Materials Research Express

PAPER

Photocarrier transport dynamics in lifetime and relaxation regimes of semiconductors containing traps

Jingyi Yu , Lingyan Xu, Binbin Zhang and Wanqi Jie1

State Key Laboratory of Solidification Processing and MIIT Key Laboratory of Radiation Detection Materials and Devices, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi’an, Shaanxi 710072, People’s Republic of China

1 Author to whom any correspondence should be addressed.

E-mail: jwq@nwpu.edu.cn

Keywords: transport properties, charge carriers, lifetime regime, relaxation regime, traps, CdTe

Abstract

High resistivity semiconductors used in various optoelectronic devices, such as radiation detectors and photoconductive switches, usually require electrical compensation involving deep level defects, which are also closely related to the photocarrier transport dynamics. In this paper, one-dimensional spatiotemporal evolution of photocarriers is numerically investigated in semiconductors containing traps. After introducing a high concentration of traps, the dynamics can be divided into three categories: relaxation, lifetime and intermediate regimes. Photocarriers will separate in the relaxation regime and transport ambipolarly in the lifetime regime. Captured space charges enhance the internal electric field between photogenerated electrons and holes, thus reduce carriers’ transport velocities in all three regimes. Storage of photocarriers in traps also weakens the majority carrier depletion in the relaxation regime, and could pin the majority carriers to the injection spot in the lifetime regime. In the intermediate regime, both semiconductor type and relative magnitudes of the dielectric relaxation time and carrier lifetimes determine the photocarrier transport behavior. By combining the three-energy-level compensation model and the trap-mediated recombination model, the criterion for different regimes and photocarrier transport dynamics are investigated in deep donor compensated CdTe semiconductors.

1. Introduction

Understanding the relation between photocarrier transport dynamics and material’s electrical properties plays a key role in optimizing the performance of various photoelectric devices. For example, high resistivity is an essential requirement for semiconductors used in certain applications, such as radiation detectors [1] and photoconductive switches [2]. However, a high resistivity semiconductor could exhibit generically different carrier transport behaviors from that of a low resistivity one. In 1960s, to interpret the difference, van Roosbroeck proposed concepts of the ‘relaxation regime’ (or ‘relaxation semiconductor’) and the ‘lifetime regime’ (or ‘lifetime semiconductor’) [3, 4]. The dielectric relaxation time [5] is larger than the carrier lifetime [6] in relaxation semiconductors, while smaller in lifetime semiconductors. Because the dielectric relaxation time is proportional to the resistivity, relaxation semiconductors typically have high resistivity and exhibit several novel transport phenomena, including majority carrier depletion induced by minority carrier injection [7, 8], quasi-Ohmic voltage-current characteristics over a wide voltage range [9, 10] and spatial separation of photogenerated electrons and holes [11]. On the other hand, lifetime semiconductors typically have low resistivity [12] and exhibit ambipolar transport phenomenon [13, 14], i.e. photogenerated electrons and holes transport together with intermediate effective drift mobility and diffusion coefficient.

At room temperature, high resistivity in most compound relaxation semiconductors is achieved by electrical compensation involving deep level defects. Blanc and Weisberg [15] first proposed a three-energy-level compensation model (two opposite shallow levels and a deep donor level) to interpret the occurrence of high resistivity GaAs. Similar models were then adopted for semi-insulating II–VI compounds [16]. For example,
CdTe with resistivity in orders of $10^9$ $\Omega$cm is widely used in room temperature x-ray detectors [17]. The mechanism of achieving such high resistivity just by an exact compensation of shallow impurities can be excluded because of the technical difficulty, therefore compensation by deep donor levels, mainly Te antisites ($\text{Te}_{\text{Cd}}$), is commonly accepted for interpreting the high resistivity [18, 19]. Apart from the resistivity and related dielectric relaxation time, deep level defects also determine the carrier recombination process and thus carrier lifetimes [20]. For effective compensation, the deep level defects need to locate near the intrinsic Fermi level, so they are also effective traps, which significantly reduce the lifetimes through the defect-mediated recombination [21, 22]. For example, in CdTe solar cells Te antisites are proved to be the dominant recombination centers limiting the minority carrier lifetime [23].

Photocarrier transport dynamics in lifetime and relaxation regimes of semiconductors have generated considerable recent research interest. Separation of photocarriers has been observed in hydrogenated amorphous silicon [24]. In theory, it is proved that in trap–free semiconductors, locally–photogenerated electrons and holes will transport ambipolarly in the lifetime regime, and separate spatially in the relaxation regime [25]. However, real materials, especially high resistivity compound semiconductors, do contain traps originated from deep level defects, which can remarkably change carrier’s transport behavior [6]. For example, variation of trap ionization states may result in significant space charges that influence the photocarrier transport dynamics [26]. Besides, because deep level defects directly link to both the carrier lifetimes and the dielectric relaxation time, they could alter the criterion dividing the relaxation and lifetime semiconductors [27, 28]. In this work, one-dimensional photocarrier transport dynamics in semiconductors containing traps are numerically investigated. After introducing high concentrations of traps into the material, the majority and minority carrier lifetimes are no equal, therefore a new intermediate regime emerges where the dielectric relaxation time is in between of the two lifetimes. Spatiotemporal evolution of photogenerated carriers in the lifetime, relaxation and intermediate regime is simulated. As an application, the criterion for different regimes is investigated for deep donor compensated CdTe material.

