THE INFLUENCE OF POINT DEFECTS ON THE LOW TEMPERATURE ELECTRON MOBILITY IN $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) SMALL-GAP SEMICONDUCTING ALLOYS. II

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(Received June 10, 1980)

Experimental and theoretical analysis of electron mobility in $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) semiconducting alloys at 4.2K has been done. The applied theory included all the scattering mechanisms which dominate at the low temperatures, i.e. scattering by charged and neutral centers as well as disorder scattering. The analysis has taken into account the model of native point defects structure of $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) given previously in Part I. It has pointed out the significant role of the native defects (both ionized and neutral) in carrier scattering processes in the crystals studied.

PACS numbers: 61.70.−r

1. *Introduction*

Point defects, i.e. native defects as well as foreign impurities, constitute scattering centers both ionized and neutral ones for electrons (current carriers) in a crystal. Their influence on electron mobility (and other kinetic coefficients) could be easily verified at the low temperatures where phonon scattering mechanisms can be neglected. In the previous papers [2, 3] concerning the analysis of the low temperature electron mobility in $Cd_xHg_{1-x}Se$ ($x \leqslant 0.25$) mixed crystals only charged centers scattering [2] or charged centers together with disorder scattering [3] were considered. However, no discussion concerning the origin of these charged centers was inserted there. Recent studies of a heat treatment and electrical properties of undoped $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) crystals [1] (I in our notation) gave some insight into the structure of native point defects in these small-gap semiconducting alloys.

The purpose of this work is to determine the influence of point defects (both ionized and neutral) on the low temperature electron mobility in undoped $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) on a base of the simplified model of the native point defects structure put forward in I.

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A brief theoretical description of the main scattering mechanisms is made in § 2. The material parameters and the calculation procedure is outlined in § 3. § 4 is devoted to the analysis of electron mobility; § 5 contains final conclusions.

2. The mechanisms of electron scattering at low temperatures

The analysis of electron mobility in $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) at 4.2 K has been performed taking into account the scattering on charged and neutral centers as well as disorder scattering which occurs in mixed crystals. The mobility calculations have been done in the strong degeneracy approximation due to the relatively high (and almost temperature independent) electron concentration and high value of the Fermi energy ($\varepsilon_F \gg k_0 T$; ε_F calculated from the bottom of the conduction band — see [4, 5] at 4.2 K in the crystals studied.

2.1. Scattering by charged centers

This mechanism is usually considered as elastic scattering of electrons on the screened Coulomb-type potentials of the ionized point defects (native defects and impurities).

In the case of zero- and small-gap semiconductors the electron mobility calculated for this scattering mode in high degeneracy limit is given by the formula [6, 7]:

$$\mu_{cc} = \frac{\hbar^3}{2\pi e^3} \frac{\kappa_s^2}{N_I} \frac{k_F^3}{m_F^{*2}} \frac{1}{F_{cc}}, \tag{1}$$

where N_I is the concentration of ionized centers, donors and acceptors ($N_I = N_D + N_A$), whereas κ_s is the static dielectric function for $q = 0$. m_F^* is the electron effective mass at the Fermi level. The function F_{cc}, in which a proper symmetry of the electron wave functions and screening of the Coulomb potential by free carriers is taken into account, has a standard form [7, 8].

2.2. Disorder scattering

Disorder (alloy) scattering of the conduction electrons occurs in the mixed crystals due to random distribution of the constituent atoms in the lattice sites (the so-called chemical disorder).

According to Kossut [3, 9], in the case of zero- and small-gap semiconductors electron mobility limited by disorder scattering is given by the formula (high degeneracy approximation):

$$\mu_d = \pi e \hbar^3 \frac{1}{Nx(1-x)V^2} \frac{1}{k_F m_F^{*2}} \frac{1}{F_d}. \tag{2}$$

Here, N is the number of all sites in cation (Cd, Hg) sublattice per unit volume. For $Cd_xHg_{1-x}Se$, where the spin-orbit splitting parameter does not change with composition ($\Delta(x) = \text{const.}$) [4], the function F_d can be written in a form [9] (see also [3]):

$$F_d = a^4 - \tfrac{2}{3} a^2(b^2+c^2)y + \tfrac{1}{3}\left[(b^2+c^2)^2 + 2b^2\left(\frac{b}{2} - \sqrt{2}\,c\right)^2\right] y^2. \tag{3}$$

