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Fractional differential approach to dispersive transport in semiconductors

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Abstract. A novel approach using equations with fractional order derivatives to describe dispersive transport in disordered semiconductors is described. A relationship between the self-similarity of dispersive transport, stable limiting distributions, and kinetic equations with fractional derivatives is established. It is shown that unlike the well-known Scher – Montroll and Arkhipov – Rudenko models, which are in a sense alternatives to the normal transport model, fractional differential equations provide a unified mathematical framework for describing normal and dispersive transport. The fractional differential formalism allows the equations of ambipolar dispersive transport to be written down and transport in systems with a distributed dispersion parameter to be described. The relationship between fractional differential equations and the generalized limiting theorem reveals the probabilistic aspects of the phenomenon in which a dispersive-to-Gaussian transport transition occurs in a time-of-flight experiment as the applied voltage is decreased and/or the sample thickness increased.

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1. Introduction

Dispersive (non-Gaussian) transport (DT) [1, 2] occurs in many disordered materials of different microscopic structures, such as amorphous hydrated silicon [3, 4], amorphous selenium [5, 6], amorphous chalcogenides [7, 8], organic semiconductors, polymers [9–11], porous solids [12–14], nanostructured materials [15], polycrystalline films [16], and liquid crystals [17] and some others. A comparison of available data suggests the presence of *universal* transport properties unrelated to the detailed atomic and molecular structure of a substance [18]. DT is considered to be an alternative to Gaussian transport, although some authors (see, e.g., Ref. [19]) try to describe dispersive diffusion by a usual diffusion equation and a Gaussian packet of particles. The fractional differential approach reviewed in the present paper reflects budding prospects for the development of normal and anomalous kinetics in the framework of unified mathematical formalism.

Fractional derivatives were first introduced into the theory of semiconductors by Babenko [20] to find time dependence of concentration at the boundary of p – n junction during normal transport at a given current density by means of factorization of the normal diffusion operator:

$$\frac{\partial}{\partial t}-\frac{\partial^2}{\partial x^2}=\left(\frac{\partial^{1/2}}{\partial t^{1/2}}-\frac{\partial}{\partial x}\right)\left(\frac{\partial^{1/2}}{\partial t^{1/2}}+\frac{\partial}{\partial x}\right).$$

The Riemann–Liouville type fractional derivatives [21]

$$\frac{\partial^\alpha}{\partial t^\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t \frac{f(t')}{(t-t')^\alpha}, \qquad 0 < \alpha < 1$$

were for the first time applied to the dispersive transport theory by Arkhipov, Popova, and Rudenko [22] in 1983; these authors expressed the relationship between concentrations of free and localized carriers through the fractional integral. In later papers (see, e.g., Refs [23–29]), they chose to use a different approximate relation between concentrations of localized and free carriers, which they called 'the master DT equation'. This relation is believed to hold for any density of localized states and permits expressing results through elementary functions in the case of an exponential density. The Arkhipov–Rudenko master DT equation leads to a diffusion equation with a variable diffusion coefficient and mobility [25].

Based on kinetic trapping–emission equations written by Noolandi [6, 30], Tiedje [31] derived, in terms of Laplace integral transformation and neglecting diffusion, a transport equation for free carrier concentration. The inverse Laplace transform of this equation represents a fractional differential equation [32].

Barkai [33] made use of the Fokker–Planck fractional differential equation proposed by Metzler, Barkai, and Klafter [34] to account for transient photocurrent relaxation in amorphous semiconductors. He showed the agreement between selected results obtained by the fractional differential approach and predicted by the Scher–Montroll model [35]. The author of Ref. [33] justified introduction of the fractional differential equation as follows: "Transport in ordered media is often modeled using diffusion equation, this approach being the simplest and most widely used. Dispersive Scher–Montroll transit time type experiments, observed in a large number of disordered systems, can be described phenomenologically using the fractional Fokker–Planck equation. This is only one example of physical phenomena in which a different type of calculus, i.e., noninteger calculus, plays a central role." The authors of Ref. [34] did not derive the equation strictly from certain initial premises but substantiated its adequacy to anomalous transport by a fulfillment of the following requirements:

(1) In the absence of an external force, the subdiffusion relation for time dependence of the particle packet width is satisfied.

(2) In the presence of a time-independent nonlinear external force, the stationary solution of the equation has the form of the Boltzmann distribution.

(3) The generalized Einstein relation is fulfilled.

(4) If the fractional exponent tends to unity, the equation transforms into the ordinary Fokker–Planck equation.

Another fractional differential diffusion equation obtained in Ref. [36] by the simple replacement of the fractional derivative for the time derivative in the standard diffusion equation was considered by Bisquert [37] with respect to transport through multiple trapping. The function in this equation with nonconserved normalization is interpreted as the concentration of delocalized carriers. References [37, 38] do not contain solutions to the equation of interest, nor do they report results of its application to the description of time-of-flight experiments. The author of Ref. [38] uses this equation for explaining power-law attenuation of photoconduction and power-law relaxation of luminescence in semiconductors with exponential density of localized states.

Power-law decay of photoluminescence in amorphous semiconductors was described in Refs [39, 40] based on the generalized random walk model with recombination by tunnel radiative transitions. Recombination was limited by dispersive diffusion of the carriers. In the framework of this model, the authors of Ref. [40] compiled a fractional differential equation for the first passage time distribution density. The recombination rate [40] was found using the integral Laplace transform of this equation.

As shown in Refs [41, 42], the main asymptotic terms of solutions to random walk equations in the Scher–Montroll model are solutions of fractional differential equations, the Green functions of which are fractionally stable densities. Solution of the equation proposed in Bisquert's paper [37] was found in terms of stable densities [43].

The present work shows that fractional differential kinetics is a consequence of DT self-similarity. The universal behavior of transient photocurrent testifies to the presence of self-similarity. The fractional differential approach is shown to be related to the Scher–Montroll model and the multiple trapping model. Moreover, the Fokker–Planck fractional differential equation applied by Barkai [33] and the equation for delocalized carrier concentration used in Ref. [37] and generalized in Ref. [32] to the case of drift diffusion are related via the expression obtained by Arkhipov, Popova, and Rudenko [22]. We shall take into account monomolecular recombination and recombination through tunnel radiative transitions. In addition, a case of a distributed dispersion parameter for simulating disordered inhomogeneous media is considered. Fractional differential equations of ambipolar DT are proposed. The adequacy of these equations and their solutions is verified by comparing analytical results with the data of time-of-flight experiments. In certain cases, Monte Carlo simulation is employed in the framework of the continuous-time random walk paradigm.

2. Universality of transient current curves and self-similarity of dispersive transport

Let us consider a classical 'time-of-flight' experiment for determining the drift mobility of charge carriers. Electrons and holes are usually generated in a sample by a pulse of laser radiation from the side of the semitransparent electrode. The voltage applied to the electrodes is such that the corresponding electric field inside the sample is significantly stronger than the field of nonequilibrium charge carriers. Generated electrons (or holes, depending on the voltage sign) enter the semitransparent electrode, while holes (or electrons) drift to the opposite electrode. In the case of normal transport, free-drifting carriers in the field E give rise to a rectangular photocurrent pulse:

$$I(t) \propto \begin{cases} \text{const}, & t < t_{\mathrm{tr}}, \\ 0, & t > t_{\mathrm{tr}}, \end{cases} \tag{1}$$

where the *time of flight* t_{tr} is given by drift velocity v and sample length L: $t_{\mathrm{tr}} = L/v$. Taken together, the scattering of delocalized carriers during the drift, trapping on localized states, and thermal emission of the carriers lead to packet spreading. Such a packet has a Gaussian shape with a mean value of $\langle x(t) \rangle \propto t$ and width $\Delta x(t) \propto \sqrt{t}$. In this case, transient current $I(t)$ remains constant until the leading

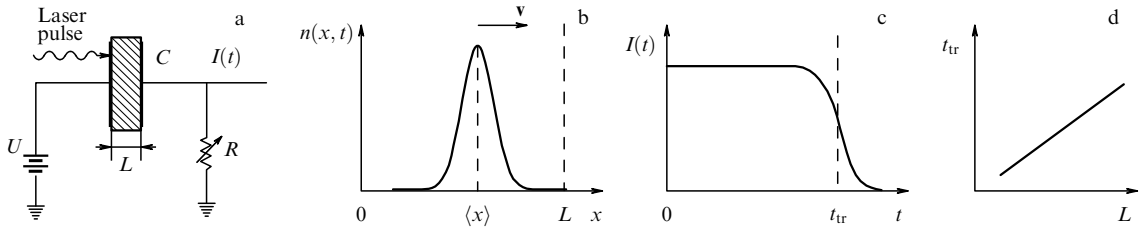

Figure 1. Experimental method for determining drift mobility: (a) electrical scheme of the experiment; (b) distribution of charge carriers in normal transport; (c) transient current curve in normal transport, and (d) time-of-flight linear dependence plotted vs. sample thickness.

edge of the Gaussian packet reaches the opposite edge of the sample. Current decrease takes a time of $\Delta x/\langle v\rangle$. As a result, the right edge of the photocurrent pulse becomes smooth (Fig. 1). Such a picture is typical of most ordered materials.

However, when determining drift mobility in certain disordered (amorphous, porous, disordered organic, strongly doped, etc.) semiconductors, a specific signal of transient current $I(t)$ is observed, having two regions with the power-law behavior of $I(t)$ and one intermediate region:

$$I(t) \propto \begin{cases} t^{-1+\alpha}, & t < t_{\rm tr}\,, \\ t^{-1-\alpha}, & t > t_{\rm tr}\,, \end{cases} \qquad \alpha < 1\,. \tag{2}$$

Exponent α, termed the *dispersion parameter*, depends on the medium characteristics and can vary with temperature. Parameter $t_{\rm tr}$ is called time of flight in analogy with normal transient processes, but has a different physical sense. It has been shown experimentally that in the dispersive transport the following relationship is valid:

$$t_{\rm tr} \propto \left(\frac{L}{U}\right)^{1/\alpha}, \tag{3}$$

where U is the voltage.

As noted in Refs [35, 44], the shape of the transient current signal in the reduced coordinates $\lg[I(t)/I(t_{\rm tr})] - \lg[t/t_{\rm tr}]$ is virtually independent of the applied voltage and sample size. This property, inherent in many (but not all: see Ref. [45]) materials, is referred to as the *property of shape universality of transient current curves* (Fig. 2). Occurrence of these features in many disordered materials confirms the *universality* of transport properties. A large number of experimental observations of this universality were reported both in early and recent publications (see Refs [1, 2, 35, 46, 47] for details).

Given dependences (2), (3), transient current curves automatically possess the *asymptotic property of universality*. Let us rewrite formulas (2) in the form

$$I(t) \sim \begin{cases} A(L, E, \alpha, \ldots)\, t^{-1+\alpha}, & t < t_{\rm tr}\,, \\ B(L, E, \alpha, \ldots)\, t^{-1-\alpha}, & t > t_{\rm tr}\,, \end{cases} \qquad \alpha < 1\,. \tag{4}$$

Time of flight $t_{\rm tr}$ is found from the intersection of asymptotes:

$$I_{\rm tr} = A(L, E, \alpha, \ldots)\, t_{\rm tr}^{-1+\alpha} = B(L, E, \alpha, \ldots)\, t_{\rm tr}^{-1-\alpha}\,.$$

Hence, $t_{\rm tr} = (B/A)^{1/2\alpha}$. The property of asymptotic universality means that the function $I(\tau t_{\rm tr})/I_{\rm tr}$ is independent of $t_{\rm tr}$. It is easy to see that this property holds for functions with

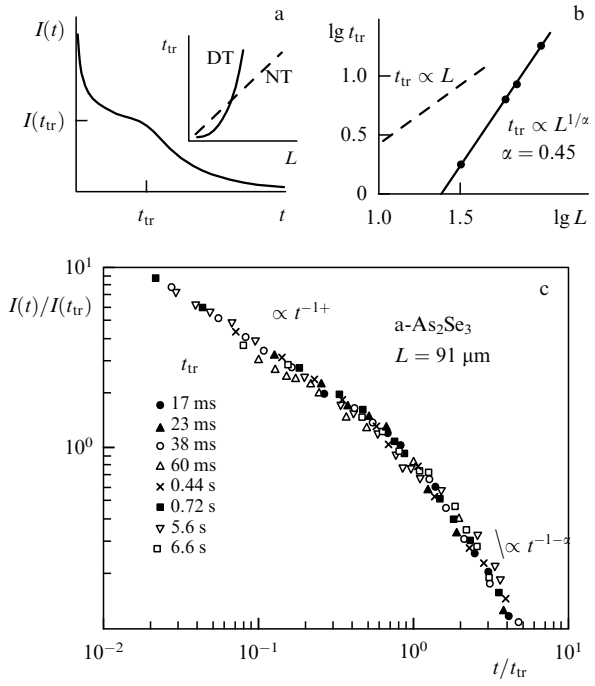

Figure 2. (a) Transient photocurrent relaxation curve; inset to this figure shows time of flight plotted vs. sample thickness for the cases of dispersive (DT) and normal (NT) transport; (b) $\lg t_{\rm tr} - \lg L$ dependence; dots — experimental data for a-As_2Se_3 from Ref. [35], solid line — power-law approximation, and (c) reduced time dependences of transient photocurrent in a-As_2Se_3 at the lg–lg scale from Ref. [35].

asymptotes (3):

$$\frac{I(\tau t_{\rm tr})}{I_{\rm tr}} \sim \begin{cases} \tau^{-1+\alpha}, & \tau < 1\,, \\ \tau^{-1-\alpha}, & \tau > 1\,, \end{cases} \qquad \alpha < 1\,.$$

It should be noted that the value of $I(t_{\rm tr})$ does not equal $I_{\rm tr}$ — point $(t_{\rm tr}, I_{\rm tr})$ is determined by intersection of asymptotics of the transient current at small and large times.

