Electron transport properties of bulk mercury–cadmium–telluride at 77 K

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A B S T R A C T

A Monte Carlo simulation of electron transport in mercury–cadmium–telluride is performed in order to extract the most important material parameters such as electron drift velocity, mean energy, effective mass, differential mobility, diffusion coefficient, impact ionization rate, velocity and energy relaxation rates. Most of these quantities are necessary for the developments of macroscopic numerical models. Moreover, for the calculated quantities, analytical interpolation formulae are given in order to achieve easy implementation in numerical codes.

The main results demonstrate that hot-electron transport and impact ionization processes occur for relatively weak electric fields, that is around 100 V/cm. The high mobility of mercury–cadmium–telluride, which makes it a good material for fast applications, is verified. Finally, a comparison between the Monte Carlo calculations, hydrodynamic simulations and experimental data is made for both stationary and transient regimes, which validates the results.

1. Introduction

Nowadays, infrared photo-detection represents a physical process with a huge number of applications in various domains, mainly led by night vision, industrial non-destructive control and medical imaging. In this context, HgCdTe (mercury–cadmium–telluride) is a widely used material. Indeed, it exhibits an energy bandgap which can be continuously adjusted from semimetal HgTe to semiconductor CdTe which corresponds to a variation from –0.3 to 1.6 eV at 77 K [1]. Then, the detected wavelengths are directly functions of the cadmium proportion, which allows to tune the photo-detection in different infrared atmospheric transmission-windows using the same material. Moreover, since the cadmium concentration has a negligible effect on the crystal parameter, all the infrared range can be covered within the same technological die. This last point is useful for multispectral photo-detection which presents a growing interest, in particular to increase target discrimination [2].

This work concerns the Hg_{0.7}Cd_{0.3}Te (hereafter indicated as MCT) at a temperature of 77 K, which allows the photo-detection of the 8–14 μm atmospheric window wavelengths. In these conditions, the semiconductor has a narrow bandgap of about 100 meV which leads to a strong non-parabolicity of the conduction band and to a small effective electron mass. As a consequence, electron transport properties differ from those of classical semiconductor materials for electronic applications and a high electron mobility, which makes MCT an optimum material for fast applications, is expected. Moreover, physical phenomena such as non-ohmic behavior and impact ionization processes are expected to be of main importance in MCT.

On the other hand, mainly due to its strategic interest, very few results concerning the MCT electron behavior are available in the literature [3,4]. In particular, input parameters of the widely used hydrodynamic and drift diffusion approaches are unavailable, which leads to the difficulty of studying the behavior of MCT-based devices using commercial or academic macroscopic simulators. As a consequence, the first step to describe correctly both transient and stationary regimes in MCT is to extract the unavailable parameters using a microscopic simulation of electron transport. To this aim, in this work, we perform a comprehensive investigation of transport parameters in MCT at 77 K based on a Monte Carlo (MC) simulation in stationary and transient regimes.

The paper is organized as follows: in Section 2, the theoretical model is described. Then, in Section 3, kinetic parameters are calculated through a Monte Carlo simulation. The obtained results are presented and analytical formulae are given. Section 4 is devoted to the study of impact ionization. Transient phenomena are treated in Section 5 where velocity and energy relaxation rates

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are given in order to develop a hydrodynamic approach. A comparison of the obtained results is done with the previous MC calculations. The main conclusions are drawn in Section 6.

2. Theoretical model

In the framework of our MC simulation of charge transport in MCT, only the dynamics of the electrons is taken into account since, in the considered n-type MCT, holes are much heavier than electrons and of negligible densities, which involves that their contribution to the charge transport can be neglected within a good approximation [4]. The MC simulator takes into account ionized impurities scattering, two modes of polar-optical phonons and alloy disorder. Acoustic phonon scattering is not accounted for because of a weak probability of occurrence which makes it negligible with respect to alloy disorder. Due to the huge difference between the characteristic times of scattering processes and the Auger recombination lifetime, that is approximately 1 ps versus 1 µs [5], this last process can be neglected. Then, as concerns the Auger generation–recombination processes, only impact ionization is accounted for in the MC model. However, we must note that, even if they have an important effect on the carrier density and, as a consequence, on the current, impact ionization processes are slower than scattering processes so that their influence on the kinetic transport parameters such as drift velocity, electron energy, mobility, etc., can be neglected. The MCT bandstructure is introduced by considering only the non-parabolic Γ valley since the energy bandgap of Hg0.8Cd0.2Te is much lower than the energy differences εL and εX separating the L and X valley, respectively, from the Γ valley. Indeed, in these conditions, the intervalley scattering probability can be considered as negligible. On the other hand, even if a strong electric field is applied which allows the electrons to accumulate energy, the narrow bandgap of the material involves the onset of the impact ionization processes before the electron have reached the energy necessary to leave the Γ valley, so that the electrons are confined at the bottom of the band. Due to the strong non-parabolicity (that is a non-parabolicity coefficient α = 11.4 eV−1⋅cm−1 [6]) and the narrow bandgap of the material, degeneracy effects must be taken into account in MCT from relatively small electron density (of the order of 1015 cm−3). Then, Pauli exclusion principle has been implemented in the MC simulator through the standard algorithm [7]. We have reported in Fig. 1 the scattering rates of MCT as functions of the electron energy for a free electron density n and an ionized impurity concentra-