The coefficients a, b and c have been determined in [8]. $y = W/V$, where V, W are the matrix elements defined as:

$$V = \langle S|U_{\mathrm{Hg,Cd}}|S\rangle, \qquad W = \langle X|U_{\mathrm{Hg,Cd}}|X\rangle. \tag{4}$$

Here $U_{\mathrm{Hg,Cd}} = U_{\mathrm{Hg}} - U_{\mathrm{Cd}}$, where U_{Hg}, U_{Cd} denote the potentials introduced by Hg and Cd atomic cores. S, X, Y, Z are the Kohn-Luttinger amplitudes.

It is worth emphasizing that formula (2) has been derived assuming that $U_{\mathrm{Hg,Cd}} \ll U_{\mathrm{Hg}}$, U_{Cd} and that $U_{\mathrm{Hg,Cd}}$ is a short range potential limited to a unit cell [9]. In our case this condition can be regarded as fulfilled due to the electron affinity of Cd and Hg.

The parameter y partially illustrates the range and shape of the scattering potential. E.g. $y = 0$ corresponds to the Dirac delta type potential centered in every lattice site whereas $y = 1$ corresponds to the potential having the nonvanishing constant value within a unit cell.

2.3. Scattering by neutral centers

As it has been proved in I, in $\mathrm{Cd}_x\mathrm{Hg}_{1-x}\mathrm{Se}$ ($x \leqslant 0.2$) alloys both neutral native defects as well as some trace impurities can form neutral scattering centers for conducting electrons. Such neutral center is assumed to have the potential $U_s(\bar{r})$ of the range limited to a unit cell.

Litwin-Staszewska and Szymańska [10] gave the formula of electron mobility for neutral centers scattering in the high degeneracy limit:

$$\mu_s = \pi e \hbar^3 \frac{1}{N_s A^2} \frac{1}{k_F m_F^{*2}} \frac{1}{F_s}. \tag{5}$$

N_s is the concentration of neutral scattering centers, whereas A is the matrix element defined by $A = \langle S|U_s|S\rangle$. The function F_s [10] contains one more matrix element $B = \langle X|U_s|X\rangle$. The form of F_s becomes identical with that of F_d (Eq. (3)) when substituting the elements V, W by A and B, respectively.

There are two unknown parameters in (5): $N_s A^2$ and $y' = B/A$. From the physical point of view we have three parameters: N_s, A, y'. Only N_s could be estimated from experiment. The estimation of A and B remains very difficult because we do not know a real shape of $U_s(\bar{r})$ which depends on the atomic potential of particular defect or impurity.

3. *Material parameters and calculation procedure*

Electron mobility has been calculated in the high degeneracy approximation taking into account the contributions of all the scattering mechanisms mentioned in § 2:

$$\mu_{\mathrm{tot}} = \left(\frac{1}{\mu_{\mathrm{cc}}} + \frac{1}{\mu_{\mathrm{d}}} + \frac{1}{\mu_{\mathrm{s}}}\right)^{-1}. \tag{6}$$

The calculations took into account the finite value of spin-orbit splitting (Δ) and the influence of higher bands on the density of states [3] (see also [4]). The dependence of energy gap on composition in $Cd_xHg_{1-x}Se$ for 4.2 K has been assumed according to [5, 11, 12] in the form:

$$E_0(x) = -0.274+2.174\,x \text{ [eV]}. \tag{7}$$

The values of remaining band structure parameters used in the calculations are the same as in HgSe:

$$P = 7.2\times10^{-8}\text{ eVcm [13, 4]};\quad \Delta = 0.45\text{ eV [4, 13]};$$

$$A' = -1.0,\quad M = -3.5,\quad L' = -2.0,\quad L'-M-N' = 4.0,\ [14]$$

and their independence of composition has been assumed.

The q-independent part of the static dielectric function, κ_s, (see Eq. (1)) has been calculated following the procedure given in [4, 5] and using the same values of dielectric constants κ_L and κ_∞.