2. Models and parameters

In this paper, carrier lifetimes are calculated through the mechanism of trapping. If the majority carrier concentration is much larger than the trap concentration, variation of charged trap density can be neglected. Excess electron and hole concentrations are always equal so as to preserve charge neutrality [25]. In this condition, the carrier lifetime $\tau_0$ can be simply calculated by [21]

$$\tau_0 = \frac{\tau_{\rho 0}(n_0 + n_l) + \tau_{\sigma 0}(p_0 + p_l)}{n_0 + p_0}, \quad (1)$$

where $n_0$ and $p_0$ are concentrations of equilibrium electrons and holes, $n_l$ and $p_l$ are electron and hole concentrations when the Fermi level coincides with the defect energy level, $\tau_{\rho 0} = 1/\sigma_{\rho 0}v_l N_l$ and $\tau_{\sigma 0} = 1/\sigma_{\sigma 0}v_l N_l$, where $\sigma_{\rho, \sigma}$ are electron and hole capture cross-sections, $v_l$ is the thermal velocity and $N_l$ is the trap concentration. However, if a semiconductor contains much larger amount of traps compared with the free carrier concentration, variation of charged trap density could result in unequal excess electron and hole concentrations. In this condition, electron and hole lifetimes are unnecessarily equal given by [21]

$$\tau_n = \frac{\tau_{\rho 0}(n_0 + n_l) + \tau_{\sigma 0}(p_0 + p_l) + N_l(1 + p_0/p_l)^{-1}}{n_0 + p_0 + N_l(1 + p_0/p_l)^{-1}(1 + p_l/p_0)^{-1}}, \quad (2a)$$

$$\tau_p = \frac{\tau_{\rho 0}(p_0 + p_l) + \tau_{\sigma 0}(n_0 + n_l) + N_l(1 + n_0/n_l)^{-1}}{n_0 + p_0 + N_l(1 + n_0/n_l)^{-1}(1 + n_l/n_0)^{-1}}. \quad (2b)$$

It is obvious that if $N_l \rightarrow 0$ both lifetimes will reduce to equation (1). On the other hand, the dielectric relaxation time $\tau_D$, which is proportional to the resistivity, is given by [29]

$$\tau_D = \varepsilon \rho = \frac{\varepsilon}{q(\mu_n n_0 + \mu_p p_0)}, \quad (3)$$

where $\varepsilon$ is the permittivity, $\rho$ the resistivity, $q$ the electron charge and $\mu_{n,p}$ the carrier mobilities.

The dielectric relaxation time and lifetime characterize different recovery-to-equilibrium routes [26] after a carrier concentration disturbance. The dielectric relaxation time governs the re-establishment rate of space charge neutrality from drawing a flow of free carriers by Coulombic interactions. The lifetime determines the timescale of achieving the Mass Action Law ($n_p p_0 = n_n^2$) [30] by carrier recombination or generation. In lifetime semiconductors, local net charges will rapidly be balanced by charge flows, therefore the material can be assumed in charge neutrality spatiotemporally. By contrast, charge neutrality in relaxation semiconductors is no longer held and space charges will significantly alter the carrier transport behavior. As a result, lifetime and
relaxation semiconductors are distinguished by their different carrier transport dynamics. For semiconductors containing a single monovalent trapping level, the normalized one-dimensional transport equations can be written as [27]

\[
\frac{\partial (\Delta N)}{\partial t} = \frac{\partial [(1 + \Delta N) E]}{\partial X} + \frac{\partial^2 (\Delta N)}{\partial X^2} - A_n U_n, \tag{4}
\]

\[
\frac{\partial (\Delta P)}{\partial t} = -\frac{\partial [(P_0 + \Delta P) E]}{\partial X} + \frac{\partial^2 (\Delta P)}{\partial X^2} - A_p U_p, \tag{5}
\]

\[
\frac{\partial M}{\partial t} = A_n U_n - A_p U_p, \tag{6}
\]

where the normalizations are \(x = X L_{D,n} \tau_{D,n} = \tau D_n, n = (1 + \Delta N) n_0, p = (P_0 + \Delta P) n_0,\) \(E_{real} = E kT/q \mu D_0,\) and \(L_D = (kT^2/\mu n_0)^{1/2}\) the dielectric relaxation time and Debye length defined for equilibrium electrons. Therefore, \(\Delta N, \Delta P\) and \(P_0\) are normalized concentrations of excess electrons, excess holes and thermal equilibrium holes respectively. For simplicity, we suppose the mobilities of electrons and holes are equal. In equation (6), \(A_n = \tau_{D,n}/\tau_{n0}\) and \(A_p = \tau_{D,n}/\tau_{p0}\) which can be viewed as constants for a low injection level in respect to the equilibrium majority carrier concentration, \(M\) is the concentration of traps filled with electrons normalized by \(n_0, U_{n,p}\) are trap’s capture rate for electrons and holes, which can be written as