Fig. 1. Hg0.8Cd0.2Te scattering rates at a temperature T = 77 K for x = 0.2, and n = N1 = 5.4 × 1014 cm−3 as functions of the carrier energy. The reported scattering rates are those of: the total rate (curve 1), the impact ionization (2), the emission through the two considered modes of polar-optical phonons (3 and 5), the ionized impurities (4), the alloy disorder (7) and the absorption through the two modes of polar-optical phonons (6 and 8).

3. Kinetic parameters

We have calculated the electron drift velocity in steady-state conditions and reported it as a function of the electric field for a zero-field free electron density n0 = 5.4 × 1014 cm−3 in Fig. 2 (curve 1). In the same figure, we have reported (curve 2) the theoretical results for drift velocity taken from Ref. [3], and we observe a good agreement for all the considered values of the electric field. Finally, we have plotted with curve 3 the experimental results obtained by Dornhaus et al. [8]. In order to allow a comparison with the theoretical results, the measured current density has been divided by the zero-field charge density qn0 to give a quantity homogeneous to a velocity. We observe a good agreement with the theoretical results for low values of the electric field, that is below 200 V/cm. Above this field, a strong increase of the experimental values is found, which leads to a discrepancy between theoretical and experimental results. This increase cannot be associated with an increase of the drift velocity, as demonstrated by MC results, and is attributed to the raise of the electron density due to the activation of impact ionization processes.

Fig. 3 reports the electron drift velocity as a function of the electric field for different values of the free electron density. The reported symbols are MC results while the lines are plots of the analytical expression [9]

\[ \nu(E) = \nu_0 \frac{E/E_0}{1 + (E/E_0)^3} \]

(1)

whose parameters have been calculated on the basis of MC simulation and are given for each considered value of the electron density.
Electron drift velocity versus electric field calculated by the Monte Carlo simulator (symbols) and its analytical expressions (lines) for the reported carrier densities.

Table 1
Values of the parameters used to fit the drift velocity and the differential mobility with Eqs. (1) and (6), respectively.

<table>
<thead>
<tr>
<th>Electron density $n$ (cm$^{-3}$)</th>
<th>$v$ (cm/s)</th>
<th>$E_c$ (V/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{14}$</td>
<td>5.90 $\times$ 10$^7$</td>
<td>148</td>
</tr>
<tr>
<td>$5.4 \times 10^{14}$</td>
<td>6.46 $\times$ 10$^7$</td>
<td>218</td>
</tr>
<tr>
<td>$10^{15}$</td>
<td>6.79 $\times$ 10$^7$</td>
<td>268</td>
</tr>
<tr>
<td>$5.4 \times 10^{15}$</td>
<td>8.00 $\times$ 10$^7$</td>
<td>494</td>
</tr>
</tbody>
</table>

The value $\zeta$ is taken equal to unity since it provides the best fitting. At low electric fields, that is below 50 V/cm, the drift velocity increases linearly with the electric field, as expected in ohmic regime. Above 50 V/cm, hot-electron effects appear which produce a sub-linear behavior with the electric field. We remark that, for a given value of the electric field, the electron velocity is higher when the electron density is lower. This phenomenon is related to the low electron effective mass and to the relatively small polar-optical phonon energy which allow impurity scattering to be still noticeable when polar-optical scattering is important.

Fig. 4 represents the average electron energy as a function of the electric field for different values of the free electron density. The analytical expression used to fit the data is given by:

$$
\epsilon(E) = \epsilon_0 \left[1 + \left(\frac{E}{E_c}\right)^\zeta\right]^{\beta/\gamma}
$$

(2)

Table 2
Parameters used in Eq. (2) to fit analytically the electron average energy as a function of the electric field and for different values of the electron density.

