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On weakly dispersive multiple-trapping transport

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ABSTRACT

Equations for multiple-trapping carrier transport, corresponding to the time-of-flight method are approximately solved under the assumption that the majority of carriers are in a thermal quasi-equilibrium. The solutions show a Gaussian shape of the carrier packet. The mean velocity of the carrier sheet for the dispersive transport regime decreases in time and its dispersion grows faster than the square root of time. The accuracy of the obtained formulas is verified by Monte Carlo calculations for exponential and Gaussian trap distributions. A satisfactory agreement is obtained up to the effective carrier transit time, provided that the trap density falls-off sufficiently fast in the energy gap. A new method of determining energetic trap profiles in disordered solids from the time-of-flight measurements is proposed.

1. Introduction

The time-of-fight (TOF) technique is a straightforward, frequently applied method of investigating the carrier transport in low-conductivity solids, both crystalline and amorphous. The sample is sandwiched between two electrodes with a constant voltage applied, and the excess carriers are generated by a short light pulse. The carrier motion in the sample induces a current transient in the measuring circuit. Information about the carrier transport mechanism can be inferred from the transient form as well as from its dependence on the experimental parameters.

As regards disordered solids, there exist two basic carrier transport mechanisms – multiple-trapping (MT) and hopping. Transitions of carriers between extended states and localized states (traps) gap occur in case of MT, whereas straightforward carrier transitions between localized states take place in case of hopping. For both mechanisms, the carrier transport may be either Gaussian or dispersive. The former transport regime is characterized by constant velocity and a Gaussian carrier sheet shape in a solid, the latter – by a gradual decrease in the mean velocity and an extremely large dispersion of the carrier packet. The first successful theory of dispersive transport was developed by Scher and Montroll [1], who attributed this phenomenon to very slow equilibration of charge carriers over localized states.

The Scher–Montroll theory initiated extensive investigations on dispersive transport (see the reviews [2,3] for earlier works). In spite of this, some problems seem to be still unresolved. In particular, this concerns the simplified description of MT dispersive transport, given by Tiedje and Rose [4] and by Orenstein and Kastner [5]. Their main idea was that the majority of trapped carriers for specific trap distributions are in a thermal quasi-equilibrium with the free carriers. This approach has been utilized in many subsequent papers. However, its validity has been questioned by Arkhipov et al. [6], since it does not describe the carrier packet broadening. The main aim of this paper is to resolve this controversy.

2. Transport equations

The present investigations are based on a standard MT model, assuming very small trap occupancy, electric field uniformity in the sample as well as negligible carrier diffusion. It should be borne in mind that the first assumption may be incorrect at the final stage of the carrier transport, due to the gradual filling of deeper traps. However, it is difficult to provide an analytical description of the MT transport taking into account the trap occupancy saturation. Only some special cases have been studied so far [7].

In the following formulas, the free and trapped carrier densities are denoted by $n(z,t)$ and $n_t(z,t)$, respectively, where $z = x/\mu_0 E$ is the reduced space variable (x is the space variable, μ_0 – the free carrier mobility and E – the electric field strength) and t is the time variable. The MT carrier transport can be described by the continuity equation:

$$\frac{\partial}{\partial t}[n(z,t)+n_t(z,t)]+\frac{\partial n(z,t)}{\partial z}=0, \tag{1}$$

and the equation relating the free and trapped carrier densities [8]:

$$n_t(z,t)=\int_0^t \Phi(t')n(z,t-t')\mathrm{d}t'. \tag{2}$$

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Here, the function $\Phi(t)$ determines the probability that the carrier is trapped in a time unit and remains in the trap until time t. This function is given by the formula:

$$\Phi(t) = C_t \int_0^\infty N_t(\varepsilon) \exp\left[-t/\tau_r(\varepsilon)\right] \mathrm{d}\varepsilon, \tag{3}$$

where C_t is the carrier capture coefficient, $N_t(\varepsilon)$ is the trap density at the energy level ε per unit energy, and

$$\tau_r(\varepsilon) = \nu_0^{-1} \exp\left(\varepsilon/kT\right) \tag{4}$$

is the mean lifetime of the trapped carrier (ν_0 is the frequency factor, k – the Boltzmann constant and T – the sample temperature). The energy ε is measured from the edge of the allowed band.

The current intensity $I(t)$, registered in the TOF experiment, equals the conduction current intensity in the sample, averaged over its thickness. Therefore

$$I(t) = \frac{I_0}{n_0 \tau_0} \int_0^{\tau_0} n(z,t) \mathrm{d}z, \tag{5}$$

where n_0 is the density of generated carriers, averaged over sample thickness, $\tau_0 = d/\mu_0 E$ and $I_0 = e n_0 \mu_0 E S$ are respectively the carrier time-of-flight and the initial current intensity in a trap-free sample (with d being the sample thickness, e – the elementary charge and S – the sample cross-sectional area). For times smaller than the effective carrier transit time τ_e through the sample, Eq. (5) may be rewritten as

$$I(t) = I_0 \frac{\mathrm{d}\bar{z}(t)}{\mathrm{d}t}, \quad t < \tau_e, \tag{6}$$

where the dash denotes averaging over the spatial carrier distribution. The transit time τ_e is implicitly given by the formula

$$\bar{z}(\tau_e) = \tau_0. \tag{7}$$

3. Thermal quasi-equilibrium approximation

The progress of carrier thermalization in trapping states is characterized by the demarcation level $\varepsilon_0(t)$ [4,5,8], defined implicitly by the formula $\tau_r[\varepsilon_0(t)] = 1.8t$, which gives:

$$\varepsilon_0(t) = kT \ln(1.8 \nu_0 t). \tag{8}$$

The level separates the traps approximately with equilibrium ($\varepsilon < \varepsilon_0(t)$) and non-equilibrium ($\varepsilon > \varepsilon_0(t)$) occupancy.