Transient photocurrent in a sample of thickness L is defined as conduction current density averaged over thickness:

$$I(t) = \frac{1}{L}\int_0^L j(x, t)\, {\rm d}x\,. \tag{5}$$

Evidently, the integral in the last formula is independent of L at the initial stage for $t \ll t_{\rm tr}$. According to relationship (3), one finds $t_{\rm tr} \propto L^{1/\alpha}$. Therefore, it is possible to write out

for A, B, and $I_{\rm tr}$ the following relations:

$$A \propto L^{-1}\,, \qquad B \propto A t_{\rm tr}^{2\alpha} \propto L\,, \qquad I_{\rm tr} \propto L^{-1/\alpha}\,.$$

Current density $j(x,t)$ is proportional to probability flux $q(x,t)$:

$$j(x,t) = eNq(x,t)\,,$$

where e is the elementary charge, and N is the number of photoinjected carriers per unit area of the illuminated electrode. The probability flux is equivalent to the first passage time distribution density $p(t|x)$:

$$q(x,t) \equiv p(t|x)\,.$$

Product $p(t|x)\,{\rm d}t$ is the probability that a walking particle (in our case, a charge carrier) will reach coordinate x within a time interval $(t, t+{\rm d}t)$. The coordinate distribution density $p(x|t)$ of the walking particle and probability flux $p(t|x)$ are related by the probability conservation equation

$$\frac{\partial p(x|t)}{\partial t} + \frac{\partial p(t|x)}{\partial x} = \delta(x)\delta(t)\,. \tag{6}$$

In the mathematical sense, the shape universality of transient current curves constitutes a self-similarity property at the time scales:

$$I(t;L_2) \approx \left(\frac{L_2}{L_1}\right)^{-1/\alpha} I\left(t\left(\frac{L_2}{L_1}\right)^{-1/\alpha};L_1\right), \tag{7}$$

where $I(t;L_1)$ and $I(t;L_2)$ are the time dependences of transient current in samples of thickness L_1 and L_2, respectively. According to relationships (2), the long-time asymptotics of transient current and the first passage time distribution density follow the power law with exponent α. By substituting first passage time density for conduction current density in formula (5), taking into account the shape universality of transient current curves (7), it is possible to show that functions $p(t|x)$ are self-similar at the time scales:

$$p(t|x_2) = \left(\frac{x_2}{x_1}\right)^{-1/\alpha} p\left(t\left(\frac{x_2}{x_1}\right)^{-1/\alpha}\middle| x_1\right).$$

Thus, the property of shape universality of transient current curves with respect to variations in sample thickness and the external field intensity is self-similar over time (scaling) upon a change in parameter $t_{\rm tr}$.

3. From self-similarity to stable laws and fractional derivatives

Time $\tau(kx)$ during which coordinate kx is reached (k is any natural number) is a random quantity, in fact the sum of k terms representing independent random times during which a carrier passes through the layers $(0,x),(x,2x),\ldots,((k-1)x,kx)$: $\tau(kx) = \sum_{j=1}^{k}\tau_j(x)$. The corresponding distribution is expressed as a k-fold convolution of the passage time distributions for each layer:

$$p(t|kx) = k^{-1/\alpha}p(tk^{-1/\alpha}|x) = p^{*k}(t|x)\,,$$

$$p^{*k}(t|x) = \int_0^t {\rm d}t'\, p(t-t'|x)\, p^{*(k-1)}(t'|x)\,.$$

Applying Laplace transformation

$$\tilde{p}(s|x) = \int_0^\infty {\rm d}t\; p(t|x)\exp(-st)\,,$$

we arrive at

$$\tilde{p}(s|kx) = \tilde{p}(k^{1/\alpha}s|x) = \left[\tilde{p}(s|x)\right]^k.$$

Taking the logarithm of the latter relation and raising it to the $1/\alpha$ power yields

$$\left[\ln\tilde{p}(s|kx)\right]^{1/\alpha} = \left[\ln\tilde{p}(k^{1/\alpha}s|x)\right]^{1/\alpha} = k^{1/\alpha}\left[\ln\tilde{p}(s|x)\right]^{1/\alpha}.$$

The latter equalities lead to

$$\left[\ln\tilde{p}(s|x)\right]^{1/\alpha} = s\left(-\frac{x}{K}\right)^{1/\alpha},$$

where K is a certain constant. For $\tilde{p}(s|x)$, we have the following expression

$$\tilde{p}(s|x) = \exp\left(-\frac{x}{K}\,s^\alpha\right). \tag{8}$$

This function is the Laplace transform of one-sided stable density with characteristic exponent α (see, for instance, Refs [48, 49]):

$$\begin{aligned} p(t|x) &= \frac{1}{2\pi{\rm i}}\int_C {\rm d}s\; p(s|x)\exp(st) \\ &= \left(\frac{x}{K}\right)^{-1/\alpha} g^{(\alpha)}\left(t\left(\frac{x}{K}\right)^{-1/\alpha}\right). \end{aligned} \tag{9}$$

Thus, the first passage time distribution density represents a one-sided stable density with a characteristic exponent equaling the dispersion parameter.

Substitution of the expression for conduction current density

$$j(x,t) = eNp(t|x) = eN\left(\frac{x}{K}\right)^{-1/\alpha} g^{(\alpha)}\left(t\left(\frac{x}{K}\right)^{-1/\alpha}\right) \tag{10}$$

into formula (5) leads to

$$I(t) = \frac{eKN\alpha}{L}\,t^{\alpha-1}\int_{\zeta_0}^\infty \zeta^{-\alpha}g^{(\alpha)}(\zeta)\,{\rm d}\zeta\,, \qquad \zeta_0 = t\left(\frac{L}{K}\right)^{-1/\alpha}. \tag{11}$$

Figure 3a displays transient current curves constructed using formula (11) for different values of the dispersion parameter. Comparison with experimental data taken from Refs [8] and [50] for vitreous As_2S_3 and a-As_2Se_3, respectively, undergoing self-similar dispersive transport, is presented in Fig. 3b.

Asymptotic analysis of expression (11) shows that ζ_0 is small when $t \ll t_{\rm tr}$ (the expression for $t_{\rm tr}$ will be derived below). Using the formula for the moments of one-sided stable distributions [48], namely

$$\int_0^\infty s^{-\alpha}g^{(\alpha)}(s)\,{\rm d}s = \frac{1}{\Gamma(1+\alpha)}\,,$$

yields

$$I(t) \cong \frac{e\,KN}{L\,\Gamma(\alpha)}\,t^{\alpha-1}\,, \qquad t < t_{\rm tr}\,. \tag{12}$$

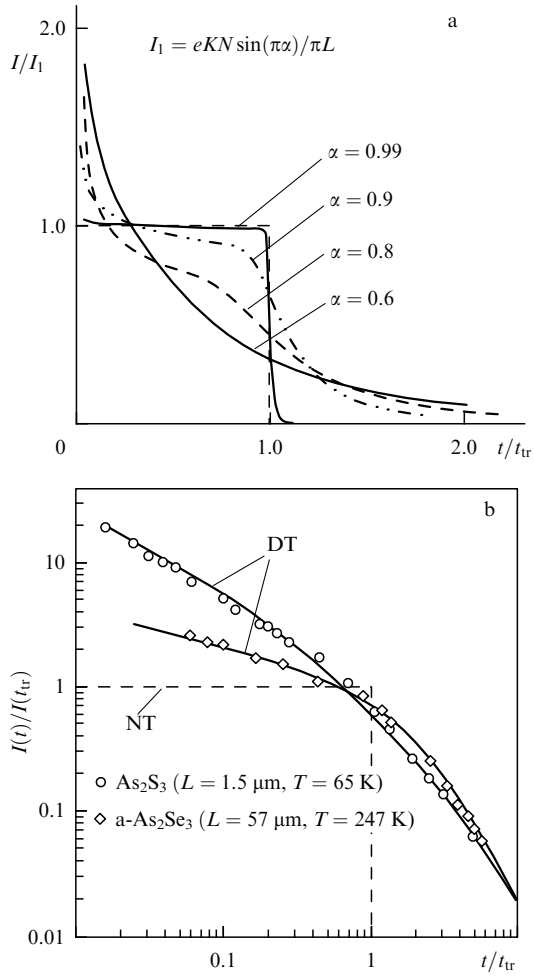

Figure 3. Theoretical transient photocurrent curves for different values of the dispersion parameter. (b) Reduced transient current density (circles — experimental data for vitreous As_2S_3 [8], rhombi — data for a-As_2Se_3 [50], solid lines — calculations from formula (11) with adjustable parameters α and t_{tr}).

At long time scales, $t \gg t_{tr}$ and $\zeta_0 \gg 1$, density $g^{(\alpha,1)}(s)$ can be represented as [48]

$$g^{(\alpha,1)}(s) \cong \frac{\Gamma(1+\alpha)\sin\pi\alpha}{\pi s^{\alpha+1}},$$

leading to the following asymptotics

$$I(t) \cong \frac{eNL}{2K\Gamma(1-\alpha)}\, t^{-\alpha-1}, \qquad t > t_{tr}. \tag{13}$$

Equating expressions (12) and (13), we find the relationship for parameter t_{tr}:

$$t_{tr} = \left(\frac{L}{K}\sqrt{\frac{\Gamma(\alpha)}{2\Gamma(1-\alpha)}}\right)^{1/\alpha}. \tag{14}$$

This formula implies that relation $t_{tr} \propto (L/E)^{1/\alpha}$ [35] is experimentally confirmed at a fixed temperature. Drift mobility is defined as

$$\mu_d = \frac{L}{Et_{tr}} = \frac{L}{E}\left(\frac{L}{K}\sqrt{\frac{\Gamma(\alpha)}{2\Gamma(1-\alpha)}}\right)^{-1/\alpha}.$$

It follows from Eqns (6) and (9) that the carrier concentration $n(x,t)$ is given by

$$n(x,t) = Np(x|t) = -N\frac{\partial}{\partial x}\int_0^t p(t|x)\,\mathrm{d}t = \frac{Nt}{\alpha K}\left(\frac{x}{K}\right)^{-1/\alpha-1} g^{(\alpha)}\left(t\left(\frac{x}{K}\right)^{-1/\alpha}\right). \tag{15}$$

Transient current is expressed through the total concentration of carriers according to the formula (see Ref. [2] for details)

$$I(t) = \frac{e}{L}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L (x-L)\,n(x,t)\,\mathrm{d}x.$$

Substituting carrier concentration (15) into this formula as a check, we come back to formula (11).

Reduced coordinate and first passage time distribution densities for dispersive motion of carriers in an electric field are shown in Fig. 4. Plots in Fig. 4a, b were calculated from formulas (15) and (9), respectively.

Time dependence of a charge that passed through the sample, as found from the formula

$$Q(t) = \int_0^t j(L,t)\,\mathrm{d}t = eNG^{(\alpha)}\left(t\left(\frac{L}{K}\right)^{-1/\alpha}\right),$$

is presented in Fig. 5.