\[
U_n = (1 + \Delta N) \left(1 - \frac{M}{M_0}\right) - N_i M \frac{M}{M_0}, \tag{7}
\]

\[
U_p = (P_0 + \Delta P) \frac{M}{M_0} - P_1 \left(1 - \frac{M}{M_0}\right), \tag{8}
\]

with the normalizations \(N_i = M_0 n_0, n_1 = N_i n_0\) and \(p_1 = P_1 n_0, N_i\) is the total trap concentration and \(M_0\) is its normalized value. In the simulation, we mainly consider n-type semiconductors with donor-type traps, i.e. the trap has a positive and a neutral state (0, +). Therefore, the Poisson equation can be expressed as

\[
\frac{\partial E}{\partial X} = \Delta P - \Delta N = (M - M_0), \tag{9}
\]

where \(M_0\) represents the value of \(M\) in equilibrium. In the simulation, the trap level is set to the most effective recombination level, i.e. the intrinsic Fermi level \(E_F\), and both electrons and holes can be captured and re-captured by the trap. Photocarriers are generated at the middle of a one-dimensional device \((X = 0)\). The initial photocarrier profile is Gaussian-shaped with the standard deviation being equal to \(1 \times 10^{-6}\), which results from an optical spot generation pulse. Maximum photocarrier concentration is set to \(n_0/10^6\) \((\max[Delta N(t = 0)] = 1 \times 10^{-6})\), therefore the injection level is small to ensure the applied electric field is not shielded by excited and trapped charges and parameters \((\tau_{D,n}, L_{D,n}, A_n, A_p, \mu_n, \mu_p)\) are independent of the excitation. Carrier dynamics are controlled by equations (4)–(9) in semiconductors containing traps, which are solved by the finite element method (FEM).

3. Results and discussion

3.1. Relaxation regime

Simulated evolution of excess filled trap charge concentration \(-\Delta M = -(M - M_0)\) and excess carrier concentrations \(\Delta N\) and \(\Delta P\) in an n-type material \((P_0 = 0.1N_0)\) is shown in figure 1. In the simulation, \(A_n\) and \(A_p\) are set to 5, so both \(\tau_n\) and \(\tau_p\) are smaller than \(\tau_{D,n}\) which is approximately equal to \(\tau_{D,p}\) in an n-type semiconductor. As a result, the semiconductor is in the relaxation regime. Time is between 0.1 to 1.0 \(\tau_{D,n}\) after the excitation with an interval of 0.1 \(\tau_{D,n}\). All concentrations are normalized to the maximum \(\Delta N\) at \(t = 0\), and the applied electric field \(E_0\) is equal to 5. Photogenerated electrons and holes separate after the excitation as expected. In figure 1(a), the trap concentration is much smaller than the majority carrier concentration \((M_0 = 0.1 N_0)\). Therefore the space charge of ionized traps is negligible in the photocarrier transport process. The majority carrier depletion as shown in the dashed box can also be observed in this situation. On the other hand, in figure 1(b), the trap concentration is larger than the majority carrier concentration \((M_0 = 10 N_0)\). In this circumstance, the remarkable amount of traps strongly influences the photocarrier dynamics in two ways. First, a large amount of photogenerated carriers is captured by the traps along the drift path rather than quick recombination. As a result, high-concentration traps in the material serve as a ‘buffer’ to store photocarriers and significantly reduce the net recombination rate. Because the majority carrier depletion (electrons in this case) in a trap-free semiconductor originates from the high recombination rate in the minority carrier peak region [25], the depletion is greatly weakened in the trap-dominated material as shown in figure 1(b). It should be noted that the influence of trapped charge on steady-state minority carrier injection, e.g. in a forward-biased p–i–n diode, and related majority carrier depletion phenomenon have been extensively studied both theoretically and
experimentally. For example, numerical simulations [27] reveal that traps as charge-storage localities reduce the tendency for majority carrier depletion in the relaxation regime, which is in good agreement with the experimental current-voltage \((I-V)\) characteristics of trap-dominated semi-insulating GaAs diodes [31, 32]. Second, trapped holes contribute to positive space charges in the hole peak region, while trapped electrons contribute to negative ones. These space charges enhance the internal electric field between the two photocarrier peaks, result in a slower peak transport velocity compared to that in a trap-free material. Despite the high trap concentration, spread of the photocarrier pulses due to the carrier diffusion is similar in figures 1\((a)\) and \((b)\), because the Coulombic attraction is weak in the relaxation regime [25]. Figure 2 illustrates the evolution of photocarrier crest positions after the excitation in trap-free and trap-dominated semiconductors, corresponding to figure 1. The crest positions basically rise linearly, but in the trap-free case drift lengths of photocarrier profile crests are about 1.2 times larger than that in the trap-dominated case \(\tau_{Dn}\) after the excitation. As a result, the high concentration of trapped space charges can significantly reduce the drift velocities of both excess electron and hole peaks. This effect can also be observed in other regimes of semiconductors containing a high concentration of traps.