In the case of weakly dispersive transport, when the approximate thermal equilibrium between free carriers and the majority of the trapped carriers is established, Eq. (2) describing the trapping/detrapping kinetics can be simplified. If the trap density in the energy gap decreases sufficiently fast, the main contribution to the integral in Eq. (3) should proceed from the energy region $\varepsilon < \varepsilon_0(t)$. The exponential function argument in the integrand is then much larger than unity for almost all values of energy ε, and the function $\Phi(t)$ should differ significantly from zero only for very small time values. The free carrier density in Eq. (2) can be then replaced by the initial terms of its Taylor series,

$$n(z, t - t') \approx n(z,t) - t' \frac{\partial n(z,t)}{\partial t}. \tag{9}$$

This results in an approximate equation, describing carrier trapping/detrapping processes,

$$n_t(z,t) \approx \left[\Theta^{-1}(t) - 1\right] n(z,t) - \tau_s(t) \frac{\partial n(z,t)}{\partial t}, \tag{10}$$

where the functions:

$$\Theta^{-1}(t) = 1 + C_t \int_0^\infty N_t(\varepsilon) \tau_r(\varepsilon) [1 - \exp\left[-t/\tau_r(\varepsilon)\right]] \mathrm{d}\varepsilon, \tag{11}$$

$$\tau_s(t) = C_t \int_0^\infty N_t(\varepsilon) \tau_r^2(\varepsilon) \{1 - [1 + t/\tau_r(\varepsilon)] \exp\left[-t/\tau_r(\varepsilon)\right]\} \mathrm{d}\varepsilon. \tag{12}$$

The last factors in integrands in Eqs. (11) and (12) may be approximated by the unit step function, $H[\varepsilon_0(t) - \varepsilon]$, provided that the functions $N_t(\varepsilon)\tau_r(\varepsilon)$ and $N_t(\varepsilon)\tau_r^2(\varepsilon)$ vary sufficiently slowly with energy. Then,

$$\Theta^{-1}(t) \approx 1 + C_t \int_0^{\varepsilon_0(t)} N_t(\varepsilon) \tau_r(\varepsilon) \mathrm{d}\varepsilon, \tag{13}$$

$$\tau_s(t) \approx C_t \int_0^{\varepsilon_0(t)} N_t(\varepsilon) \tau_r^2(\varepsilon) \mathrm{d}\varepsilon. \tag{14}$$

It should be stressed that both integrals are calculated over the energy interval $0 \leqslant \varepsilon \leqslant \varepsilon_0(t)$, where the trapped carriers are in a thermal quasi-equilibrium.

Equations equivalent to Eq. (10), with the last term having been omitted, have been obtained in [4,5] under the assumption of an exact thermal equilibrium between free carriers and carriers trapped in the energy region $\varepsilon \leqslant \varepsilon_0(t)$. As has been already indicated, this approach has been criticized [6], as it does not describe the spatial carrier dispersion. The mentioned term approximately takes into account the deviations of carrier densities from their equilibrium values. It will be seen that the presence of the term results in a finite spread of the carrier packet.

4. Solution of transport equations

An approximate solution of the equations identical to (1) and (10) has been already obtained in the paper [9], dealing with non-isothermal carrier transport, and has the form of

$$n(z,t) \approx \frac{n_0 \tau_0 \Theta(t)}{2[\pi \xi(t)]^{1/2}} \exp\left\{-\frac{[z - \zeta(t)]^2}{4\xi(t)}\right\}, \tag{15}$$

$$n_t(z,t) \approx \left[\Theta^{-1}(t) - 1\right] n(z,t), \tag{16}$$

where the functions

$$\zeta(t) = \int_0^t \Theta(t') \mathrm{d}t', \tag{17}$$

$$\xi(t) = \int_0^t \tau_s(t') \Theta^3(t') \mathrm{d}t'. \tag{18}$$

Thus, the carrier packet in the considered approximation has a Gaussian shape. The 'centroid' and the RMS spread of carrier distribution are given respectively by the formulas:

$$\bar{z}(t) = \zeta(t), \tag{19}$$

$$\sigma(t) = [2\xi(t)]^{1/2}. \tag{20}$$

The above results constitute a straightforward extension of those obtained for the Gaussian carrier transport [10,11]. In such a case the functions $\Theta(t)$ and $\tau_s(t)$ are constant which implies that $\bar{z}(t) \propto t$ and $\sigma(t) \propto t^{1/2}$.

Inserting the free carrier density (15) into the integral (5) the following formula for the current transient intensity is obtained:

$$I(t) = \frac{I_0 \Theta(t)}{2} \left\{1 + \mathrm{erf}\left[\frac{\tau_0 - \zeta(t)}{2\xi^{1/2}(t)}\right]\right\}, \tag{21}$$

where $\mathrm{erf}(\ldots)$ is the error function. The initial current decay and the effective carrier transit time τ_e, corresponding approximately to the transition to faster final current decay are given by

$$I(t) \approx I_0 \Theta(t), \quad t < \tau_e, \tag{22}$$

$$\zeta(\tau_e) = \tau_0. \tag{23}$$

It follows from Eqs. (15)–(17) as well as Eqs. (22),(23) that the carrier packet's effective mobility determined by the trapping/detrapping events is given by $\mu_{\mathrm{eff}}(t) = \mu_0 \Theta(t)$. The effective carrier