Functions (9) and (15) are the solutions of equations with fractional derivatives as shown below. The transform of the first passage time distribution density (8) satisfies the equation

$$\frac{s^\alpha}{K}\,\tilde{p}(s|x) + \frac{\partial}{\partial x}\,\tilde{p}(s|x) = \delta(x).$$

Taking into account that inverse Laplace transform gives

$$s^\alpha\tilde{p}(s|x) \mapsto \frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial t}\int_0^t \frac{p(t'|x)}{(t-t')^\alpha}\,\mathrm{d}t' = \frac{\partial^\alpha}{\partial t^\alpha}\,p(t|x),$$

we arrive at a fractional differential equation for density $p(t|x)$:

$$K^{-1}\,\frac{\partial^\alpha}{\partial t^\alpha}\,p(t|x) + \frac{\partial}{\partial x}\,p(t|x) = \delta(x)\delta(t).$$

Formula (10) implies that an analogous equation holds true for conduction current density and free carrier concentration. Here, $\partial^\alpha/\partial t^\alpha$ is the Riemann–Liouville fractional derivative of order $0 < \alpha < 1$.

The Laplace image of normalized total carrier concentration (15), taking the form

$$\tilde{n}(x,s) = -N\frac{\partial}{\partial x}\frac{\tilde{p}(s|x)}{s} = -N\frac{\partial}{\partial x}\frac{1}{s}\exp\left(-\frac{x}{K}s^\alpha\right) = N\frac{s^{\alpha-1}}{K}\exp\left(-\frac{x}{K}s^\alpha\right) = N\frac{s^{\alpha-1}}{K}\,\tilde{p}(s|x), \tag{16}$$

is the solution of the equation

$$s^\alpha\tilde{n}(x,s) + K\frac{\partial}{\partial x}\,\tilde{n}(x,s) = Ns^{\alpha-1}\delta(x),$$

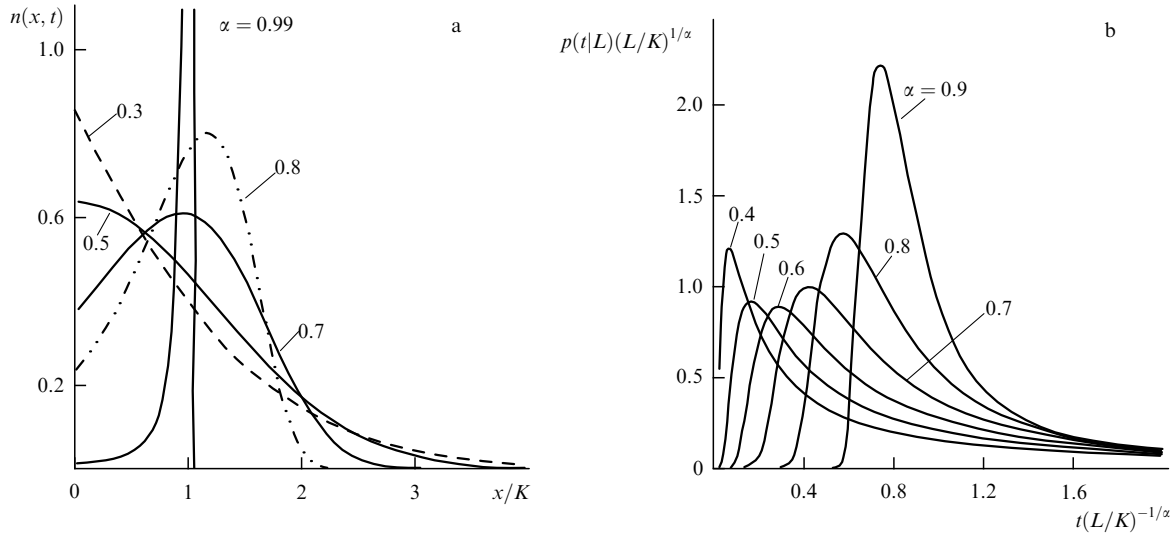

Figure 4. (a) Coordinate distribution densities for dispersive drift at different values of the dispersion parameter. (b) First passage time distribution density.

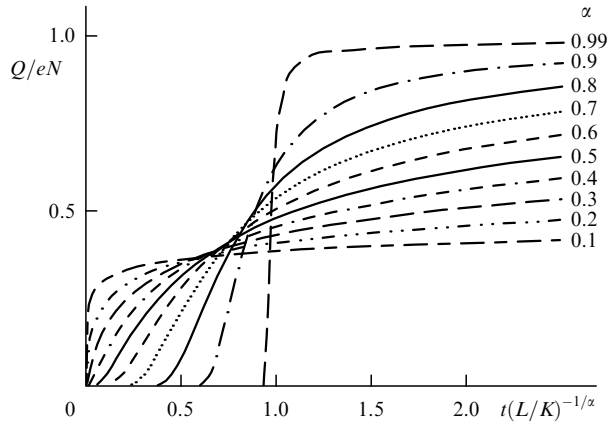

Figure 5. Time dependence of a charge that passed through the sample for different values of the dispersion parameter.

the inverse transformation of which yields a fractional differential equation for dispersive drift:

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}}\, n(x,t) + K\,\frac{\partial}{\partial x}\, n(x,t) = \frac{N t^{-\alpha}}{\Gamma(1-\alpha)}\,\delta(x)\,. \qquad (17)$$

To conclude, it follows from the shape universality of transient current curves and the power-law dependence of flight time on sample thickness, that the first passage time without additional assumptions as regards the transfer mechanism is distributed according to a stable law with the characteristic exponent equalling the dispersion parameter. Such time distribution accounts for the presence of power-law asymptotics of transient current at long and short time scales. Moreover, conduction current density, free carrier concentration, and total carrier concentration are the solutions of fractional differential equations. It is also worth noting that the form of stable transient current density agrees with the Scher–Montroll hypothesis [35] for power-law distribution of the times of carrier residence in localized states during DT.

4. The Scher–Montroll model

Continuous time random walk (CTRW) model, introduced in the famous paper [35] by Scher and Montroll in 1975, provided the first detailed explanation of all the main patterns of current behavior in time-of-flight experiments with amorphous semiconductors.

The main assumptions of this model are as follows:

(1) The transport of charge carriers is a jumplike walking process in which the walkers change their positions jumpwise at random instants of time.

(2) Carrier jumps are independent of one another, and time intervals between them (*waiting times*) are independent, identically distributed random quantities τ.

(3) Waiting times are characterized by a broad power-law distribution:

$$\mathsf{P}\{\tau > t\} \propto t^{-\alpha}\,, \qquad t \to \infty\,, \qquad 0 < \alpha < 1\,. \qquad (18)$$

Power-law asymptotics of transient current (2) were for the first time explained by Shlesinger [51] based on the CTRW model. The power-law waiting time distribution in the hopping transport model was deduced from *ab initio* calculations done by Tunaley [52] and Scher and Lax [18] in 1972. The authors of Ref. [35] simulated charge transfer in disordered semiconductors as carrier hoppings within the model grid of localized states. The grid constitutes a regular cubic lattice, each cell of which contains randomly distributed sites (localized states). The waiting time till the next hopping depends on the distance to the nearest neighbor sites. As shown in Ref. [35], the cell residence time distribution can obey the power law owing to site spatial disorder in a cell.

Assumption (18) is of fundamental importance because such a time distribution having an infinite mean value leads to result (2), whereas any distribution with a finite mean waiting time, e.g., exponential distribution, produces a normal signal (1) [41]. Why the infinite mean value does not contradict the physical sense was plausibly explained in Ref. [52]. The divergence of integral

$$\lim_{T\to\infty} \int_0^T \psi(t)\, t\, \mathrm{d}t = \infty$$

actually means only the impossibility of using $\langle\tau\rangle$ for calculations. Because

$$\lim_{T\to\infty}\int_T^\infty \psi(t)\,\mathrm{d}t = 0\,,$$

all observed realizations of τ are finite, and there is no paradox.

As is known, the description of normal transport is based on the central limit theorem of the probability theory. For random quantities distributed according to law (18), divergence of dispersion for $\alpha < 2$ and divergence of mathematical expectation for $\alpha < 1$ make this theorem inapplicable, which necessitates the application of the generalized limit theorem.

The generalized limit theorem. Let random quantities X_j be independent and identically distributed, and satisfy the following conditions

$$\mathsf{P}(X > x) \sim a_+ x^{-\alpha}\,, \qquad x\to\infty\,,$$
$$\mathsf{P}(X < -x) \sim a_- x^{-\alpha}\,, \qquad x\to\infty\,,$$

$0 < \alpha \leqslant 2$, $a_+ \geqslant 0$, $a_- \geqslant 0$, and $a_+ + a_- > 0$. Then, A_n and $B_n > 0$ sequences exist such that, as $n\to\infty$, one finds

$$\frac{\sum_{j=1}^n X_j - A_n}{B_n} \overset{d}{\sim} S^{(\alpha,\beta)}\,,$$

where $S^{(\alpha,\beta)}$ is the stable random variable with exponent α and asymmetry parameter $\beta = (a_+ - a_-)/(a_+ + a_-)$. Stable random quantities can be defined through characteristic functions having the form (form A) [48]

$$g^{(\alpha,\beta)}(k) = \exp\left\{-|k|^\alpha\left[1 - \mathrm{i}\beta\tan\left(\frac{\alpha\pi}{2}\right)\operatorname{sgn}(k)\right]\right\}, \quad \alpha\neq 1\,,$$
$$g^{(1,\beta)}(k) = \exp\left(-|k|\right).$$

Certainly, there are an infinite number of sequences of normalizing coefficients A_n, B_n showing similar asymptotic behavior as $n\to\infty$. By way of example, they can be defined in the following way ($a = \langle X\rangle$ and $c = a_+ + a_-$):

at $\alpha = 2$ $\quad A_n = na\,, \quad B_n = \sqrt{cn\ln n}\,,$

at $\alpha\in(1,2)$ $\quad A_n = na\,, \quad B_n = \left(\dfrac{\pi cn}{2\Gamma(\alpha)\sin(\alpha\pi/2)}\right)^{1/\alpha}\,,$

at $\alpha = 1$ $\quad A_n = \beta cn\ln n\,, \quad B_n = \dfrac{\pi cn}{2}\,,$

at $\alpha\in(0,1)$ $\quad A_n = 0\,, \quad B_n = \left(\dfrac{\pi cn}{2\Gamma(\alpha)\sin(\alpha\pi/2)}\right)^{1/\alpha}\,.$

In the Scher–Montroll model, waiting times τ (positive random quantities) are distributed according to the asymptotically power law, which means that at macroscopic scales much greater than the average distance between localized states the first passage time distribution, conduction current density, and concentration of delocalized carriers considered as functions of time should have the form of stable density distribution in agreement with formulas (9) and (10) obtained in Section 3.

The main characteristics of the CTRW model are waiting time (τ) and path (λ) distributions. Let us denote densities of these distributions as $\psi(t)$ and $p(\mathbf{r})$. Coordinate distribution density $p(\mathbf{r},t)$ of a particle executing jumpwise walking and initially located at the origin of coordinates is defined in terms of the Fourier–Laplace transform [53]:

$$\hat{\tilde{p}}(\mathbf{k},s) = \frac{1-\tilde{\psi}(s)}{s\left[1-\hat{p}(\mathbf{k})\tilde{\psi}(s)\right]}\,, \tag{19}$$

where

$$\hat{\tilde{p}}(\mathbf{k},s) = \int_{\mathbf{R}}\mathrm{d}\mathbf{r}\,\exp(\mathrm{i}\mathbf{k}\mathbf{r})\int_0^\infty \mathrm{d}t\,\exp(-st)\,p(\mathbf{r},t)$$

is the Fourier–Laplace transform of normalized particle concentration, $\hat{p}(\mathbf{k})$ is the Fourier transform of path distribution density, and $\tilde{\psi}(s)$ is the Laplace transform of waiting time distribution density. Substituting into Eqn (19) the asymptotic series expansion of the Laplace image of waiting time distribution density with the power-law tail

$$\tilde{\psi}(s) \sim 1 - \frac{s^\alpha}{c^\alpha}\,, \qquad s\ll c\,,$$

along with asymptotic expansion of the Fourier image of path distribution density:

$$\hat{p}(\mathbf{k}) \sim 1 + \mathbf{c}_1\mathrm{i}\mathbf{k} - c_2k^2\,, \qquad |\mathbf{k}| \ll \frac{1}{|\mathbf{c}_1|}\,,$$

and applying the Tauberian theorem [54], we shall obtain

$$\hat{\tilde{p}}(\mathbf{k},s) = \frac{c^{-\alpha}s^{\alpha-1}}{-\mathbf{c}_1\mathrm{i}\mathbf{k} + c_2k^2 + s^\alpha/c^\alpha}\,.$$

Rewriting the last expression in the form

$$\left[s^\alpha - \mathbf{c}_1c^\alpha\mathrm{i}\mathbf{k} + c_2c^\alpha k^2\right]\hat{\tilde{p}}(\mathbf{k},s) = s^{\alpha-1}\,,$$

and applying inverse Fourier and Laplace transformations yield

$$\frac{\partial^\alpha}{\partial t^\alpha}\,p(\mathbf{r},t) + \mathbf{K}\nabla p(\mathbf{r},t) - C\nabla^2 p(\mathbf{r},t) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\,\delta(\mathbf{r})\,. \tag{20}$$

This equation in a one-dimensional case with $C = 0$ coincides with equation (17) obtained in Section 3.