<table>
<thead>
<tr>
<th>Electron density $n$ (cm$^{-3}$)</th>
<th>$\epsilon_0$ (meV)</th>
<th>$E_c$ (V/cm)</th>
<th>$\beta$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{14}$</td>
<td>11.54</td>
<td>148</td>
<td>2.20</td>
<td>0.350</td>
</tr>
<tr>
<td>$5.4 \times 10^{14}$</td>
<td>11.54</td>
<td>218</td>
<td>1.95</td>
<td>0.560</td>
</tr>
<tr>
<td>$10^{15}$</td>
<td>11.60</td>
<td>268</td>
<td>1.76</td>
<td>0.690</td>
</tr>
<tr>
<td>$5.4 \times 10^{15}$</td>
<td>14.97</td>
<td>494</td>
<td>1.65</td>
<td>1.11</td>
</tr>
</tbody>
</table>

Fig. 4. Average energy versus electric field calculated by the MC simulator (symbols) and its analytical expressions (lines) for $n = 10^{14}$ cm$^{-3}$ and $n = 5.4 \times 10^{14}$ cm$^{-3}$ (a) and for $n = 10^{15}$ cm$^{-3}$ and $n = 5.4 \times 10^{15}$ cm$^{-3}$ (b).

Fig. 5. Average electron effective mass as a function of the electric field for $n = 10^{14}$ cm$^{-3}$ and $n = 5.4 \times 10^{14}$ cm$^{-3}$ (a) and for $n = 10^{15}$ cm$^{-3}$ and $n = 5.4 \times 10^{15}$ cm$^{-3}$ (b). Symbols refer to MC calculations and lines refer to analytical formula (5).
and its parameter values are given in Table 2. As previously, Fig. 4 can be separated into the same two regions. In the former one, below 50 V/cm, the average energy is practically constant with the electric field and equal to the thermal equilibrium energy. We remark that, due to degeneracy effects, the equilibrium energy value differs with the electron density, and it increases for the higher electron densities. In the latter region, above 50 V/cm, the energy increases with the electric field due to the heating of electrons. We remark that the increase is higher for lower densities, involving that transition from ohmic to hot-electron regime occurs for higher fields when the electron concentration is higher. As a matter of fact, the increase of the electron concentration strengthens the electron screening, which favors the polar-optical scattering and then energy dissipation.

The analysis of both average energy and drift velocity show that non-ohmic regime begins for relatively weak electric fields, that is around 50 V/cm.

Table 3
Values of parameters $a$, $b$ and $c$ used to express analytically the average electron effective mass through Eq. (5).

<table>
<thead>
<tr>
<th>$n$ (cm$^{-3}$)</th>
<th>$a$ (10$^{-39}$ kg m$^2$ V$^{-2}$)</th>
<th>$b$ (10$^{-36}$ kg m V$^{-1}$)</th>
<th>$c$ (10$^{-35}$ kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10$^{14}$</td>
<td>3.91</td>
<td>8.70</td>
<td>8.82</td>
</tr>
<tr>
<td>5.4 × 10$^{14}$</td>
<td>5.98</td>
<td>7.37</td>
<td>8.74</td>
</tr>
<tr>
<td>10$^{15}$</td>
<td>7.18</td>
<td>6.47</td>
<td>8.73</td>
</tr>
<tr>
<td>5.4 × 10$^{15}$</td>
<td>9.64</td>
<td>3.74</td>
<td>9.50</td>
</tr>
</tbody>
</table>

We have calculated, for the considered free electron densities, the mean longitudinal free electron effective mass $m'$ versus the electric field. This quantity is obtained by averaging the inverse electron longitudinal effective mass $1/m_e$, which is defined by the relation

$$\frac{1}{m_e} = \frac{e^2}{\hat{p}^2_e}$$  \hspace{1cm} (3)

where $p_e$ is the momentum component along the electric field. By deriving Eq. (3), one obtains

$$\frac{1}{m'_e} = \frac{1}{m_e(1+2xe)} \left[ 1 - \frac{2x p_e^2}{m_e(1+2x e)^2} \right]$$  \hspace{1cm} (4)

where $m_e$ is the electron effective mass at the bottom of the conduction band, that is for an energy equal to zero.

The MC results are reported as symbols in Fig. 5 where the reported lines refer to analytical formula

$$m'(E) = ae^2 + bE + c$$  \hspace{1cm} (5)

whose parameters $a$, $b$ and $c$ are given in Table 3. The increase of the electron effective mass with the electric field is due to the strong non-parabolicity of the material and depends weakly on the electron density. At zero-field, we observe the degeneracy effects since the electron effective mass, in this case, increases for the highest electron densities.

Fig. 6. Electron static differential mobility as a function of the electric field for $n = 10^{14}$ cm$^{-3}$ and $n = 5.4 \times 10^{14}$ cm$^{-3}$ (a) and for $n = 10^{15}$ cm$^{-3}$ and $n = 5.4 \times 10^{15}$ cm$^{-3}$ (b) at temperature $T = 77$ K. Symbols refer to MC calculations and lines refer to analytical formula (6).