Electron mobility for disorder scattering mode has been calculated taking the modified values of matrix elements V, W [5, 15] ($V/\Omega_0 = 1.77$ eV, $y = -0.22$) which correspond to the $E_0(x)$ dependence given by Eq. (7).

4. *The influence of point defects on the electron mobility at low temperatures*

Experimental and theoretical analysis of the electron mobility in $Cd_xHg_{1-x}Se$ at 4.2 K as a function of electron concentration has been performed. It concerns mainly the crystals of the composition $x = 0.1$ for which the most complete information from the heat treat-

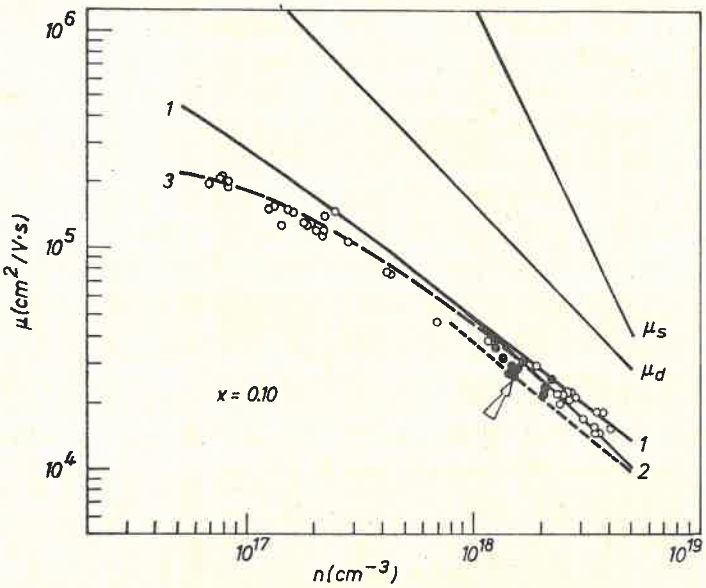

Fig. 1. Experimental and theoretical electron mobility vs concentration in $Cd_{0.1}Hg_{0.9}Se$ semiconducting alloys at 4.2 K. Further explanation in the text

ment and X-ray investigations has been gathered (see I). Additionally, the results of similar analysis for $Cd_{0.2}Hg_{0.8}Se$ will be presented.

Fig. 1 gives experimental values of electron mobility vs concentration for $Cd_{0.1}Hg_{0.9}Se$ at 4.2 K. Points corresponding to the as-grown crystals have been denoted by full circles. Curve *1–1* is the total mobility, μ_{tot} calculated with the assumption $n_{4.2\,K} = N_D$ (N_D — concentration of singly ionized donors). This approximation does not take into account additional scattering centers, namely ionized acceptors and neutral defects (native defects, impurities). Here $\mu_{tot} = (1/\mu_{cc}+1/\mu_d)^{-1}$. The contribution μ_d has been also plotted in the figure.

It can be seen that the theory (curve *1–1*) describes well the experimental $\mu(n)$ dependence only for the purest samples for particular values of n.

First of all it is worth discussing what the origin of the ionized donor centers is. It has been deduced in I, that ionized interstitial Hg atoms form the dominant donor centers in $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$), i.e. at the low temperature $N_D \simeq [Hg_i]$. There can also appear some minority donor centers due to existence of certain trace impurities and other point defects (see I). However their concentration does not change within the applied heat treatment processes (I) which determine electron concentration at 4.2 K.

It is seen from Fig. 1 that the major part of the points corresponding to electron mobility of the crystals studied lies below the theoretical values. These discrepancies reach even 100% for the samples of the low concentration ($n \gtrsim 10^{17}$ cm^{-3}). Then it becomes necessary to consider a real structure of the crystal by including to this analysis the additional scattering centers, both neutral and ionized.

4.1. Neutral centers

The discrepancy between theoretical (curve *1–1*) and experimental mobility can be observed for the high concentration samples, i.e. for $n \gtrsim 10^{18}$ cm^{-3} (Fig. 1). It concerns mainly the as-grown crystals. Usually one considers two competitive factors which can give a decrease of electron mobility: the compensation (here — by ionized acceptors) and/or neutral scattering centers (see e.g. [16]). It has been shown in I that the second factor is a dominating one in $Cd_{0.1}Hg_{0.9}Se$ with $n > 10^{18}$ cm^{-3} due to the existence of the neutral Hg microprecipitations.