Thus, fractional differential equations and their solutions are consistent with the Scher–Montroll random walk model.

5. The Arkhipov–Rudenko approach

In 1982, Arkhipov and Rudenko proposed an approach in the framework of the concept of multiple trapping transport that yields analytical results for the description of dispersive transport [23, 24]. The Arkhipov–Rudenko theory is rather popular and widely used in ongoing research (see, e.g., Refs [55, 56]). Here is a quotation from their work, giving an idea of this approach [23]: "The carriers make transitions between the conduction state and localized levels. This process finally results in equilibrium between the mobile and immobile carrier fractions. Before thermal equilibrium is established, the energy interval, in which the localized states are distributed, may be divided into two regions: (1) The regions of shallow traps is situated between the mobility edge and some boundary energy $\varepsilon_*(t)$. In this region the equilibrium between the conduction state and traps is established at some time t. ... (2) The region of deep traps lies below the boundary energy $\varepsilon_*(t)$. No carriers are realized from these

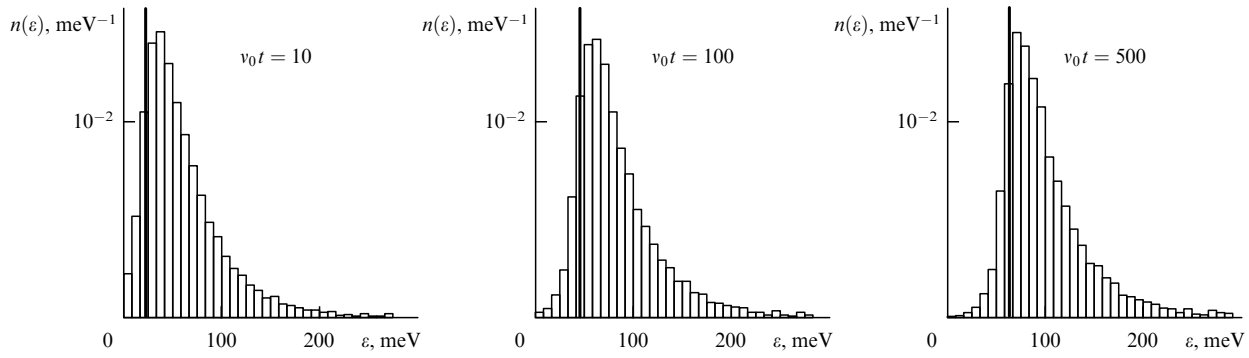

Figure 6. Variation of carrier energy distribution with time: $\varepsilon_0 = 40$ meV, and $kT = 10$ meV.

traps until the time t. The concentration of carriers captured by the deep traps changes only due to trapping. Consequently we may neglect the 'release term'... ." Although this approach is an approximate one, it fairly well describes the main features of transient current behavior in time-of-flight experiments. Specifically, it explains the power-law asymptotics of transient current for exponential density of states, power-law dependence of drift mobility on sample thickness, electric field strength, etc. [24].

By dividing localized states into shallow and deep ones, an equation for nonequilibrium transport with time-dependent diffusion coefficient D and mobility μ was derived [23]:

$$\frac{\partial n(x,t)}{\partial t} + \mu_1(t)E\,\frac{\partial n(x,t)}{\partial x} - D_1(t)\,\frac{\partial^2 n(x,t)}{\partial x^2} = -\lambda(t)\big[n(x,t) - n(x,0)\big]\,, \tag{21}$$

where time functions are defined by the relationships

$$\mu_1(t) = \frac{1}{1+1/\theta(t)}\,\mu\,, \qquad D_1(t) = \frac{1}{1+1/\theta(t)}\,D\,,$$
$$\lambda(t) = \frac{1}{1+1/\theta(t)}\,\frac{1}{\tau(t)}\,, \tag{22}$$
$$\frac{1}{\theta(t)} = \int_0^{\varepsilon_*(t)} \mathrm{d}\varepsilon\;\frac{\rho(\varepsilon)}{N_\mathrm{c}}\exp\left(\frac{\varepsilon}{kT}\right), \qquad \frac{1}{\tau(t)} = \int_{\varepsilon_*(t)}^{\infty} \mathrm{d}\varepsilon\, c(\varepsilon)\,\rho(\varepsilon)\,,$$

and the demarcation level position is found by solving the equation

$$c(\varepsilon_*)N_\mathrm{c}\exp\left(-\frac{\varepsilon_*}{kT}\right)t = 1\,.$$

In the case of weak energy dependence of the capture coefficient, $c(\varepsilon) \approx c_0$, the demarcation level equals $\varepsilon_* = kT\ln(v_0t)$, where $v_0 = N_\mathrm{c}c_0$ is the mean attempt-to-escape frequency.

The authors of Refs [23, 26] distinguish a strongly nonequilibrium transport regime in which most carriers are captured in rather deep traps (below the demarcation level) and are unlikely to be released by the instant of time t. This regime corresponds to the values of dispersion parameter $\alpha < 0.5$. The equation called by Arkhipov and Rudenko the 'master DT equation' has the form

$$n_\mathrm{c}(\mathbf{r},t) = \frac{\partial}{\partial t}\big[\tau(t)\,n(\mathbf{r},t)\big]\,, \tag{23}$$

where the function $\tau(t)$ is given by the expression

$$\tau(t) = \left[v_0\int_{kT\ln(v_0t)}^{\infty}\mathrm{d}\varepsilon\;\rho(\varepsilon)\right]^{-1}.$$

Here, $\rho(\varepsilon)$ is the density of localized states.

In this regime, it is possible to neglect the contribution of carriers occupying shallow traps, which is equivalent to neglecting the time derivative in equation (21) (see Ref. [23] for details):

$$n(x,t) + \mu E\tau(t)\,\frac{\partial}{\partial x}\,n(x,t) - D\tau(t)\,\frac{\partial^2}{\partial x^2}\,n(x,t) = n(x,0)\,. \tag{24}$$

Equation (24) can be obtained directly from the continuity equation using relationship (23). Given the initial condition $n(x,0) = N\delta(x)$, the solution is the exponential function:

$$n(x,t) = \frac{N}{\mu E\tau(t)}\exp\left(-\frac{x}{\mu E\tau(t)}\right). \tag{25}$$

Solutions obtained using relationship (23) and their comparison with the solutions we found in the framework of the fractional differential approach will be presented below.

As follows from Eqn (23), delocalized carrier density has the form

$$n_\mathrm{c}(x,t) = Nx\,\frac{\tau'(t)}{\big[\mu E\tau(t)\big]^2}\exp\left(-\frac{x}{\mu E\tau(t)}\right). \tag{26}$$

Then, transient current is defined as follows:

$$I(t) = \frac{e\mu E}{L}\int_0^L \mathrm{d}x\,n_\mathrm{c}(x,t) = eN\mu EL^{-1}\tau'(t)\left[1 - \left(1+\frac{L}{\mu E\tau(t)}\right)\exp\left(-\frac{L}{\mu E\tau(t)}\right)\right].$$

For the exponential energy distribution of band tail states, under the conditions of weak energy dependence of the capture coefficient, function $\tau(t)$ takes the form [26, 29]

$$\tau(t) = \frac{N_\mathrm{c}}{N_\mathrm{t}}\,v_0^{-1}(v_0t)^{\alpha}\,. \tag{27}$$

Figures 6 and 7 present histograms of carrier energy distribution obtained by numerical Monte Carlo simulation of the filling of localized states in a time-of-flight experiment at two temperatures: 115 and 290 K. Exponential density of states $\rho(\varepsilon) = (N_\mathrm{t}/\varepsilon_0)\exp(-\varepsilon/\varepsilon_0)$ of width $\varepsilon_0 = 40$ meV was used for the purpose of simulation. The solid line shows the

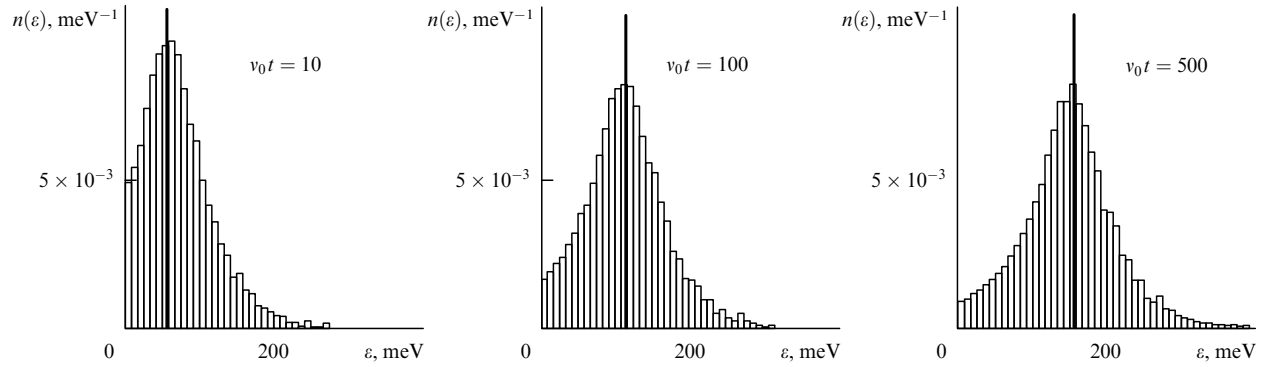

Figure 7. Variation of carrier energy distribution with time: $\varepsilon_0 = 40$ meV, and $kT = 25$ meV.

position of demarcation level $\varepsilon_*(t) = kT \ln(v_0 t)$. It follows that τ-approximation is rough for the second case, i.e., for $T = 290$ K and $\alpha \approx 0.6$; in other words, the fraction of carriers in shallow traps, $\varepsilon < \varepsilon_*$, is large enough to be taken into account in calculations.

The approximation based on Eqns (23) and (24) is sometimes called the τ-approximation [11, 56]. It allows all the results for the exponential density of localized states to be expressed in elementary functions, but poorly describes transport at dispersion parameters $\alpha > 0.5$, because the main condition of this approximation is violated. For $\alpha > 0.5$, the fraction of shallow-trap carriers cannot be neglected. Doubtless, the authors of Ref. [23] understood this when they derived the τ-approximation for strongly nonequilibrium transport. Not surprisingly, equation (24) does not go over into the equation of normal transport for $\alpha > 1$, where $\alpha = kT/\varepsilon_0$ for the exponential density of states. It should be noted, however, that the more general equation (21) does not satisfy the correspondence principle either, i.e., it does not go over into the normal transport equation upon enhancement of the dispersion parameter.

By way of example, the following equation for exponential density of states is obtained from Eqn (22):

$$\frac{1}{\theta(t)} = \frac{\alpha N_t}{(1-\alpha)N_c}\left[(v_0 t)^{1-\alpha} - 1\right].$$

For $v_0 t \gg 1$, one finds

$$\alpha < 1\,, \quad \frac{1}{\theta(t)} \approx \frac{\alpha N_t}{(1-\alpha)N_c}(v_0 t)^{1-\alpha}\,,$$
$$\mu_1(t) \propto t^{\alpha-1}\,, \quad D_1(t) \propto t^{\alpha-1};$$
$$\alpha \geqslant 1\,, \quad \frac{1}{\theta(t)} \approx \frac{\alpha N_t}{(\alpha-1)N_c}\,,$$
$$\mu_1(t) \approx \text{const}\,, \quad D_1(t) \approx \text{const}\,.$$

When $\alpha = kT/\varepsilon_0 > 1$, it follows from the Scher–Montroll model [35], numerical and analytical calculations in the framework of the multiple trapping model [31], and the fractional differential approach [33, 32] that the normal transport regime must take place in long-time asymptotics. Equation (21) for $\alpha \geqslant 1$ has the form

$$\frac{\partial n(x,t)}{\partial t} + \mu_1 E \frac{\partial n(x,t)}{\partial x} - D_1 \frac{\partial^2 n(x,t)}{\partial x^2} = -A(v_0 t)^{-\alpha}\left[n(x,t) - n(x,0)\right],$$

where μ_1 and D_1 are constants, and

$$A = \frac{(\alpha-1)v_0 N_t}{\alpha(N_c + N_t) - N_c}\,.$$

The Green function of the latter equation is not a Gaussian function, even though its left-hand side contains the standard Fokker–Planck operator with constant coefficients.