Fig. 7. Diffusion coefficient versus electric field at $T = 77$ K for $n = 10^{14}$ cm$^{-3}$ and $n = 5.4 \times 10^{14}$ cm$^{-3}$ (a) and for $n = 10^{15}$ cm$^{-3}$ and $n = 5.4 \times 10^{15}$ cm$^{-3}$ (b). Symbols refer to Monte Carlo simulation and lines to analytical expression Eq. (7) with suitable parameters (see Table 4).
Fig. 6 represents the electron static differential mobility versus electric field for different values of the free electron density. By definition of the differential mobility, its analytical expression can be deduced by deriving Eq. (1) with \( \zeta = 1 \), which gives

\[
\mu'(E) = \frac{\text{d} v}{\text{d} E} = \nu_0 \frac{1}{(1 + E/E_c)^2}\]  

(6)

The used parameter values are still the same as those of drift velocity, and are therefore given in Table 1. We can observe a high ohmic mobility, higher than \( 10^5 \) cm\(^2\)/Vs, which is typical of this material. Moreover, due to an increased scattering efficiency at high fields, the differential mobility decreases with the electric field. For the lowest electric fields, that is below 100 V/cm, the ohmic mobility is higher for the lowest electron concentrations. However, this situation is inverted for highest electric fields, that is above 200 V/cm, for which higher electron concentrations present a higher differential mobility.

Fig. 7 reports the diffusion coefficient as a function of the electric field for different values of the electron density. To calculate it, we used the autocorrelation functions of velocity fluctuations and neglected degeneracy effects, as explained in Ref. [10]. Additionally, the diffusion coefficient has been fitted using the expression

\[
D(E) = \frac{D_0}{[1 + (E/E_b)\gamma]^\beta},
\]

(7)

whose parameter values are given in Table 4. The results show that the diffusion coefficient decreases monotonously with the electric field. At high electric fields, the diffusion coefficient becomes almost independent of the electric field. Moreover, a comparison of the ohmic mobility and diffusion coefficient calculated independently have shown a good agreement with Einstein relation.

In order to validate the MC simulator, we have reported in Fig. 8 the ohmic mobility as a function of the electron density. A comparison is made between MC simulations and experimental results taken from the literature [3,11,5], and a good agreement is observed.

<table>
<thead>
<tr>
<th>Electron density (cm(^{-3}))</th>
<th>( D_0 ) (m(^2)/s)</th>
<th>( E_c ) (V/cm)</th>
<th>( \beta )</th>
<th>( \gamma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^{14} )</td>
<td>0.23</td>
<td>148</td>
<td>1.14</td>
<td>1.08</td>
</tr>
<tr>
<td>( 5.4 \times 10^{14} )</td>
<td>0.19</td>
<td>218</td>
<td>0.93</td>
<td>1.24</td>
</tr>
<tr>
<td>( 10^{15} )</td>
<td>0.17</td>
<td>268</td>
<td>0.87</td>
<td>1.25</td>
</tr>
<tr>
<td>( 5.4 \times 10^{15} )</td>
<td>0.09</td>
<td>494</td>
<td>1.26</td>
<td>0.89</td>
</tr>
</tbody>
</table>

Fig. 8. Ohmic mobility as a function of the free electron density calculated with our Monte Carlo simulator (■), and values taken from Ref. [3] (▲ and ▽), [11] (▼) and [5] (○). The dotted line represents a guide for the eyes.

Fig. 9. Current as a function of the electric field. Experimental results taken from reference [8] (1) and Monte Carlo simulations for \( P_0 = 5 \times 10^{-15} \) s\(^{-1} \) and \( \psi = 2 \) (2), for \( P_0 = 10^{-16} \) s\(^{-1} \) and \( \psi = 3 \) (3), for \( P_0 = 5 \times 10^{13} \) s\(^{-1} \) and \( \psi = 3 \) (4) and for \( P_0 = 5 \times 10^{12} \) s\(^{-1} \) and \( \psi = 2 \) (5). The lines are guides for the eye.

Fig. 10. Evolution of normalized electron density for a zero-field electron density \( n_0 = 5.4 \times 10^{14} \) cm\(^{-3} \) and for an applied electric field \( E = 300 \) V/cm, \( E = 310 \) V/cm and \( E = 320 \) V/cm (a) and \( E = 300 \) V/cm, \( E = 330 \) V/cm and \( E = 350 \) V/cm (b). Symbols refer to MC calculations and lines to analytical expression Eq. (10).
4. Impact ionization (Auger generation)