3.2. Lifetime regime
Simulated evolution of \(-\Delta M, \Delta N\) and \(\Delta P\) in the lifetime regime is shown in figure 3. In the simulation, the material is n-type \((P_0 = 0.1N_0)\) with a high trap concentration \((M_0 = 10N_0)\). Time is between 0.2 to 2.0\(\tau_{Dn}\) after the excitation with an interval of 0.2\(\tau_{Dn}\). All concentrations are normalized to the maximum \(\Delta N\) at \(t = 0\), and the applied electric field \(E_0\) is equal to 2. In figure 3\((a)\), \(A_n = A_p = 1\) thus \(\tau_n = 3.19\tau_{Dn}\) and \(\tau_p = 1.41\tau_{Dn}\). Capture velocities of excess electrons and holes are similar. Trapped electrons form a negative space charge region on the left of the injection spot, and trapped holes form a positive one on the right. Despite trap-induced space charges, the photocarrier dynamics are similar to the dynamics in the lifetime regime of a trap-free semiconductor. Photogenerated electrons as majority carriers finally drift following the minority carriers, as the arrow marked. This separating-ambipolar transport process indicates the internal electric field related drift current term can overcome the external electric field related term [25].

However, trapped charges do alter the photocarrier dynamics in the lifetime regime, especially in the case of strong minority carrier trapping. In figure 3\((b)\), \(A_p\) is 100 times larger than \(A_n\), thus the capture velocity for excess holes is much larger than that for electrons. Because of the significant trapping effect, excess hole concentration quickly shrinks after the excitation and converts to a large amount of trapped positive charges, which has a great impact on the transport process of photogenerated electrons. At the beginning of the transport process, electrons trend to drift along the electric field. However, because the material is in the lifetime regime, the
positive trapped charges strongly attract photogenerated electrons. As a result, most excess electrons remain at the injection spot. This procedure can still be regarded as a separating-ambipolar transport process, except that it originates from the internal electric field between the free and trapped charges rather than two mobile photocarrier pulses. Besides, the strong Coulombic attraction effect also leads to a significant spread of photogenerated electrons, while the spread of photogenerated holes is greatly weakened by the large hole capture velocity.

3.3. Intermediate regime
Electron and hole lifetimes are different in trap-dominated semiconductors, therefore a new intermediate regime emerges where the dielectric relaxation time is in between of the two lifetimes. Figure 4 illustrates evolution of
−ΔM, ΔN and ΔP in two typical situations, i.e. $\tau_n > \tau_{Dn} > \tau_p$ and $\tau_p > \tau_{Dn} > \tau_n$. In the simulation, the material is n-type ($P_0 = 0.1N_0$) and trap-dominated ($M_0 = 10N_0$). Time is between 0.2 to $2.0\tau_{Dn}$ after the excitation with an interval of $0.2\tau_{Dn}$. All concentrations are normalized to the maximum $\Delta N$ at $t = 0$, and the applied electric field $E_0$ is equal to 2. In figure 4(a), $A_n = A_p = 2$ thus $\tau_n > \tau_{Dn} > \tau_p$. Photogenerated holes drift along the applied electric field to the cathode, while excess electrons drift following the holes after a separating-ambipolar transition. In this case, photocarrier transport dynamics are basically similar to the case of the lifetime regime as shown in figure 3(a), although $\tau_p$ is smaller than $\tau_{Dn}$. In figure 4(b), $A_n = 20$ and $A_p = 1$ thus $\tau_p > \tau_{Dn} > \tau_n$. Because capture velocity for electrons is very large, photogenerated electrons are quickly trapped after injection, creating a significant negative charge region at the injection spot. Despite the significant negative charge region, photogenerated holes still drift to the cathode, therefore photocarriers are separated by applied electric field.

Simulated photocarrier transport dynamics indicate that the intermediate regime can be viewed as that one kind of carriers behaves as in the lifetime regime and the other as in the relaxation regime. In figure 4(a), excess holes behave as in the relaxation regime, therefore they drift along the electric field after the injection. By contrast, excess electrons behave as in the lifetime regime. The strong Coulombic attraction between the two pulses produces the separating-ambipolar transition of electrons as majority carriers. In figure 4(b), excess holes behave as in the lifetime regime. Because the semiconductor is n-type, holes as minority carriers still drift to the cathode. On the other hand, excess electrons drift to the anode, which is in line with the electron transport dynamics in the relaxation regime. Besides, the strong trapping effect diminishes the majority depletion phenomenon, and negative space charges reduce the hole peak drift velocity. Despite the transport directions, it should be noted that the spreading behavior of photocarriers in the intermediate regime can be different from that in other regimes. In figure 4(a), the trapping effect is moderate thus the spread of excess electrons and holes is similar to the corresponding regimes as in figures 1(a) and 3(a). However, the strong electron trapping as in figure 4(b) weakens the spread of excess electrons comparing to figure 1(b), but the spread of excess holes is basically not influenced by trapped negative charges, which is different from the case of electrons in the lifetime regime as in figure 3(b).