6. Physical basis of power-law waiting time distribution

The physical foundations of a broad power-law waiting time distribution (18) have been discussed in many studies. It was shown in Ref. [57] that such distribution underlain by a multiple trapping mechanism may be a consequence of exponential energy distribution of localized states. The exponential form of the density of band tail states was extensively used in model calculations and discussions of the results of experiments on transport and luminescence in disordered semiconductors [57–59]. However, as mentioned in Refs [25, 26], the main features of carrier packet propagation during dispersive transport controlled by carrier capture in localized states may be just as well retained in other, sufficiently broad energy distributions of traps. Transport in a purely hopping model occurs via tunneling between adjacent traps, and power-like waiting time distribution results from dispersion of distances between localized states [31]. Dispersive transport is observed in disordered semiconductors of a different nature. It is worthwhile to study the common mathematical principles accounting for anomalous transport in different physical models.

Random waiting time τ in a given localized state is characterized by the probability

$$\mathsf{P}\{\tau > t\} = \exp\left(-\frac{t}{\theta}\right), \tag{28}$$

where the parameter θ is the mean residence time in a given trap.

In a model of transport controlled by multiple trapping (see, for instance, Refs [6, 25, 60]), one finds

$$\theta = \omega_\varepsilon^{-1} \exp\left(\frac{\varepsilon}{kT}\right), \tag{29}$$

where ω_ε is the carrier capture rate in a trap with energy ε.

In the tunneling transport model proposed in Ref. [61], one has

$$\theta = \beta\left[\exp(\gamma d) - 1\right], \tag{30}$$

where d is the distance to the neighbor site, γ is the positive constant, and the parameter β is inversely proportional to the applied field strength.

In the Miller–Abrahams random grid model for hopping conductivity (see, e.g., Ref. [62]), the mean residence time is defined as

$$\theta = \left[v_0 \sum_j \exp\left(-\frac{2d_{ij}}{a} - \frac{\varepsilon_{ij}}{kT} \right) \right]^{-1}, \tag{31}$$

where v_0 is the characteristic carrier hopping rate, a is the localization radius, d_{ij} is the distance between the ith and jth sites, and ε_{ij} is the corresponding energy difference.

The lack of long-range order, dispersion of intertrap distances, and fluctuations of localized state energy in disordered semiconductors account for different values of the parameter θ in individual localized states. In averaging over a certain sample volume, quantity θ behaves like a random one. As follows from formulas (29)–(31), a weak dispersion of intertrap distances and/or localized state energies result in a broad distribution of the parameter θ that may have a 'heavy' power-law tail.

Let us consider the case specified by formula (30). It is assumed in this model that carriers undergo one-dimensional motion along the positive direction of the x-axis, given by the direction of the applied field. Randomly positioned on the axis are potential wells, between which the carriers are tunnelled. In a quasiclassical approximation, the distribution of random time τ during which a charge carrier resides at a selected site is given by probability (28).

On the assumption of uniform potential well distribution along the straight line, the probability of interest equals

$$\mathsf{P}\{d > x\} = \exp\left(-\frac{x}{d_0} \right);$$

hence, one arrives at

$$\mathsf{P}\{\theta > t\} = \mathsf{P}\Big\{ \beta\big[\exp(\gamma d) - 1\big] > t \Big\} = \frac{1}{(1 + t/\beta)^{\alpha_1}}, \tag{32}$$

where

$$\alpha_1 = \frac{1}{\gamma d_0}.$$

According to formula (28), conditional probability at a given θ equals

$$\mathsf{P}\{\tau > t|\theta\} = \exp\left(-\frac{t}{\theta} \right),$$

and it follows from relationship (32) that θ has the distribution density

$$p_\theta(t) = \frac{\alpha_1}{\beta(1 + t/\beta)^{\alpha_1 + 1}}.$$

Then, the absolute (i.e., averaged over θ) probability for the residence time of the carrier in a site takes the form

$$\mathsf{P}\{\tau > t\} = \int_0^\infty \mathsf{P}\{\tau > t \,|\theta = t'\}\, p_\theta(t')\, \mathrm{d}t'$$
$$\sim \alpha_1 \Gamma(\alpha_1) \left(\frac{t}{\beta} \right)^{-\alpha_1}, \qquad t \gg \beta. \tag{33}$$

As shown in Ref. [35], the dispersive behavior may be a consequence of multiple trapping in localized states distributed by energies. The assumption that the density of states below the mobility edge exponentially falls off with energy may lead to formula (2) with the parameter α_1 depending on temperature T. In the case of exponential tail of the density of states, namely

$$\rho(\varepsilon) \propto \exp\left(-\frac{\varepsilon}{\varepsilon_0} \right),$$

assuming that the capture rate weakly depends on trap energy $\omega_\varepsilon \approx \omega_0$, we obtain

$$p_\theta(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\, \mathsf{P}\{\theta > t\} = -\frac{\mathrm{d}}{\mathrm{d}t}\, \mathsf{P}\left\{ \omega_0^{-1} \exp\left(\frac{\varepsilon}{kT} \right) > t \right\}$$
$$= -\frac{\mathrm{d}}{\mathrm{d}t} (\omega_0 t)^{-\alpha_1} = \alpha_1 \omega_0 (\omega_0 t)^{-\alpha_1 - 1},$$

where

$$\alpha_1 = \frac{kT}{\varepsilon_0}.$$

The absolute probability for the residence time of a carrier in the localized state is equal to

$$\mathsf{P}\{\tau > t\} = \int_0^\infty \mathsf{P}\{\tau > t \,|\theta = t'\}\, p_\theta(t')\, \mathrm{d}t'$$
$$\sim \alpha_1 \Gamma(\alpha_1) (\omega_0 t)^{-\alpha_1}, \qquad t \gg \omega_0^{-1}. \tag{34}$$

Naturally, energy and spatial distributions of localized states in most cases differ from exponential ones. Notice that exponential distribution has a methodological deficiency of being characterized by a single parameter: the mathematical expectation of this distribution equals the root-mean-square deviation. Varying this parameter, it is impossible to theoretically determine changes in transport properties during transition from an ordered to a disordered position of trapping centers.

Let us consider the multiple trapping mechanism at greater length. Take a gamma-distribution, instead of an exponential one, and write its normalized density in the form

$$\rho(\varepsilon) = \frac{\varepsilon_0}{\sigma_\varepsilon^2\, \Gamma(\varepsilon_0^2/\sigma_\varepsilon^2)} \left(\frac{\varepsilon_0\, \varepsilon}{\sigma_\varepsilon^2} \right)^{-1 + \varepsilon_0^2/\sigma_\varepsilon^2} \exp\left(-\frac{\varepsilon_0\, \varepsilon}{\sigma_\varepsilon^2} \right), \tag{35}$$

where ε_0 and σ_ε^2 are the mean level depth and mean square of energy fluctuations of localized states, respectively. Plots of gamma-distribution densities are depicted in Fig. 8. Parameter σ_ε represents the localized state distribution width and thereby characterizes the degree of semiconductor disorder. If σ_ε tends to zero, we have a crystalline semiconductor model with a single trapping level: $\rho(\varepsilon) \to \delta(\varepsilon - \varepsilon_0)$. If $\sigma_\varepsilon = \varepsilon_0$, we arrive at an exponential tail of the density of localized states: $\rho(\varepsilon) = \varepsilon_0^{-1} \exp(-\varepsilon/\varepsilon_0)$, and

$$p_\theta(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\, \mathsf{P}\{\theta > t\} = -\frac{\mathrm{d}}{\mathrm{d}t}\, \mathsf{P}\left\{ \omega_0^{-1} \exp\left(\frac{\varepsilon}{kT} \right) > t \right\}$$
$$= -\frac{\mathrm{d}}{\mathrm{d}t}\, \mathsf{P}\{\varepsilon > kT \ln \omega_0 t\} = \rho(kT \ln \omega_0 t)\, \frac{kT}{t}.$$

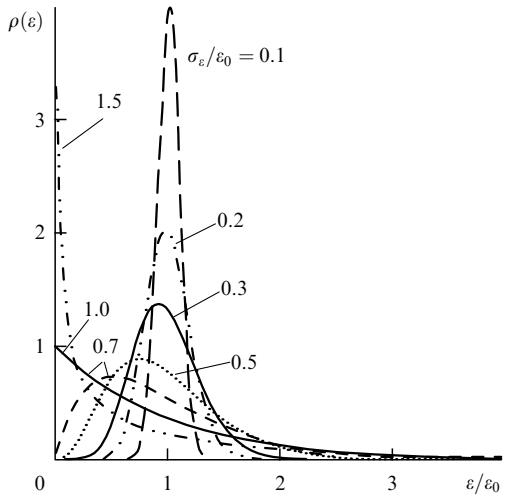

Figure 8. Gamma-distribution density for different $\sigma_\varepsilon/\varepsilon_0$ values.

Thus, for the distribution density of parameter θ, one obtains

$$p_\theta(t) = \frac{\varepsilon_0 kT}{\omega_0 \sigma_\varepsilon^2\, \Gamma(\varepsilon_0^2/\sigma_\varepsilon^2)} \left(\frac{\varepsilon_0 kT}{\sigma_\varepsilon^2} \ln \omega_0 t\right)^{-1+\varepsilon_0^2/\sigma_\varepsilon^2} (\omega_0 t)^{-1-kT\varepsilon_0/\sigma_\varepsilon^2}.$$

Then, the probability for waiting time distribution is defined as

$$\mathsf{P}\{\tau > t\} = \int_0^\infty \mathsf{P}\{\tau > t\,|\theta = t'\}\, p_\theta(t')\, \mathrm{d}t' \sim u(t)(\omega_0 t)^{-\alpha_1},$$
$$t \gg \omega_0^{-1}, \qquad \alpha_1 = kT\,\frac{\varepsilon_0}{\sigma_\varepsilon^2}, \tag{36}$$

where $u(t)$ is a slowly varying function.

The relationship of the theory of dispersive transport with stable laws and the generalized limit theorem allows the dispersive transport condition (18) to be defined more exactly:

$$\mathsf{P}\{\tau > t\} \sim h(t) t^{-\alpha_1}, \qquad t \to \infty, \qquad \alpha_1 < 1,$$

where $h(t)$ is the slowly varying function in Karamat's sense (see Ref. [54] for details), i.e., such a positive function set on $[0, \infty)$ that satisfies the condition

$$\frac{h(ta)}{h(t)} \to \text{const} < \infty, \qquad t \to \infty$$

for any $a > 0$.

Function $u(t)$ in expression (36) is a slowly varying one. Dispersive transport corresponds to $\alpha_1 < 1$. In accordance with expression (36), this condition is satisfied if the mean square σ_ε^2 of energy fluctuations of localized states, characterizing semiconductor disorder, is greater than product $kT\varepsilon_0$.

In the tunneling model proposed in Ref. [61] for the dispersion parameter, one has

$$\alpha_1 = \frac{d_0}{\sigma_d^2 \gamma},$$

where d_0 and σ_d^2 are the mathematical expectation and root-mean-square deviation of random distance between adjacent sites; if $\sigma_d^2 > d_0/\gamma$, the semiconductor satisfies the dispersive transport condition. In other words, in the case of tunneling the transport is dispersive when fluctuations squared of the intertrap distance exceed the mean hopping length multiplied by the half-radius of wave function localization.

7. Fractional differential equations of dispersive transport

As shown in Section 3, fractional differential equations of dispersive transport for a time-of-flight experiment can be obtained based on the shape universality of transient current curves and the power-law dependence of the flight time on sample thickness. In the present section, we propose more general equations for a three-dimensional case taking into account the diffusion term.

