at low temperatures ($T < 60$ K) the main scattering mechanism is static strain scattering and disorder scattering (for $x > 0$). At high temperatures, the contribution of the polar optical phonon scattering becomes dominant. Other scattering mechanisms, such as acoustic and piezoacoustic scattering, piezooptic and nonpolar optical phonon one, ionized impurity one, give negligibly small contributions.

Table.

x	γ_{PO}	γ_{PZ}	γ_{II}	$N_{SS}\gamma_{SS}\times10^{-14}$ cm^{-3}
0	0.61	0.32	0.26	1.9
0.05	0.64	0.32	0.26	2.8
0.10	0.7	0.32	0.26	4.5
0.2	0.70	0.32	0.26	2.2
0.268	0.68	0.32	0.26	2.9
0.353	0.64	0.32	0.26	2.3
0.547	0.59	0.32	0.26	7.5

4. Conclusion

On the base of the short-range principle, the electron scattering processes with participation of various lattice defects in the solid solution $Cd_xHg_{1-x}Se$ were considered. A good agreement between the theory and experimental data within the investigated temperature range was established.

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