The electron mobility for neutral centers scattering has been calculated from Eq. (5). For neutral Hg microprecipitations we assume $A/\Omega_0 = 10$ eV. This choice is not quite accidental because for such a neutral center (Hg_I) the matrix element A is practically of the form $A = \langle S|U_{Hg}|S\rangle$. On the other hand (see § 3) the best fit value of disorder scattering parameter V is $V/\Omega_0 = (1/\Omega_0)\times\langle S|U_{Hg}-U_{Cd}|S\rangle = 1.77$ eV. It should be reminded here that formula (2) is valid and can be applied under condition $U_{Hg}-U_{Cd} \ll U_{Hg}$. In other words it means that $A \gg V$.

We should emphasize here that in this formalism the neutral Hg microprecipitations are treated as quasi-point defects with their dimensions limited to the unit cell. Hence, $y' = 1$ has been assumed. The concentration of neutral centers, N_s, usually depends on n and can be estimated from the experiment.

In the first step the mobility calculations have been performed for N_s independent of n. Lower dashed line in Fig. 1 represents the total electron mobility after introducing the contribution of neutral center scattering, μ_s (N_s = const.), to the former calculations (curve *1–1*). Theoretical mobility has been fitted to the experimental point, showed by an arrow, using N_s as fitting parameter. The best fit has been obtained for $N_s = 6\times10^{19}$ cm^{-3}. The experimental point mentioned above corresponds to the mobility for the as-grown crystal with $n = 1.5\times10^{18}$ cm^{-3}. Its lattice constant ($a_0 = 6.0900$ Å) has been marked in Fig. 5 of the paper I.

In I, the concentration of the neutral interstitial Hg atoms in this crystal has been estimated as $[\mathrm{Hg_I}] \simeq 1.3\times10^{20}$ cm^{-3}. Hence the value of N_s obtained from above discussed fitting seems quite reasonable. It results from the fact that within the previously assumed model of the native point defects structure of $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) (see I) the following relation should take place: $N_s \leqslant \frac{1}{2}[\mathrm{Hg_I}]$.

The $\mu_{tot}(n, N_s)$ calculated for $N_s = 6\times10^{19}$ cm^{-3} can be treated as the estimated limit of the lowest values of electron mobility in this concentration range, i.e. $n \geqslant 10^{18}$ cm^{-3}. It is seen from Fig. 1 that these low mobility values are reached primarily by the as-grown crystals.

It has been pointed out in I that the neutral Hg microprecipitations can be also created in Hg-saturated samples due to the quenching process and passive annealing of a crystal.

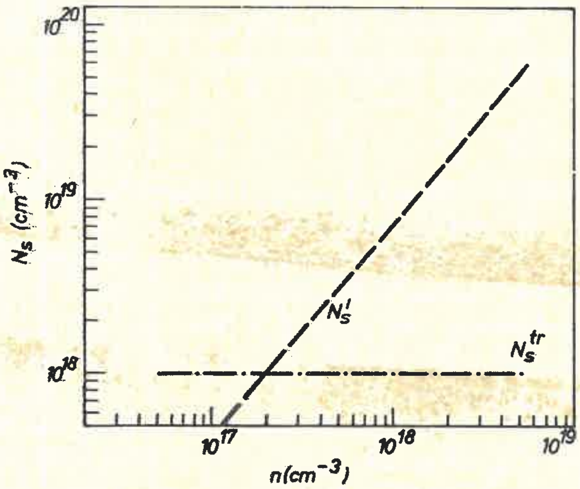

Fig. 2. Hypothetical dependence of neutral scattering centers concentration on n in $Cd_{0.1}Hg_{0.9}Se$ semiconducting alloys. N_s' and N_s^{tr} denote the concentration of neutral centers connected with native point defects ($\mathrm{Hg_I}$) and with trace impurities, respectively