In the multiple trapping model, carriers are divided into delocalized and trapped ones. The delocalized carriers in the external electric field $\mathbf{E}$ are scattered on phonons and inhomogeneities to drift with an average velocity $\mathbf{v} = \mu\mathbf{E}$, where μ is mobility. As noted in Ref. [31], the overwhelming majority of carriers involved in dispersive transport are captured in traps, whereas it is free ones that are actually responsible for the transport. In the classical theory of charge transfer in crystalline semiconductors, most kinetic equations are written for the concentration of free carriers. In the hopping model, all carriers are localized, and tunneling from one trap to another and/or thermodynamic hoppings occur almost instantaneously. The hopping model implies zero concentration of free carriers; therefore, the equation for them makes sense only in the case of a multiple trapping mechanism. Let us use a mathematical trick to avoid derivation for each mechanism of a separate generalized drift–diffusion equation for total concentration. After having composed equations for delocalized and trapped carriers, for the hopping transport mechanism we turn the number of free charges to zero and velocity v to infinity. The passage from integral equations of the CTRW model to a generalized one-dimensional fractional differential diffusion equation for the total concentration is realized in Ref. [42] on the assumption of asymptotic power-law waiting time distribution.

We assume that particles are transported in a regular medium, i.e., particles in identical macroscopic volumes of a material are involved in a roughly similar mean number of capture events. Trap density is much higher than the number density of carriers involved in the transport process. The number of transitions $w_{\mathrm{M}\to\mathrm{R}}(\mathbf{r}, t)$ from motion to rest per unit time in a unit volume, i.e., the number of capture events, is proportional to the concentration of delocalized carriers:

$$w_{\mathrm{M}\to\mathrm{R}}(\mathbf{r}, t) = \tau_0^{-1}\, n_\mathrm{c}(\mathbf{r}, t).$$

Here, τ_0 is the mean time of particle's motion between two entrapments to the localized state; in the hopping model, $\tau_0 \to 0$. The total concentration of carriers is the sum of concentrations of mobile, $n_\mathrm{c}(\mathbf{r}, t)$, and trapped, $n_\mathrm{t}(\mathbf{r}, t)$, carriers:

$$n(\mathbf{r}, t) = n_\mathrm{c}(\mathbf{r}, t) + n_\mathrm{t}(\mathbf{r}, t);$$

in this case, the relation

$$n_\mathrm{t}(\mathbf{r}, t) = \int_0^t \tau_0^{-1} n_\mathrm{c}(\mathbf{r}, t')\big[1 - \Psi(t - t')\big]\, \mathrm{d}t' \tag{37}$$

is fulfilled, where $\Psi(t)$ is the distribution function of random residence time in the localized state (see Section 2).

Let $\Psi(t)$ be the asymptotically power-law distribution function

$$1-\Psi(t)=\mathsf{P}\{\tau>t\}=\int_t^\infty \psi(t')\,\mathrm{d}t'\sim\frac{(ct)^{-\alpha}}{\Gamma(1-\alpha)}\,,\quad \alpha\leqslant 1\,;$$

then, relation (37) can be rewritten as

$$\frac{\partial n_\mathrm{t}(\mathbf{r},t)}{\partial t}=(\tau_0 c^\alpha)^{-1}\,\frac{1}{\Gamma(1-\alpha)}\,\frac{\partial}{\partial t}\int_0^t\frac{n_\mathrm{c}(\mathbf{r},t')}{(t-t')^\alpha}\,\mathrm{d}t'\,. \tag{38}$$

In this expression, the integro-differential operator is a Riemann–Liouville fractional derivative of order $\alpha\leqslant 1$ (see, for instance, Ref. [21]):

$$\frac{\partial^\alpha n_\mathrm{c}(\mathbf{r},t)}{\partial t^\alpha}=\frac{1}{\Gamma(1-\alpha)}\,\frac{\partial}{\partial t}\int_0^t\frac{n_\mathrm{c}(\mathbf{r},t')}{(t-t')^\alpha}\,\mathrm{d}t'\,.$$

Let us rewrite expression (38) in the form

$$\frac{\partial n_\mathrm{t}(\mathbf{r},t)}{\partial t}=\frac{1}{\tau_0 c^\alpha}\,\frac{\partial^\alpha n_\mathrm{c}(\mathbf{r},t)}{\partial t^\alpha}\,. \tag{39}$$

The last formula relates concentrations of free and localized carriers. This relation was written in terms of the Laplace transform for the multiple trapping model in Refs [6, 31] and interpreted in terms of fractional derivatives in Ref. [42]. Expression (38) coincides up to coefficients with the one obtained by Arkhipov, Popova, and Rudenko [22].

The flux is expressed through the concentration of delocalized carriers by the formula

$$\mathbf{q}(\mathbf{r},t)=\mathbf{v}n_\mathrm{c}(\mathbf{r},t)-D\nabla n_\mathrm{c}(\mathbf{r},t)\,. \tag{40}$$

Here, $\mathbf{v}=\mu\mathbf{E}$ is the average velocity of the particle's directional motion, and D is the diffusion coefficient.

Substituting relation (40) into continuity equation

$$\frac{\partial n(\mathbf{r},t)}{\partial t}+\operatorname{div}\mathbf{q}(\mathbf{r},t)=n(\mathbf{r},0)\,\delta(t) \tag{41}$$

and taking account of expression (39) yields the *fractional differential drift–diffusion equation* for a concentration of *delocalized* carriers:

$$\frac{\partial n_\mathrm{c}(\mathbf{r},t)}{\partial t}+\frac{l}{\tau_0 K}\,\frac{\partial^\alpha n_\mathrm{c}(\mathbf{r},t)}{\partial t^\alpha}+\operatorname{div}\left(\mu\mathbf{E}\,n_\mathrm{c}(\mathbf{r},t)-D\nabla n_\mathrm{c}(\mathbf{r},t)\right)=n(\mathbf{r},0)\,\delta(t)\,,\qquad K=c^\alpha l\,. \tag{42}$$

The equation for the total concentration is obtained taking into account that the overwhelming number of carriers are captured in traps for times $t\gg c^{-1}$, so that

$$n(\mathbf{r},t)\approx n_\mathrm{t}(\mathbf{r},t)\,.$$

This expression stems from Eqn (39). Then, using Eqns (39)–(41), we obtain the *fractional differential drift–diffusion equation* for the *total* concentration:

$$\frac{\partial n(\mathbf{r},t)}{\partial t}+\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\operatorname{div}\left(\mathbf{K}n(\mathbf{r},t)-C\nabla n(\mathbf{r},t)\right)=n(\mathbf{r},0)\,\delta(t)\,, \tag{43}$$

where $\mathbf{K}=\tau_0 K\mathbf{v}/l$, and $C=\tau_0 KD/l$.

Application of the Riemann–Liouville fractional integral operator of order $(1-\alpha)$ to this equation leads to

$$\frac{\partial^\alpha n(\mathbf{r},t)}{\partial t^\alpha}+\operatorname{div}\left(\mathbf{K}n(\mathbf{r},t)-C\nabla n(\mathbf{r},t)\right)=\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\,n(\mathbf{r},0)\,. \tag{44}$$

Concentration $n(\mathbf{r},t)$ satisfies the normalization condition

$$\int_\infty n(\mathbf{r},t)\,\mathrm{d}V=N\,,$$

where N is the number of charge carriers participating in the transport. In a time-of-flight experiment, N is the number of photoinjected carriers.

The fractional equation of symmetric diffusion,

$$\frac{\partial^\alpha n(\mathbf{r},t)}{\partial t^\alpha}=C\nabla^2 n(\mathbf{r},t)+\frac{t^{-\alpha}}{\Gamma(1-\alpha)}\,\delta(\mathbf{r})\,, \tag{45}$$

was derived by Nigmatullin [63, 64] for diffusion on fractal structures simulating porous and disordered media, and, independently, by Balakrishnan [65] for a one-dimensional case when generalizing Brownian motion. The Fokker–Planck fractional differential equation describing random walks of a particle in the external field was investigated in Refs [66–69, 33]. Barkai [33] was the first to show that the Fokker–Planck fractional equation written for the total carrier distribution density normalized to unity describes the anomalous transient current behavior (2).

Replacement of the first derivative with respect to time by fractional derivative of order α in the normal diffusion equation yields the equation for carrier density with non-conserved normalization:

$$\frac{\partial^\alpha n(x,t)}{\partial t^\alpha}=C\,\frac{\partial^2 n(x,t)}{\partial x^2}\,,$$

which was investigated by Hilfer [36, 70]. It was interpreted in Refs [37, 38, 43] as a macroscopic diffusion equation for free carriers in the multiple trapping regime, i.e., $n(x,t)\equiv n_\mathrm{c}(x,t)$. The expression for transient photocurrent obtained in Ref. [42] by solving an analogous fractional differential dispersive-drift equation

$$\frac{\partial^\alpha n_\mathrm{c}(x,t)}{\partial t^\alpha}=K\,\frac{\partial n_\mathrm{c}(x,t)}{\partial x}\,,$$

coincides with the formula from paper [71], derived in the framework of the multiple trapping theory [72].

8. Solutions to fractional differential equations of dispersive transport

A carrier in the above model can reside in two dynamic states: rest and motion. If there is an instantaneous hopping from one trap to another, the particle may be regarded as having been in motion during an infinitely small time. The total walking time of a carrier is the sum of trap residence time t_R and motion time t_M:

$$t=t_\mathrm{R}+t_\mathrm{M}\,.$$

For the overwhelming majority of particles involved in dispersive transport, one has $t_\mathrm{R}\gg t_\mathrm{M}$. The displacement of a carrier from its initial position is directly related to motion

time. An equivalent of equation (44) is a system of two equations, one of which relates carrier coordinates to motion time, and the other of which links time of carrier's motion to total walking time.

Conditional distribution density $p(t_M|t)$ can be found using the random walk model. Let us assume time t_M to be the process coordinate. Relation $t_R \gg t_M$ being valid for dispersive transport (hence, $t \approx t_R$), the density $p(t_M|t)$ satisfies the equation of one-sided fractal jumpwise walks (see Ref. [49] for details):

$$\frac{\partial^\alpha p(t_M|t)}{\partial t^\alpha} + \frac{\tau_0 K}{l}\frac{\partial p(t_M|t)}{\partial t_M} = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\,\delta(t_M)\,, \tag{46}$$

the solution of which is expressed through one-sided stable density with the characteristic exponent α:

$$p(t_M|t) = \frac{ct}{\alpha t_M}\left(\frac{t_M}{\tau_0}\right)^{-1/\alpha} g^{(\alpha)}\left(ct\left(\frac{t_M}{\tau_0}\right)^{-1/\alpha}\right). \tag{47}$$

Conditional distribution density of carrier coordinate $\mathbf{r}$ provided that the motion time is t_M satisfies the ordinary Fokker–Planck equation

$$\frac{\partial p(\mathbf{r}|t_M)}{\partial t_M} + \operatorname{div}\left(\mu\mathbf{E}\,p(\mathbf{r}|t_M) - D\nabla p(\mathbf{r}|t_M)\right) = \delta(t)\,p(\mathbf{r}|0)\,. \tag{48}$$

The sought-for distribution $n(\mathbf{r}, t)$ is found using the formula

$$n(\mathbf{r}, t) = \int_0^t p(\mathbf{r}|t_M)\,p(t_M|t)\,\mathrm{d}t_M\,. \tag{49}$$

Multiplying equation (46) by $p(\mathbf{r}|t_M)$ and integrating it over time from 0 to t, and taking Eqn (48) into account, we arrive at equation (44). This means that fractional differential equation (44) can be obtained by substituting the solution of integer-order partial differential equation (48) and expression (47) into formula (49). The solution of the (43) type Fokker–Planck fractional equation, an equivalent of equation (44), was first proposed in Ref. [33].