To complete the theoretical investigations and allow a comprehensive description of the electron behavior of MCT, the impact ionization rate must be calculated since it has not been the object of a systematic study. Nevertheless, previous works of Gelmont [3,4] and Dornhaus and Nimtz [8,5] emphasized the strong influence of Auger generation (also called impactionization) and recombination processes on the current density-electric field characteristics of MCT from relatively low electric fields. As a matter of fact, Auger processes represent the main recombination channel in MCT [12] while the narrow gap of the semiconductor favors impact ionization events. In agreement with references [4,12], since we consider n-type material, impact ionization processes involving two holes and one electron can be neglected, and then only conduction–conduction–heavy-hole–conduction band (CCHC) and conduction–conduction–light-hole–conduction band (CCLC) processes must be considered. Moreover, due to the band-edge electron conduction related to the narrow energy gap of the material, CCLC processes can be neglected and only CCHC Auger processes have to be taken into account. Then, since hot-electron regime is activated for relatively weak electric fields for which holes remain cold, we can neglect the impact ionization processes initiated by holes and only consider Auger generation due to the electrons.

Auger lifetime has been calculated to be of the order of the microsecond [5], which is a characteristic time much longer than those associated with usual scattering processes (that is optical phonons, ionized impurities, etc.) and can then be neglected in the MC simulator. As concerns generation processes, they are introduced in the microscopic model through a collision with a

![Fig. 11. Ionization rate as a function of the electric field for a zero-field electron density \( n_0 = 5.4 \times 10^{14} \) cm\(^{-3}\). Symbols refer to MC calculations and lines to Eq. (10) whose parameters are given in Table 5.](image)

```
Table 5
Values of parameters \( g_0 \) and \( E_0 \) obtained by comparing analytical formula Eq. (11) and MC simulations.

<table>
<thead>
<tr>
<th>Electron density ( n_0 ) (cm(^{-3}))</th>
<th>( g_0 ) (s(^{-1}))</th>
<th>( E_0 ) (V/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^{14} )</td>
<td>10,000</td>
<td>43.2</td>
</tr>
<tr>
<td>( 5.4 \times 10^{14} )</td>
<td>8400</td>
<td>42.9</td>
</tr>
<tr>
<td>( 10^{15} )</td>
<td>7900</td>
<td>42.8</td>
</tr>
<tr>
<td>( 5.4 \times 10^{15} )</td>
<td>5600</td>
<td>42.7</td>
</tr>
</tbody>
</table>
```

![Fig. 12. Velocity \( v_v \) and energy relaxation rates \( v_\epsilon \) as functions of the electric field for the reported values of the free electron density.](image)
MC results have been fitted, as shown in Fig. 13, with the Shockley formula [13] of the form [14]

\[ P_0(\varepsilon) = P_0 \left( \frac{\varepsilon - \varepsilon_{th}}{\varepsilon_{th}} \right)^g \]  

(8)

where \( \varepsilon_{th} \) is the impact ionization threshold energy, while \( P_0 \) and \( \psi \) represent adjustable parameters. The impact ionization threshold energy can be calculated with the relation [4]

\[ \varepsilon_{th} = \left( 1 + \frac{2m_e}{m_h} \right) \varepsilon_g \]  

(9)

where \( m_h \) is the heavy hole effective mass. In order to find the suitable values of \( P_0 \) and \( \psi \), we have performed Monte Carlo simulations for different values of these parameters. This allowed us to calculate at the same time electron drift velocity and the electron multiplication, and then to extract the electron current density as a function of the electric field. The obtained results have been compared with experimental data taken from reference [8], which are reported in Fig. 9, by considering a simulated sample of the same geometry that the experimental one. We observe that the best fitting is obtained for \( \psi = 3 \) and \( P_0 = 10^{12} \text{ s}^{-1} \).

Note that, due to their relatively long characteristic time, impact ionization processes do not affect drift velocity but mainly affect electron density.

Then, we have calculated the ionization rate \( g \). For this purpose, we have simulated the evolution in time of the electron density, for different values of the electric field and of the zero-field value of the electron density \( n_0 \). The recombination processes have been neglected, so the time evolution of the electron density verifies the relation [12]

\[ \frac{n(t)}{n_0} = \exp(gt) \]  

(10)

We have reported as symbols in Fig. 10 some of the obtained results for the case \( n_0 = 5.4 \times 10^{14} \text{ cm}^{-3} \). The analytical formula (10) has been plotted as lines with the suitable values of the generation rate \( g \). In the same time, the generation rate has been analytically expressed as a function of the electric field for different values of the electron density. For this sake, the different MC results have been fitted, as shown in Fig. 11, with the Shockley formula [12]

\[ g = g_0 \exp(E/E_0) \]  

(11)

The suitable values of \( g_0 \) and \( E_0 \) are reported in Table 5 for the different considered values of the free electron density.