### 3.4. Application to CdTe materials

CdTe and related CdZnTe have long been viewed as the most promising material used for room-temperature X/γ-ray detection [17]. As radiation detectors, the semiconductor should be in the relaxation regime in order to separate radiation-generated electrons and holes under an applied electric field [23]. Considering the fact that carrier lifetimes should be much longer than the carrier transit time through the device to achieve a complete...
Charge collection, high resistivity and thus a large dielectric relaxation time are necessary for CdTe crystals used as radiation detectors. It is widely accepted that high resistivity CdTe is achieved by compensation involving deep donor levels [18], mainly Te antisites (Te\(_{\text{Cd}}\)). As a result, here we use a three-energy-level compensation model, i.e. a shallow donor, a shallow acceptor, and a deep donor, with concentrations of \(N_d, N_a\) and \(N_p\), respectively. Two shallow levels can be assumed completely ionized at room temperature, while the filling rate of the deep donor varies a lot depending on the compensation ratio \(N_f/(N_a-N_d)\). Because the carrier lifetime in detector-grade CdTe is several \(\mu\)s, the deep donor concentration can be estimated [17, 33] in orders of \(10^{12}\) cm\(^{-3}\) for typical electron and hole capture cross-sections \(\sigma_n, \sigma_p\).

Calculated \(\tau_D, \tau_n, \tau_p\) in CdTe as a function of \(N_f/(N_a-N_d)\) is illustrated in figure 5. The parameters used are \(E_i = E_f - 0.65\) eV, \(N_a - N_d = 1 \times 10^{12}\) cm\(^{-3}\), \(\sigma_n = 1 \times 10^{-15}\) cm\(^2\) and \(\sigma_p = 1 \times 10^{-14}\) cm\(^2\), which are extracted from experimental results [18]. The semiconductor is low-resistivity p-type in the range \(N_f/(N_a-N_d) < 1\). By introducing more deep donors, a type-inversion happens at \(N_f/(N_a-N_d) \approx 1\). After that, CdTe is over-compensated and turns into a high resistivity n-type semiconductor. It is evident that compensation by deep levels is very effective because the high resistivity is maintained even in a mild over-compensated situation [34]. On the other hand, deep levels could also be effective recombination centers which significantly reduce carrier lifetimes. From figure 5, if \(N_f/(N_a-N_d) \ll 1\) and \(n_0 + p_0 \gg N_f\), the discrepancy between \(\tau_n\) and \(\tau_p\) is small and they can be replaced by \(\tau_0\). With increasing trap concentration, \(\tau_n\) and \(\tau_p\) start to split after \(N_f > n_0 + p_0\). Near the type-inversion point, \(\tau_p\) decreases while \(\tau_n\) reaches its maximum. After the type-inversion, \(\tau_p\) keeps decreasing with an increasing compensation ratio, while \(\tau_n\) basically remains as a constant.

The compensation ratio influences both the dielectric relaxation time and the lifetimes, therefore the criterion for semiconductor regimes becomes more complicated in deep donor compensated CdTe than trap-free materials. Figure 6 shows CdTe semiconductors satisfying \(\tau_D > \tau_n\) or \(\tau_D > \tau_p\) as a function of trap’s capture cross-sections \(\sigma_n, \sigma_p\). In figure 6(a), \(N_f/(N_a-N_d) = 0.1\) so the CdTe is low resistivity. However, the material could still be a relaxation semiconductor if carrier lifetimes are small enough with very large \(\sigma_n, \sigma_p\). When \(N_f/(N_a-N_d) = 1\), \(\tau_p\) reaches its peak value near the type-inversion compensation ratio, which becomes the major restriction for CdTe to be a relaxation semiconductor. As a result, a large \(\tau_D > \tau_D > \tau_n\) intermediate regime appears in this case, as shown in figures 6(b). In figure 6(c) and (d), CdTe is over-compensated with increasing compensation ratio, but the region \(\tau_D > \tau_p\) remains similar, thus the region is almost irrelevant to \(\sigma_n\). On the other hand, when \(N_f/(N_a-N_d)\) rises, the region \(\tau_D > \tau_n\) requires a larger \(\sigma_n\) because of a decreasing \(\tau_D\) and a constant \(\tau_n\), as indicated in figure 5. It should be noted that for CdTe radiation detectors, long carrier drift length given by the product of the carrier mobility, lifetime and the electric field strength is essential for complete charge collection. As a result, achieving the relaxation semiconductor by a very short lifetime in heavily doped CdTe is not preferred. Besides, although deep donors located near the midgap are effective compensation levels, they are also effective recombination centers reducing carrier lifetimes. All in all, there is a trade-off between compensation and recombination.
Simulated photocarrier evolution also verifies the criterion for relaxation and lifetime regimes in deep donor compensated CdTe, as shown in figure 7. Time is between 10 ns to 100 ns after the excitation with an interval of 10 ns. Photocarriers are generated at the middle of a one-dimensional device \((x = 0)\). The initial distribution of injected electrons and holes is a Gaussian-shaped pulse with a standard deviation of 1 \(\mu\)m and a maximum concentration of \(1 \times 10^{15} \text{ cm}^{-3}\). The device is large enough so the injection can be viewed as a local small