We shall find the solution to fractional differential equation (42) for a delocalized carrier concentration, making sense only in the multiple trapping model, using relationship (39) rewritten in the form

$$n_c(\mathbf{r}, t) = \tau_0 c^\alpha \frac{\partial^{1-\alpha} n(\mathbf{r}, t)}{\partial t^{1-\alpha}}\,.$$

Substituting expression (49) for $n(\mathbf{r}, t)$ in this formula gives

$$n_c(\mathbf{r}, t) = \tau_0 c^\alpha \int_0^t p(\mathbf{r}|t_M)\,\frac{\partial^{1-\alpha} p(t_M|t)}{\partial t^{1-\alpha}}\,\mathrm{d}t_M\,.$$

Function $\tau_0 c^\alpha\,\partial^{1-\alpha} p(t_M|t)/\partial t^{1-\alpha}$ in this expression represents conditional distribution density $p(t|t_M)$. Indeed, it follows from the law of conservation of probability,

$$\frac{\partial p(t_M|t)}{\partial t} + \frac{\partial p(t|t_M)}{\partial t_M} = \delta(t)\delta(t_M)\,,$$

and from equation (46) rewritten in the form

$$\frac{\partial p(t_M|t)}{\partial t} + \tau_0 c^\alpha \frac{\partial}{\partial t_M}\frac{\partial^{1-\alpha} p(t_M|t)}{\partial t^{1-\alpha}} = \delta(t)\delta(t_M)$$

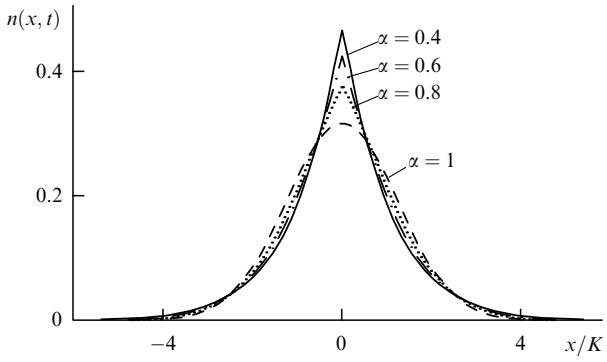

Figure 9. Coordinate distribution densities in dispersive diffusion.

that

$$p(t|t_M) = \tau_0 c^\alpha \frac{\partial^{1-\alpha} p(t_M|t)}{\partial t^{1-\alpha}}\,. \tag{50}$$

Conditional distribution density $p(t|t_M)$ satisfies the equation

$$\frac{\partial p(t|t_M)}{\partial t_M} + (\tau_0 c^\alpha)^{-1}\frac{\partial^\alpha p(t|t_M)}{\partial t^\alpha} = \delta(t)\delta(t_M)\,.$$

By expressing the solution of the last equation through stable densities (see Ref. [49] for details), we have

$$p(t|t_M) = c\left(\frac{t_M}{\tau_0}\right)^{-1/\alpha} g^{(\alpha)}\left(ct\left(\frac{t_M}{\tau_0}\right)^{-1/\alpha}\right). \tag{51}$$

Therefore, the concentration of delocalized carriers is given by

$$n_c(\mathbf{r}, t) = \int_0^t p(\mathbf{r}|t_M)\,p(t|t_M)\,\mathrm{d}t_M\,, \tag{52}$$

where function $p(t|t_M)$ is defined by Eqn (51), and density $p(\mathbf{r}|t_M)$ satisfies the ordinary Fokker–Planck equation (48).

Carrier distribution profiles for dispersive diffusion are presented in Fig. 9.

9. Relationship with other theories

The fractional differential approach rests on four interrelated cornerstones: self-similarity, power-law relaxation, stable distributions, and fractional differential equations. Self-similarity of dispersive transport is evidenced by the shape universality of transient current curves. Stable distributions are limiting for sums of independent random variables distributed according to the asymptotically power law. Stable distributions themselves have power-law 'tails', satisfy equations with fractional derivatives, and describe power-law kinetics. These fractional differential equations have self-similar solutions.

The consistency between the fractional differential approach and the Scher–Montroll model was discussed in Section 4. Specifically, it contains a derivation of a dispersive transport equation with the Riemann–Liouville fractional derivative from the Montroll–Weiss equation for jumpwise walking.

Let us consider the relationship between the multiple trapping model and fractional differential equations. The model of multiple trapping monopolar conduction is based on the continuity equation and the following balance equations [6, 73, 74]:

$$\frac{\partial n_i(\mathbf{r},t)}{\partial t} = \omega_i n_c(\mathbf{r},t) - r_i n_i(\mathbf{r},t)\,, \tag{53}$$

$$n(\mathbf{r},t) = n_c(\mathbf{r},t) + n_t(\mathbf{r},t), \qquad n_t(\mathbf{r},t) = \sum_i n_i(\mathbf{r},t)\,,$$

where $n_i(\mathbf{r},t)$ is the concentration of carriers captured in traps with energy ε_i. The rates of capture (ω_i) and release (r_i) are related by the detailed balance condition

$$\omega_i = r_i \exp\left(\frac{\varepsilon_i}{kT}\right).$$

We assume the capture rate to be weakly dependent on the trap energy: $\omega_i \approx \omega_0$.

Solving equations (53) by the Laplace transform method for exponential tail distribution of the density of states,

$$\rho(\varepsilon) = \frac{1}{\varepsilon_0}\exp\left(-\frac{\varepsilon}{\varepsilon_0}\right),$$

Tiedje [31] arrived at the result

$$\frac{s}{\omega_0}\,\tilde{n}_t(\mathbf{r},s) = \frac{\pi\alpha}{\sin\pi\alpha}\,\frac{s^\alpha}{\omega_0^\alpha}\,\tilde{n}_c(\mathbf{r},s)\,, \tag{54}$$

where

$$\tilde{n}_t(\mathbf{r},s) = \int_0^\infty \mathrm{d}t\, n_t(\mathbf{r},t)\exp(-st)\,.$$

When diffusion of delocalized carriers can be neglected, conduction current density $j = evn_c(x,t) = eNp(t|x)$. Taking into account formula (54), the continuity equation for the transformant of delocalized carrier concentration assumes the form

$$\omega_0\,\frac{\pi\alpha}{\sin\pi\alpha}\left(\frac{s}{\omega_0}\right)^\alpha \tilde{n}_c(x,s) + v\,\frac{\partial}{\partial x}\,\tilde{n}_c(x,s) = N\delta(x)\,. \tag{55}$$

The solution to this equation, viz.

$$\tilde{n}_c(x,s) = Nv^{-1}\exp\left(-\frac{x}{K}\,s^\alpha\right), \qquad c = \omega_0\left(\frac{\pi\alpha}{\sin\pi\alpha}\right)^{-1/\alpha},$$

$$K = c^\alpha l, \qquad l = \frac{v}{\omega_0}\,,$$

is the Laplace transform of the stable density

$$n_c(x,t) = Nv^{-1}\left(\frac{x}{K}\right)^{-1/\alpha} g^{(\alpha)}\left(t\left(\frac{x}{K}\right)^{-1/\alpha}\right),$$

in agreement with formula (9).

It is worthwhile to note that equations (53) disregard the filling of band tail states. Arkhipov, Popova, and Rudenko [22] took account of the finiteness of the trap number for the exponential model of localized state density and obtained the relationship

$$n(\mathbf{r},t) = \Gamma(1+\alpha)\left(\frac{N_t}{N_c}\right)^\alpha \omega_0^{(1-\alpha)}\int_0^t \mathrm{d}t'\,\frac{n_c(\mathbf{r},t')}{(t-t')^\alpha} \times \exp\left[-\frac{\omega_0}{N_t}\int_{t'}^t \mathrm{d}t''\, n_c(\mathbf{r},t'')\right],$$

which goes over into fractional differential relationship (39) in the approximation of weak trap population. Here, N_c and N_t are the density of mobile states and total trap density, respectively.

Noolandi [30] was the first to show that the multiple trapping model in the asymptotic limit is mathematically equivalent to the Scher–Montroll random walk model. However, the latter model does not explain certain effects associated with transport by the multiple trapping mechanism, for instance, current saturation as a result of filling the band tail states [22].

A comparison of solutions obtained in the framework of the fractional differential approach with those calculated from the Arkhipov–Rudenko master DT equation [23] is presented in Fig. 10. The difference between solutions becomes significant for $\alpha > 0.5$. It is worth mentioning some important peculiarities of solution (25), ensuing from τ-approximation equation (23) and corresponding to the main DT characteristics. According to expression (27), mean packet width (i.e., the root-mean-square deviation of normalized density) and mean carrier displacement grow with time in proportion to t^α, while the transient current density has power asymptotics observed in experiment. However, the transport must become normal as $\alpha \to 1$; in the presence of drift, carrier concentrations must transform into delta functions, and the transient current signal into a step. As follows from formulas (10) and (15), and Fig. 11, solutions of fractional differential equations satisfy this principle (*correspondence principle*), whereas solutions obtained with the help of the Arkhipov–Rudenko master DT equation adequately describe only the strong DT regime, where $\alpha \leqslant 0.5$. A comparison of photocurrent (11) with experimental data and the result obtained using the master DT equation [25] is given in Fig. 11.

It is worth noting that solutions (10) and (15) imply *probabilistic interpretation*. The concentration of free carriers (in the case of 'pure' drift) is proportional to the conduction current density and, therefore, to flight time distribution density in the layer of a given thickness. If the layer is *mentally* divided into two identical sublayers, the random flight time is the sum of flight times through each sublayer. Then the following relation is fulfilled:

$$p(t|x) = \frac{\mu E}{N}\,n_c(x,t) = \left(\frac{\mu E}{N}\right)^2 \int_0^t \mathrm{d}t'\, n_c\left(\frac{x}{2}\,, t-t'\right) n_c\left(\frac{x}{2}\,, t'\right). \tag{56}$$

The convolution of two stable densities (with identical characteristic exponents) is again stable, while the time convolution of functions (26) does not lead to the function of the same form, i.e., condition (56) for these solutions is not fulfilled.

10. Inclusion of recombination

Let us take into account recombination in fractional differential equations of dispersive transport, starting from mono-

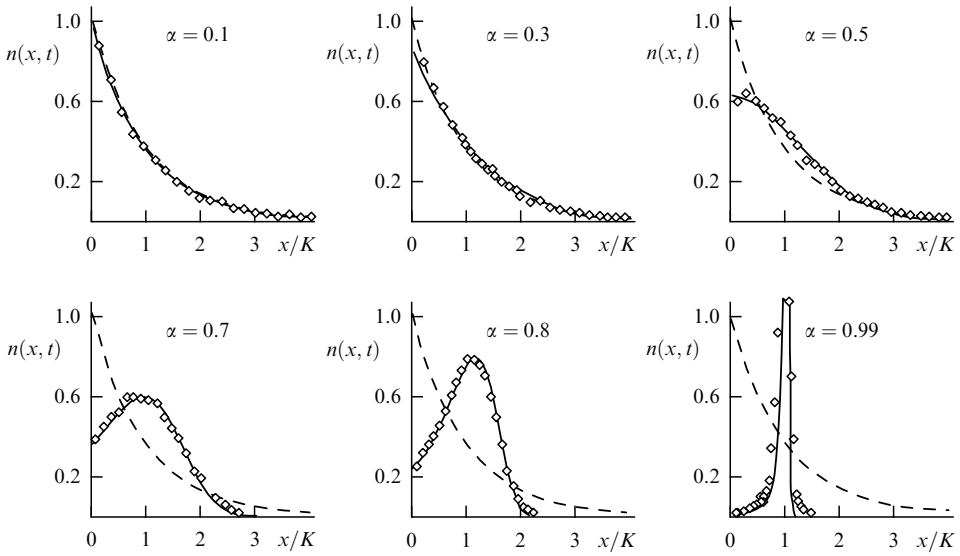

Figure 10. Total carrier concentration normalized to unity: dots — results of Monte Carlo simulation in the framework of the Scher–Montroll walking scheme; dashed lines — results obtained using the Arkhipov–Rudenko master DT equation [26], and solid lines — concentrations calculated from formula (15).