5. Transient parameters

Due to the good electron properties at high-frequency [15] and to the great time difference between scatterings and generation–recombination processes, the most appropriated approach to describe time-dependent electron transport in the material is the hydrodynamic (HD) model. If we consider low-generation regime in a bulk material, the balance equation of electron density, velocity and energy can be, respectively, rewritten as [12]

\[ \frac{dn}{dt} = gn - Rn^2p \]  

(12)

\[ \frac{dv}{dt} = \frac{qE}{m_e^v - \psi v} \]  

(13)

and

\[ \frac{d\varepsilon}{dt} = qE(v - (\varepsilon - \varepsilon_0))v_e \]  

(14)

where \( n \) and \( p \) are, respectively, the electron and the hole densities, \( v \) the average velocity and \( \varepsilon \) the average energy. The velocity and energy relaxation rates \( v_p \) and \( v_e \) as well as the effective electron mass \( m^v \) are related to the carrier dynamics, while the Auger generation and relaxation rates \( g \) and \( R \) refer to electron density variations in time.

While \( n, v, \varepsilon \) are the solutions of Eqs. (12)–(14), respectively, the quantities \( v_p, v_e, m^v, g \) and \( R \) are input parameters which describe the material electron properties and then depend strongly on it. A good approximation of the recombination rate value \( R \) can be taken as equal to \( R = 10^{-24} \text{ cm}^6 \text{ s}^{-1} \) [12]. The velocity and energy relaxation rates \( v_p \) and \( v_e \) are calculated through the relations

\[ v_p = \frac{qE}{m_e^v} \]  

(15)

and

\[ v_e = \frac{qE \varepsilon}{\varepsilon - \varepsilon_0} \]  

(16)

where the values of \( \varepsilon, \varepsilon_0 \) and \( m^v \) have been calculated by the MC simulation. We have reported them for the different values of the free electron density and as functions of the electric field in Fig. 12.

The velocity relaxation rate increases monotonously as a function of the electric field and takes higher values at increasing carrier concentrations. In contrast, the energy relaxation rate exhibits a maximum in the intermediate fields region (between 200 and 300 V/cm). It is interesting to notice that for the low values of \( n \) (Fig. 12a–c) \( v_e \) takes higher values than \( v_p \) almost in the full range of considered electric fields. This implies a faster relaxation of

![](image-url)
energy than velocity which is a quite unusual behavior for standard semiconductor materials. We have verified that this behavior is due to the strong non-parabolicity which characterize the MCT energy band.

After having extracted the suitable values of the material parameters \( v_r, v_s, m^*, g \) and \( R \) from the microscopic simulator, the HD study can be leaded by solving Eqs. (12)–(14). We have reported in Fig. 13 the time evolution of the average velocity (Fig. 13a) and energy (Fig. 13b) for different values of a step-like electric field switched-on at time \( t = 0 \) where thermodynamic equilibrium is assumed. In all cases a good agreement between the MC and HD results is found which validates the set of input parameters for the HD model. Continuous curves correspond to the MC results, while the symbols correspond to the MC results. We can observe for all the considered cases a very good agreement between MC and HD simulations.

6. Conclusion

After a description of the theoretical model, we have performed a Monte Carlo simulation of electron transport in Hg\(_{0.8}\)Cd\(_{0.2}\)Te, describing both stationary and transient conditions. The main scattering rates have been calculated, and hot-electron regime and impact ionization processes have been shown to occur for relatively weak electric fields, that is below 100 V/cm. The electron transport parameters, that is the drift velocity, average energy, electron effective mass, differential mobility, Auger generation rate, diffusion coefficient, velocity and energy relaxation rate have been extracted.

Additionally, we have provided analytical formulas of these transport parameters which are useful for an easy implementation in macroscopic simulations, such as drift diffusion and hydrodynamic. These approaches allow, from the knowledge of the field dependence of all the transport parameters for all values of electric fields, the modeling of HgCdTe-based structures and devices such as photovoltaic infrared detectors or avalanche photodiodes.

Appendix A. Scattering rates

Even if the material of interest is a narrow-gap semiconductor, standard expression of the scattering rates [16] can be used with a good accuracy [3]. Moreover, previous studies have shown that acoustic phonon contribution to the scattering processes can be neglected [3]. The MC simulator takes into account polar-optical phonons, ionized impurities, alloy and impact ionization scattering processes. The different expressions used to calculate the scattering rates in Hg\(_{0.8}\)Cd\(_{0.2}\)Te are exposed in the following.