Figure 6. Semiconductor regimes of CdTe satisfying \(\tau_D > \tau_n\) or \(\tau_D > \tau_p\) as a function of trap’s capture cross-sections \(\sigma_{n,p}\), where \(N_d - N_a = 1 \times 10^{13} \text{ cm}^{-3}\) and \(N_t/(N_d - N_a)\) is equal to (a) 0.1, (b) 1, (c) 10 and (d) 100.

Figure 7. Evolution of photogenerated carriers in CdTe with a time interval 10 ns after the excitation. The parameters used are \(N_d - N_a = 1 \times 10^{13} \text{ cm}^{-3}\), \(\sigma_n = 1 \times 10^{-14} \text{ cm}^2\) and (a) \(N_t/(N_d - N_a) = 0.1\), \(\sigma_p = 1 \times 10^{-14} \text{ cm}^2\); (b) \(N_t/(N_d - N_a) = 2\), \(\sigma_p = 1 \times 10^{-14} \text{ cm}^2\); (c) \(N_t/(N_d - N_a) = 10^6\), \(\sigma_p = 1 \times 10^{-18} \text{ cm}^2\).
perturbation where carrier dynamics can be simulated using equations (4)–(9). Excess carrier concentrations are normalized to the maximum $\Delta n$ at $t = 0$, and the applied electric field $E_0$ is equal to 1000 V cm$^{-1}$. In figure 7(a), the material is low resistivity p-type and in the lifetime regime with $N_i/(N_a - N_d) = 0.1$. Excess holes drift following electrons after injection, i.e. photocarriers transport ambipolarly, which is similar to the case of figure 3(a). In addition, a double-hump distribution of holes and the separating-ambipolar transport dynamics can also be observed. The ambipolar transport has been used to measure the minority carrier mobility in low-resistivity HgCdTe infrared photoconductive detectors [35]. By contrast, if CdTe is compensated to high resistivity ($N_i/(N_a - N_d) = 2$) as shown in figure 7(b), the material is in the relaxation regime. Excess electrons and holes will separate after the injection, i.e. electrons drift to the anode and holes drift to the cathode, which is similar to the case of figure 1(b). Note that in CdTe $\mu_p$ is approximately 10 times larger than $\mu_p$ (1000 versus 80 cm$^2$ V$^{-1}$ s$^{-1}$), therefore the electron pulse moves faster. Such separation behavior can be observed by the transient charge technique in high-resistivity CdTe radiation detectors [36]. However, the compensation ratio should not be too large, otherwise the material will be too extrinsic and might enter the intermediate or lifetime regime. For example, in figure 7(c), the compensation ratio is very large ($N_i/(N_a - N_d) = 10^8$) and $\sigma_p$ is reduced to $1 \times 10^{-18}$ cm$^2$ in order to ensure the lifetimes are not smaller than the time interval in the calculation. In this circumstance, $\tau_D$ is shorter than $\tau_n$ and $\tau_p$, thus CdTe is again in the lifetime regime except for its strong n-type. Excess holes are quickly trapped after the injection, while excess electrons remain at the excitation spot attracted by positive trapped charges. The photocarrier dynamics are in line with the ambipolar transport process of the trap-dominated lifetime regime as shown in figure 3(b).