The magnitude of $[\mathrm{Hg_I}]$ depends on n (see I). Hence, the effective concentration of additional scattering centers connected with these defects should also depend on n. Fig. 2 presents the hypothetical $N_s'(n)$ dependence for $Cd_{0.1}Hg_{0.9}Se$. For $N_s'(n)$ the linear dependence (in logarythmic scale) between the points $N_s'(n = 5\times10^{18}\ \mathrm{cm^{-3}}) = 5\times10^{19}$ cm^{-3} and $N_s'(n = 2\times10^{17}\ \mathrm{cm^{-3}}) = 10^{18}$ cm^{-3} has been assumed. Here, the results of estimations made in I within the assumed model of native point defects structure in $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) have been taken into account. The electron mobility μ_s for scattering on neutral centers calculated with the above $N_s'(n)$ dependence has been also plotted in Fig. 1.

Certain trace impurities can also be the origin of neutral scattering centers in $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) — see I. Their impurity level was below 10^{18} cm^{-3}, in a very rough estimation [5]. In the mobility calculations the upper limit of the trace impurity concentration, $N_s^{tr} = 10^{18}$ cm^{-3}, was taken independently of the electron concentration (Fig. 2). For these centers the values of matrix elements $A/\Omega_0 = 10$ eV and $y' = 0$ were assumed irrespective of the type of impurity. The calculations of total electron mobility in which the contribution $\mu_s(N_s^{tr} = 10^{18}$ cm$^{-3})$ has been taken into account indicate that its influence on the values of μ_{tot} is negligible. For the highest electron concentration considered here, $n = 5\times10^{18}$ cm^{-3}, it lowers μ_{tot} by about 1%.

Curve *1–2* in Fig. 1 represents the total mobility calculated including the contributions of both types of neutral scattering centers, i.e. $\mu_s(N_s'(n))$ and $\mu_s(N_s^{tr})$. It can be seen that within experimental error the points corresponding to the annealed samples of the concentration $n \gtrsim 10^{18}$ cm^{-3} lie between the lines *1–1* and *1–2*.

For comparison, Fig. 3 shows the experimental and theoretical electron mobility vs concentration in $Cd_{0.2}Hg_{0.8}Se$ at 4.2K. Here, μ_{tot} represents the total theoretical mobility including the contributions from scattering by charged centers (μ_{cc}) and disorder scattering

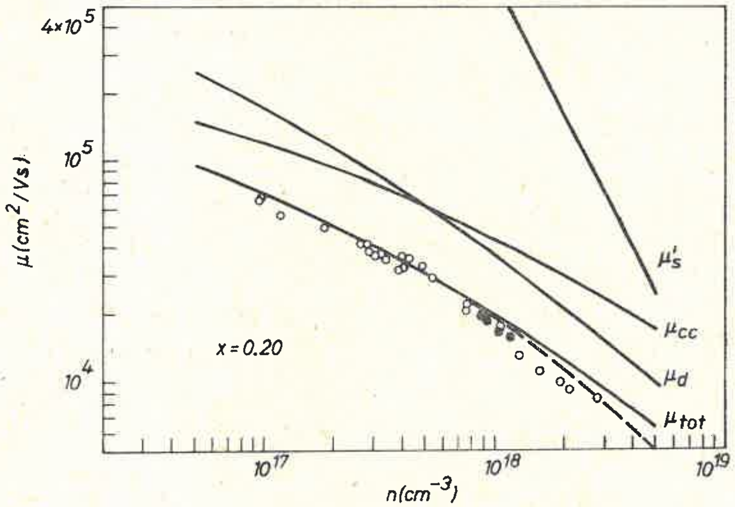

Fig. 3. Experimental and theoretical electron mobility vs concentration in $Cd_{0.2}Hg_{0.8}Se$ at 4.2 K. See explanation in the text

(μ_d). Similarly as for $x = 0.1$ (Fig. 1), certain discrepancy between theory and experiment can be observed for the crystals with $n \gtrsim 10^{18}$ cm^{-3}. μ_s' represents the mobility limited by neutral center scattering (Hg microprecipitations) assuming, for simplification, the same $N_s'(n)$ dependence as for $x = 0.1$. It has been checked that also for $x = 0.2$ the contribution given by scattering on neutral trace impurities can be completely neglected in the whole considered range of n. Dashed line in Fig. 3 is the theoretical electron mobility obtained if μ_s' is taken into account. It can be seen that including the contribution of μ_s', the discrepancy between μ_{tot} and the experimental mobility in the range $n \gtrsim 10^{18}$ cm^{-3} is partially reduced.