A.1. Polar-optical phonon scattering

Since the material is an alloy, we introduce the polar-optical phonon scattering by considering two different polar-optical phonon modes, each one corresponding to CdTe (mode 1) or HgTe (mode 2) sublattices [3]. The polar-optical phonon scattering is then included through two separate mechanisms. Each sublattice contributes to the dielectric constant value, and the contribution of the mode \( i \) can be calculated through the relation [17,3]

\[
\kappa_i(x) = \kappa_{\infty}(x) \left( \frac{\omega_{\text{LO}}}{\omega_{\text{TO}}} \right)^2 - 1
\]

where \( x \) is the cadmium proportion and where \( \kappa_{\infty} \), the high-frequency contribution of the dielectric function, is approximated by the relation [17]

\[
\kappa_{\infty}(x) = 10.4 - 3x
\]

so that, in the case of Hg\(_{0.8}\)Cd\(_{0.2}\)Te

\[
\kappa_{\infty} = 9.8
\]

The quantities \( \omega_{\text{TO}} \) and \( \omega_{\text{LO}} \), represent, respectively, the longitudinal and the transverse polar-optical phonon angular frequency for the \( i \)-th optical modes. The suitable values for Hg\(_{0.8}\)Cd\(_{0.2}\)Te are given in Table 6 [18,3]. The polar-optical scattering rate corresponding to optical mode \( i \) as a function of the electron energy is given by

\[
P_{i\text{opt}}(\epsilon) = A_{i\text{opt}} \frac{1}{1 + 2C_{18}/C_{19}} F_{i\text{opt}}(\epsilon, \epsilon') \left[ N_{i\text{opt}} + 1 - \frac{j}{2} \right]
\]

where \( k \) is the modulus of \( k \) wave-vector, \( x \) is the non-parabolicity coefficient and

\[
\epsilon' = \epsilon + j\hbar \omega_{i\text{opt}}
\]

\( \epsilon' \) being the electron energy after the scattering and \( j = 1 \) for an absorption process and \( j = -1 \) for an emission process. The optical phonon angular frequency \( \omega_{i\text{opt}} \) is taken equal to the longitudinal value \( \omega_{i\text{LO}} \). The value \( N_{i\text{opt}} \) is the occupation number of \( i \)-th mode polar-optical phonons, which verifies

\[
N_{i\text{opt}} = \frac{1}{\exp \left( \frac{h\omega_{i\text{opt}}}{k_B T} \right) - 1}
\]

where \( k_B \) is the Boltzmann constant. The function \( F_{i\text{opt}}(\epsilon, \epsilon') \) is given by

\[
F_{i\text{opt}}(\epsilon, \epsilon') = \frac{A \ln \left( \frac{\alpha + A}{\epsilon - \epsilon'} \right) + B}{C}
\]

with

\[
A = [2(1 + \alpha x)(1 + \alpha x') + \alpha(x' + x')]^2
\]

\[
B = -2x\sqrt{\gamma} [4(1 + \alpha x)(1 + \alpha x') + \alpha(x' + x')]
\]

and

\[
C = (1 + \alpha x)(1 + \alpha x')
\]

The variables \( k, \gamma \) and \( \epsilon \) refer to values before scattering and \( k', \gamma' \) and \( \epsilon' \) to the same physical quantities after the scattering process. The value \( A_{i\text{opt}} \) is given by

\[
A_{i\text{opt}} = \frac{\epsilon^2 m_e \omega_{i\text{opt}}}{16\pi^2 \hbar^2 k_{0i}^2}
\]

where \( m_e \) is the electron effective mass, \( \hbar \) the reduced Planck constant, \( k_0 \) the permittivity of vacuum. The effective dielectric constant \( k_i^2 \) is expressed as [3]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x )</td>
<td>Cadmium proportion</td>
<td>0.2</td>
</tr>
<tr>
<td>( P )</td>
<td>Momentum matrix element</td>
<td>( 8.28 \times 10^{-10} ) eV m</td>
</tr>
<tr>
<td>( \Delta E )</td>
<td>Conduction band offset</td>
<td>1.423 eV</td>
</tr>
<tr>
<td>( \kappa_{\infty} )</td>
<td>High frequency dielectric function</td>
<td>9.8</td>
</tr>
<tr>
<td>( h\omega_{\text{TO}} )</td>
<td>Longitudinal polar-optical energy (mode 1)</td>
<td>19.24 meV</td>
</tr>
<tr>
<td>( h\omega_{\text{LO}} )</td>
<td>Longitudinal polar-optical energy (mode 2)</td>
<td>17.26 meV</td>
</tr>
<tr>
<td>( h\omega_{\text{TO1}} )</td>
<td>Transverse polar-optical energy (mode 1)</td>
<td>18.51 meV</td>
</tr>
<tr>
<td>( h\omega_{\text{LO1}} )</td>
<td>Transverse polar-optical energy (mode 2)</td>
<td>15.02 meV</td>
</tr>
<tr>
<td>( \Delta E' )</td>
<td>Valence band offset</td>
<td>0.350 eV</td>
</tr>
<tr>
<td>( N_{\text{th}} )</td>
<td>Cation concentration</td>
<td>( 1.47 \times 10^{22} ) cm(^{-3} )</td>
</tr>
<tr>
<td>( R )</td>
<td>Recombination rate</td>
<td>( 10^{-4} ) cm(^{3} ) s(^{-1} )</td>
</tr>
<tr>
<td>( \epsilon_{\text{th}} )</td>
<td>Impact ionization energy threshold</td>
<td>93 meV</td>
</tr>
</tbody>
</table>
where $\kappa_t$ is given by Eq. (17).