4. Conclusion

In this work, the influence of traps on the photocarrier transport dynamics is investigated. If the amount of traps in a semiconductor is comparable with free carrier concentrations, majority and minority carrier lifetimes are not equal, therefore the photocarrier transport dynamics can be divided into three categories, i.e. relaxation, lifetime, and intermediate regimes. In the relaxation regime ($\tau_D > \tau_{n,p}$), photogenerated electrons and holes will separate by the applied electric field. High-concentration traps contribute to significant captured space charges along photocarriers’ drift path, which enhances the internal electric field between excess electrons and holes. The internal electric field reduces carriers’ transport velocities compared to a trap-free material, which can also be observed in other regimes. Besides, high-concentration traps can store photocarriers and significantly reduce the net recombination rate, therefore weaken the majority carrier depletion in the relaxation regime. In the lifetime regime ($\tau_D < \tau_{n,p}$), photocarriers will transport ambipolarly after a short separating process. A strong minority carrier trapping effect can pin excess majority carriers to the injection spot. In the intermediate regime ($\tau_n > \tau_D > \tau_p$ or $\tau_p > \tau_D > \tau_n$), both semiconductor type and relative magnitudes of $\tau_D$, $\tau_n$, and $\tau_p$ determine the photocarrier transport behavior. For n-type semiconductors, photogenerated holes will drift along the electric field followed by excess electrons if $\tau_n > \tau_D > \tau_p$, while photogenerated electrons and holes will separate if $\tau_p > \tau_D > \tau_n$. As an application, the criterion for different regimes is studied in the case of deep donor compensated CdTe, where the three-energy-level compensation model is combined with the trap-mediated recombination model. In order to obtain detector-grade CdTe, i.e. materials in the relaxation regime, the compensation ratio should be larger than one. On the other hand, larger trap capture cross-sections in detector-grade CdTe are not preferred. The criterion for relaxation and lifetime regimes in CdTe is also verified by numerical simulations of the photocarrier transport dynamics. In a mild over-compensated range where the material can be used as radiation detectors, excess electrons and holes are separated by the applied electric field. Otherwise, the material becomes too extrinsic where photogenerated carriers transport ambipolarly.

Acknowledgments

This work was supported by the National Key Research and Development Program of China (2016YFF0101301), the National Natural Science Foundation of China (NNSFC-51502244), the Fundamental Research Funds for the Central Universities (3102015B(II)ZS014) and the fund of MIIT(MJ-2017-F-05).