4.2. Ionized acceptors

It is seen in Fig. 1, that in $Cd_{0.1}Hg_{0.9}Se$ crystals with electron concentration $n \gtrsim 5 \times 10^{17}$ cm^{-3} the experimental mobility reaches much lower values than it could result from the theory (curve *1–1*) even after including the scattering by neutral centers (curve *1–2*). Hence, additional calculations including the compensation effect have been performed. Curve *3–2* corresponds to the total electron mobility $\mu_{tot}(n)$, calculated according to Eq. (6), where the contribution μ_{cc} takes into account partial compensation given by singly ionized acceptor centers with the concentration $N_A = 2.9 \times 10^{16}$ cm^{-3}. The resulting theoretical $\mu_{tot}(n)$ dependence (curve *3–2*) agrees very well with the experimental one, especially for the lowest values of n.

It is worth considering the origin of acceptor centers in the crystals studied. It has been suggested in paper I that these centers are connected with the ionized Hg vacancies, V'_{Hg}. In fact, the compensation effect is the strongest in the samples of the lowest achievable electron concentration (i.e. Se-saturated or dynamic vacuum annealed samples) where, as it has been proved before (§ 4.1), the influence of neutral defects on the mobility is negligible. Furthermore, the up-to-now data [4, 5] point out that in the purest $Cd_xHg_{1-x}Se$ crystals the compensation decreases with rising x — it also confirms the relation between N_A and $[V'_{Hg}]$. E.g., Fig. 3 shows that for low concentration $Cd_{0.2}Hg_{0.8}Se$ crystals the compensation need not to be taken into account ($N_A = 0$). It can be reminded here that in the crystals previously subjected to Se-saturation or dynamic vacuum annealing certain decrease of compensation (N_A) due to passive annealing have been observed (see I).

Also certain trace impurities detected in undoped $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) crystals, such as Ag, Cu or As [1,5] could form ionized acceptor centers. In fact, Lin [17] suggested that in undoped $Cd_xHg_{1-x}Te$ alloys the acceptor centers are mainly due to existence of Ag and Cu as trace impurities. However, in $Cd_xHg_{1-x}Se$ their influence on the electron mobility seems to be rather negligible, because of the above mentioned dependence of the compensation level on x, whereas the trace impurities level remains the same irrespective of the composition [5].

5. *Conclusions*

Experimental and theoretical investigations made in this paper point out the significant influence of native point defects on the electron mobility in undoped $Cd_xHg_{1-x}Se$ ($x \leqslant 0.2$) semiconducting alloys at 4.2 K. The mobility analysis was based on the approximate model of native point defects structure in $Cd_xHg_{1-x}Se$, given in I, and considered the scattering by charged and neutral centers as well as disorder scattering.

The results obtained in I and II point out that donor point defects in the form of ionized Hg interstitials ($Hg_i^{\cdot}$) are the dominant charged scattering centers at the low temperatures. The analysis of mobility vs electron concentration in $Cd_{0.1}Hg_{0.9}Se$ and $Cd_{0.2}Hg_{0.8}Se$ in the range $n \lesssim 10^{18}$ cm^{-3} proves the necessity of taking into account the scattering by neutral centers connected with Hg-microprecipitations which exist in the as-grown and Hg-saturated crystals (see I).

In $Cd_{0.1}Hg_{0.9}Se$ mixed crystals with low values of $n(\gtrsim 5\times 10^{17}$ cm$^{-3})$ electron mobility is significantly lowered due to the partial compensation ($N_A < N_D$) by ionized acceptors which are probably connected with the ionized Hg vacancies (V'_{Hg}).

Trace impurities can also form ionized or neutral scattering centers in $Cd_xHg_{1-x}Se$ — however the estimations performed here suggest that their influence on electron mobility in the crystals studied is rather negligible.

The author dedicates this paper to his nice little wife Jola.

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