### A.2. Ionized impurities scattering

We use the Brooks–Herring model [19] which takes into account the screening effect of space charges. The screening length is $q_1r_c^2$ where

$$q_1^2 = \frac{e^2n}{\kappa_0\kappa_t\kappa_s T}$$

where $\epsilon$ is the elementary charge, $n$ the free electron density, $\kappa_0$ the vacuum permittivity, $\kappa_t$ the dielectric constant, $\kappa_s$ the Boltzmann constant and $T$ the temperature. The Coulomb potential induced by an ionized impurity is then expressed as

$$V(r) = \frac{e^2}{\kappa_0\kappa_r} \exp(-q_1r)$$

where $r$ represents the distance. To know the static dielectric constant $\kappa_{rs}$ we must consider the two sublattice modes and the high-frequency contributions. Then, $\kappa_s$ is given by

$$\kappa_s = \kappa_s(x) + \kappa_t(x) + \kappa_s(x)$$

The ionized impurities scattering rate is given by

$$P_{\text{imp}}(\epsilon) = A_{\text{imp}} \frac{k}{1 + 2\epsilon \epsilon_c} F_{\text{imp}}(\epsilon, N_i)$$

where $N_i$ is the ionized impurity concentration, and

$$F_{\text{imp}}(\epsilon, N_i) = \frac{2f_1^2}{(4k^2 + q_1^2)^2} + 2f_1^2$$

$$+ f_2 f_3 \ln \left( \frac{q_1^2}{4k^2 + q_1^2} \right)$$

and

$$f_1 = \frac{2\epsilon}{2k}$$

and where

$$f_2 = 1 + 2\epsilon \epsilon + f_1 q_1^2$$

The value of $A_{\text{imp}}$ is given by

$$A_{\text{imp}} = \frac{e^2 N_i n_c}{2\pi \kappa_0 \kappa_s^2 \kappa_t^2 \hbar^2}$$

In MCT, at 77 K, all the donors can be considered as ionized [20]. Moreover, hole and acceptor concentrations can be considered as negligible in comparison with the free electron density. Then, we have considered in this work that $N_i \approx n$.

### A.3. Alloy scattering

The alloy scattering is introduced through the virtual crystal approximation [21]. In the case of MCT, by assuming that Hg and Cd ions are distributed in the cation lattice in a uniform and ordered way, the lattice potential can be considered as the repetition of a periodical structure whose potential corresponds to the average of those of the different components, weighted by their respective proportions. In reality, the cation layout is not perfectly ordered and a random part must be added to the periodical potential, which represents the difference between the real crystal and the virtual one [22]. This random part constitutes then a perturbation potential which allows to calculate the alloy scattering probability. The alloy scattering is an elastic transition and its occurrence rate is given by [3]

$$P(\epsilon) = \frac{x(1-x)\Delta E_c^2 m_c}{\pi \hbar^2 N_{\text{cat}} \epsilon_g} \sqrt{2m_c(\epsilon^2 + 2\epsilon \epsilon + \frac{1}{4} \epsilon^2)}$$

where $\Delta E_c$ is the cation density and where $\Delta \epsilon_c$ is the conduction band offset which verifies

$$\Delta \epsilon_c = E_c(CdTe) - E_c(HgTe) = \Delta \epsilon_g + \Delta \epsilon_e$$

where $\Delta \epsilon_g$ is the difference between HgTe and CdTe bandgaps and where $\Delta \epsilon_e$ the valence band offset, is taken as $\Delta \epsilon_e = -0.350$ eV [23].

The calculation of the alloy scattering rate needs the knowledge of the cation density $N_{\text{cat}}$. Since the material density and the mass of each composing atom are known, $N_{\text{cat}}$ can be simply deduced by the relation

$$N_{\text{cat}} = \frac{\rho}{\Delta M_{\text{Hg}_1\text{CdTe}}} \times \mathcal{A}$$

where $\mathcal{A}$ is the Avogadro number. Finally, we have calculated for the case of $Hg_{0.3}Cd_{0.7}Te$ that $N_{\text{cat}} = 1.47 \times 10^{22}$ cm$^{-3}$.

### References