ORCID iDs

Jingyi Yu @ https://orcid.org/0000-0002-8534-4624
References

[1] Závorka J, Pekárek J, Grill R, Belas E, Ridzováková K, Pipek J and Franc J 2019 Inhomogeneous resistivity and its effect on CdZnTe-based radiation detectors operating at high radiation fluxes J. Phys. D: Appl. Phys. 52 325109
[2] Islam N E, Shimomura H, Schowoiger J S H and Joshi R P 2000 Compensation mechanisms and the response of high resistivity GaAs photoconductive switches during high-power applications IEEE Trans. Plasma Sci. 28 1028–32
[3] van Roosbroeck W 1961 Current–carrier transport with space charge in semiconductors Phys. Rev. 123 474–90
[4] van Roosbroeck W and Casey H C 1970 A new regime of semiconductor behavior: Carrier transport when dielectric relaxation time exceeds lifetime Proceedings of the Tenth International Conference on the Physics of Semiconductors (Cambridge, Massachusetts) pp 832–8 U.S. Atomic Energy Commission, Division of Technical Information
[5] Neamen D A 2011 Semiconductor Physics And Devices—Basic Principles 4th edn (New York: McGraw-Hill Education)
[6] van Roosbroeck W 1960 Current–carrier transport and photoconductivity in semiconductors with trapping Phys. Rev. 109 636–52
[7] Popescu C and Henisch H K 1975 Minority carrier injection in relaxation semiconductors Phys. Rev. B 11 1563–8
[8] Manifacier J C 2010 Multiple steady-state current–voltage characteristics in drift–diffusion modelisation of N type and semi-insulating GaAs Gunn structures Solid-State Electron. 54 1511–9
[9] Manifacier J C and Henisch H K 1981 The interpretation of ohmic behavior in semi-insulating gallium arsenide systems J. Appl. Phys. 52 5195–201
[10] Jones B K, Santana J and McPherson M 1998 Ohmic I–V characteristics in semi-insulating semiconductor diodes Solid State Commun. 105 547–9
[11] Parrott J E 1985 The theory of majority-carrier motion in the Hayes-Shockley experiment Solid-State Electron. 28 1065–75
[12] Haegel N M 1991 Relaxation semiconductors: in theory and in practice Applied Physics A Solids and Surfaces 53 1–7
[13] Ruzicka B A, Werake L K, Samassekou H and Zhao H 2010 Ambipolar diffusion of photoexcited carriers in bulk GaAs Appl. Phys. Lett. 97 1–4
[14] Bose R et al 2016 Real-space visualization of energy loss and carrier diffusion in a semiconductor nanowire array using 4D electron microscopy Adv. Mater. 28 5106–11
[15] Blanc J and Weissberg L R 1961 Energy-level model for high-resistivity gallium arsenide Nature 192 155–6
[16] Castaldini A, Cavallini A, Fraboni B, Polenta L, Fernandez P and Piqueras J 1996 Compensation and deep levels in II–VI compounds Materials Science and Engineering: B 42 302–5
[17] Szoles C 2004 CdZnTe and CdTe materials for X-ray and gamma ray radiation detector applications Physica Status Solidi (B) Basic Research 241 783–90
[18] Babentsov V, Franc J and James R B 2009 Compensation and carrier trapping in indium-doped CdTe: Contributions from an important near-mid-gap donor Appl. Phys. Lett. 94 052102
[19] Lindström A, Mirbt S, Sanval B and Klintenberg M 2016 High resistivity in undoped CdTe: carrier compensation of Te antites and Cd vacancies J. Phys. D: Appl. Phys. 49 035101
[20] Dubois S, Enjalbert N and Garandet J P 2008 Effects of the compensation level on the carrier lifetime of crystalline silicon Appl. Phys. Lett. 93 032114
[21] Shockley W and Read W T 1952 Statistics of the recombination of holes and electrons Phys. Rev. 87 835–42
[22] Hall R N 1952 Electron–hole recombination in germanium Phys. Rev. 87 387–387
[23] Ma J, Kuciauskas D, Albin D, Bhattacharya R, Reese M, Barnes T, Li J, Gessert T and Wei S 2013 Dependence of the minority-carrier lifetime on the stoichiometry of CdTe using time–resolved photoluminescence and first-principles calculations Phys. Rev. Lett. 111 067402
[24] Liao B, Naja Shacham-Diamand Y and Kidron I 1984 Haynes-Shockley experiment on n-type HgCdTe J. Appl. Phys. 57 4299–4301
[25] Islam N E, Schamiloglu E, Schoenberg J S H and Joshi R P 2000 Compensation mechanisms and the response of high resistivity GaAs photoconductive switches during high-power applications IEEE Trans. Plasma Sci. 28 1028–32
[26] Mevissenko A, Grill R, Pekárek J, Belas E, Faura P, Pipek J, Lunder V and Elhadidy H 2017 Characterization of polarizing semiconductor radiation detectors by laser-induced transient currents Appl. Phys. Lett. 111 082103
[27] Popescu C and Henisch H K 1975 Minority carrier injection in relaxation semiconductors Phys. Rev. B 11 1563–8
[28] Parrott J E 1985 The theory of majority-carrier motion in the Hayes-Shockley experiment Solid-State Electron. 28 1065–75
[29] Manifacier J C and Henisch H K 1980 The concept of screening length in lifetime and relaxation semiconductors J. Appl. Phys. 52 5195–201
[30] Haegel N M 1991 Relaxation semiconductors: in theory and in practice Applied Physics A Solids and Surfaces 53 1–7
[31] Ruzicka B A, Werake L K, Samassekou H and Zhao H 2010 Ambipolar diffusion of photoexcited carriers in bulk GaAs Appl. Phys. Lett. 97 1–4
[32] Bose R et al 2016 Real-space visualization of energy loss and carrier diffusion in a semiconductor nanowire array using 4D electron microscopy Adv. Mater. 28 5106–11
[33] Blanc J and Weissberg L R 1961 Energy-level model for high-resistivity gallium arsenide Nature 192 155–6
[34] Castaldini A, Cavallini A, Fraboni B, Polenta L, Fernandez P and Piqueras J 1996 Compensation and deep levels in II–VI compounds Materials Science and Engineering: B 42 302–5
[35] Szoles C 2004 CdZnTe and CdTe materials for X-ray and gamma ray radiation detector applications Physica Status Solidi (B) Basic Research 241 783–90
[36] Babentsov V, Franc J and James R B 2009 Compensation and carrier trapping in indium-doped CdTe: Contributions from an important near-mid-gap donor Appl. Phys. Lett. 94 052102
[37] Lindström A, Mirbt S, Sanval B and Klintenberg M 2016 High resistivity in undoped CdTe: carrier compensation of Te antites and Cd vacancies J. Phys. D: Appl. Phys. 49 035101
[38] Dubois S, Enjalbert N and Garandet J P 2008 Effects of the compensation level on the carrier lifetime of crystalline silicon Appl. Phys. Lett. 93 032114
[39] Shockley W and Read W T 1952 Statistics of the recombination of holes and electrons Phys. Rev. 87 835–42
[40] Hall R N 1952 Electron–hole recombination in germanium Phys. Rev. 87 387–387
[41] Ma J, Kuciauskas D, Albin D, Bhattacharya R, Reese M, Barnes T, Li J, Gessert T and Wei S 2013 Dependence of the minority-carrier lifetime on the stoichiometry of CdTe using time–resolved photoluminescence and first-principles calculations Phys. Rev. Lett. 111 067402
[42] Liao B, Naja Shacham-Diamand Y and Kidron I 1984 Haynes-Shockley experiment on n-type HgCdTe J. Appl. Phys. 57 4299–4301
[43] Islam N E, Schamiloglu E, Schoenberg J S H and Joshi R P 2000 Compensation mechanisms and the response of high resistivity GaAs photoconductive switches during high-power applications IEEE Trans. Plasma Sci. 28 1028–32
[44] Mevissenko A, Grill R, Pekárek J, Belas E, Faura P, Pipek J, Lunder V and Elhadidy H 2017 Characterization of polarizing semiconductor radiation detectors by laser-induced transient currents Appl. Phys. Lett. 111 082103