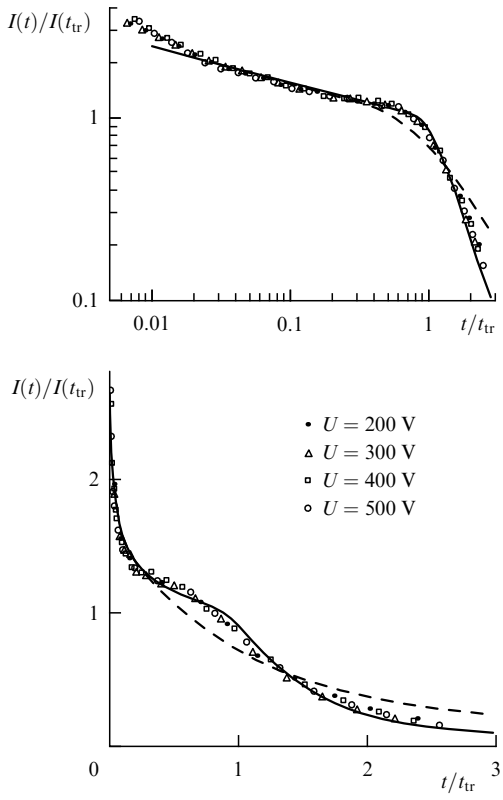

Figure 11. Transient current curves: dots (digitized from a figure in the paper by Scher and Montroll [35]) — experimental data for an organic trinitrofluorenon–polyvinyl carbazole (TNF–PVC) complex obtained by Gill; dashed lines — results obtained using the Arkhipov–Rudenko master DT equation [25], and solid line — transient current calculated from formula (11). Dispersion parameter $\alpha = 0.8$ [35].

molecular recombination of free carriers [75] and the recombination of localized carriers by tunneling transitions [40]. In the presence of monomolecular recombination, basic balance equations for the model of transport controlled by capture in localized states have the form [76–79]

$$\frac{\mathrm{d}n_\mathrm{c}(\mathbf{r},t)}{\mathrm{d}t} = -\sum_i \frac{\mathrm{d}n_i(\mathbf{r},t)}{\mathrm{d}t} - \frac{n_\mathrm{c}(\mathbf{r},t)}{\tau} + N\delta(t)\,,$$

$$\frac{\mathrm{d}n_i(\mathbf{r},t)}{\mathrm{d}t} = -r_i n_i(\mathbf{r},t) + \omega_i n_\mathrm{c}(\mathbf{r},t)\,.$$

It follows from these equations that liner recombination gives rise to the corresponding term in the continuity equation:

$$\frac{\partial n(\mathbf{r},t)}{\partial t} + \operatorname{div}\mathbf{q}(\mathbf{r},t) = -\frac{n_\mathrm{c}(\mathbf{r},t)}{\tau} + n(\mathbf{r},0)\,\delta(t)\,,$$

where τ is the lifetime of delocalized carriers prior to monomolecular recombination. The use of this equation instead of the continuity equation (41) leads to the generalized diffusion equation for nonequilibrium electron concentration $\delta n_\mathrm{c}(x,t)$, taking into consideration linear recombination:

$$\frac{\partial n_\mathrm{c}(\mathbf{r},t)}{\partial t} + \frac{1}{\tau_{0\mathrm{n}} c_\mathrm{n}^\alpha}\frac{\partial^\alpha n_\mathrm{c}(\mathbf{r},t)}{\partial t^\alpha} + \operatorname{div}\left(-\mu_n \mathbf{E}\, n_\mathrm{c}(\mathbf{r},t) - D_n \nabla n_\mathrm{c}(\mathbf{r},t)\right) + \frac{\delta n_\mathrm{c}(\mathbf{r},t)}{\tau_\mathrm{n}} = 0\,. \quad (57)$$

Then, the equation for total concentration $n(\mathbf{r},t)$, which is the sum of concentrations of free carriers and carriers localized in band tail states,

$$\delta n(\mathbf{r},t) = \delta n_\mathrm{t}(\mathbf{r},t) + \delta n_\mathrm{c}(\mathbf{r},t)\,,$$

can be written out, taking into account relationship (39), as

$$\frac{\partial n(\mathbf{r},t)}{\partial t} + \tau_{0\mathrm{n}} c_\mathrm{n}^\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left[\operatorname{div}\left(-\mu_\mathrm{n}\mathbf{E}\,\delta n(\mathbf{r},t) - D_\mathrm{n}\nabla n(\mathbf{r},t)\right) + \frac{\delta n(\mathbf{r},t)}{\tau_\mathrm{n}}\right] = \delta n(\mathbf{r},0)\,\delta(t)\,, \quad (58)$$

or

$$\frac{\partial^{\alpha} n(\mathbf{r},t)}{\partial t^{\alpha}} + \operatorname{div}\left(-\mu_{\mathrm{n}}\tau_{0\mathrm{n}}c_{\mathrm{n}}^{\alpha}\mathbf{E}\,\delta n(\mathbf{r},t) - D_{\mathrm{n}}\tau_{0\mathrm{n}}c_{\mathrm{n}}^{\alpha}\nabla n(\mathbf{r},t)\right) + \tau_{0\mathrm{n}}K_{\mathrm{n}}\frac{\delta n(\mathbf{r},t)}{\tau_{\mathrm{n}}} = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\,\delta n(\mathbf{r},0)\,. \tag{59}$$

The dispersive transport equation for tunneling transitions of localized carriers can be obtained based on the model of Seki, Wojcik, and Tachiya [39, 40]. These authors deduced a fractional differential equation for the first passage time distribution density. We derived equations for carrier concentrations and found their solutions [80].

Recombination waiting time in the absence of random walks is given by the distribution function

$$\Phi(\mathbf{r},t) = \int_0^t \phi(\mathbf{r},t)\,\mathrm{d}t\,.$$

The authors of Ref. [40] considered a case of exponential distribution

$$\phi(\mathbf{r},t) = \gamma_{\mathrm{rc}}(\mathbf{r})\exp\left[-\gamma_{\mathrm{rc}}(\mathbf{r})t\right], \tag{60}$$

where $\gamma_{\mathrm{rc}}(\mathbf{r})$ is the distance-dependent recombination rate.

The trap release time distribution density for the hopping process with recombination has the form

$$\psi_{\mathrm{out}}(\mathbf{r},t) = \psi(t)\left[1-\Phi(\mathbf{r},t)\right], \tag{61}$$

and recombination time distribution density is described by the expression

$$\psi_{\mathrm{rc}}(\mathbf{r},t) = \phi(\mathbf{r},t)\left[1-\Psi(t)\right]. \tag{62}$$

It is easy to show that the normalization condition

$$\int_0^{\infty}\mathrm{d}t\left[\psi_{\mathrm{out}}(\mathbf{r},t)+\psi_{\mathrm{rc}}(\mathbf{r},t)\right] = 1$$

is fulfilled.

In the presence of recombination, the following relation between concentrations of free and localized carriers is obtained instead of relationship (37):

$$n_{\mathrm{t}}(\mathbf{r},t) = \int_0^t \tau_0^{-1} n_{\mathrm{c}}(\mathbf{r},t')\left[1-\Psi_{\mathrm{out}}(\mathbf{r},t-t')-\Psi_{\mathrm{rc}}(\mathbf{r},t-t')\right]\mathrm{d}t'\,, \tag{63}$$

where

$$\Psi_{\mathrm{out}}(\mathbf{r},t) = \int_0^t \mathrm{d}t\,\psi_{\mathrm{out}}(\mathbf{r},t)\,, \qquad \Psi_{\mathrm{rc}}(\mathbf{r},t) = \int_0^t \mathrm{d}t\,\psi_{\mathrm{rc}}(\mathbf{r},t)\,.$$

Taking into consideration that

$$\Psi_{\mathrm{out}}(\mathbf{r},t) + \Psi_{\mathrm{rc}}(\mathbf{r},t) = \Psi(t) + \Phi(\mathbf{r},t) - \Phi(\mathbf{r},t)\Psi(t)\,,$$

relation (63) can be rewritten as

$$n_{\mathrm{t}}(\mathbf{r},t) = \int_0^t \mathrm{d}t'\,\tau_0^{-1} n_{\mathrm{c}}(\mathbf{r},t')\left[1-\Psi(t-t')\right]\left[1-\Phi(\mathbf{r},t-t')\right]. \tag{64}$$

For exponential distribution $\phi(t)$, one obtains

$$\frac{\partial n_{\mathrm{t}}(\mathbf{r},t)}{\partial t} = (\tau_0 c^{\alpha})^{-1}\frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial t}\int_0^t \mathrm{d}t'\,\frac{n_{\mathrm{c}}(\mathbf{r},t')}{(t-t')^{\alpha}}\exp\left[-\gamma_{\mathrm{rc}}(\mathbf{r})(t-t')\right]. \tag{65}$$

Substituting relation (64) into the continuity equation taking into account recombination, i.e.

$$\frac{\partial n(\mathbf{r},t)}{\partial t} + \operatorname{div}\mathbf{q}(\mathbf{r},t) + \phi(\mathbf{r},0)n_{\mathrm{t}}(\mathbf{r},t) = n(\mathbf{r},0)\delta(t)\,, \tag{66}$$

we arrive at the equation for the concentration of delocalized carriers that, in the case of exponential recombination time distribution, can be written out as

$$\frac{\partial n_{\mathrm{c}}(\mathbf{r},t)}{\partial t} + (c^{\alpha}\tau_0)^{-1}\exp\left[-\gamma_{\mathrm{rc}}(\mathbf{r})t\right]\frac{\partial^{\alpha}}{\partial t^{\alpha}}\,n_{\mathrm{c}}(\mathbf{r},t)\exp\left[\gamma_{\mathrm{rc}}(\mathbf{r})t\right] + \operatorname{div}\left[\mu\mathbf{E}n_{\mathrm{c}}(\mathbf{r},t) - D\nabla n_{\mathrm{c}}(\mathbf{r},t)\right] = \delta(t)n(\mathbf{r},0)\,. \tag{67}$$

The equation for the total concentration takes the form

$$\exp\left[-\gamma_{\mathrm{rc}}(\mathbf{r})t\right]\frac{\partial^{\alpha}}{\partial t^{\alpha}}\,n(\mathbf{r},t)\exp\left[\gamma_{\mathrm{rc}}(\mathbf{r})t\right] + (c^{\alpha}\tau_0)\times\operatorname{div}\left[\mu\mathbf{E}\,n(\mathbf{r},t) - D\nabla n(\mathbf{r},t)\right] = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\exp\left[-\gamma_{\mathrm{rc}}(\mathbf{r})t\right]n(\mathbf{r},0)\,. \tag{68}$$

The solution to the last equation is expressed through stable density [80]:

$$n(\mathbf{r},t) = \exp\left[-\gamma_{\mathrm{rc}}(\mathbf{r})t\right]\int_0^{\infty}\frac{1}{(4\pi D\tau)^{3/2}}\exp\left[-\frac{(\mathbf{r}-\mu\mathbf{E}\tau)^2}{4D\tau}\right]\times\frac{ct}{\alpha\tau_0(\tau/\tau_0)^{1+1/\alpha}}\,g^{(\alpha)}\left(ct\left(\frac{\tau}{\tau_0}\right)^{-1/\alpha}\right)\mathrm{d}\tau\,.$$

The dependence of the recombination rate $\gamma_{\mathrm{rc}}(\mathbf{r})$ on spatial coordinate $\mathbf{r}$ is defined by the distribution of recombination centers and the recombination type. In the case of the tunneling mechanism, one has $\gamma_{\mathrm{rc}}(\mathbf{r}) \propto \exp(-2\beta r)$, and in the case of the energy transition model, $\gamma_{\mathrm{rc}}(\mathbf{r}) \propto r^{-6}$ (see Ref. [40] for details).

11. Ambipolar dispersive transport

Normal diffusion and normal drift of charge carriers in the case of double injection in semiconductors are characterized by the ambipolar diffusion coefficient and ambipolar mobility. In normal transport with $D_{\mathrm{n}} > D_{\mathrm{p}}$, the diffusion electron packet expands faster than the hole packet. The arising electric field (ambipolar diffusion field) slows down electrons and accelerates holes. In a steady-state regime, hole and electron fluxes are identical. If there is drift, the inequality of carrier mobilities μ_{n} and μ_{p} in an external electric field accounts for acquiring a common, ambipolar drift velocity by electron and hole packets. Time-of-flight experiments demonstrated that drift mobility in dispersive transport depends on the sample thickness and the electric field strength; therefore, drift mobility cannot be used as a characteristic of ambipolar transport. The diffusion equation in the Arkhipov–Rudenko model contains time-depen-

dent diffusion coefficients and mobility. Moreover, these quantities depend on the initial conditions and therefore are equally unsuitable for the description of ambipolar dispersive transport.

Let us try to apply the fractional differential approach, assuming the semiconductor to be homogeneous (i.e., the diffusion coefficient and mobility to be independent of the coordinates). Let the quasineutrality condition $\delta p = \delta n$ be fulfilled. Electron and hole lifetimes are identical: $\tau_n = \tau_p$. Let us rewrite the dispersive transport equation (59) with monomolecular recombination for electrons and holes in the form

$$\frac{\partial^{\alpha_n} n}{\partial t^{\alpha_n}} - \mu_n^* n \operatorname{div}\mathbf{E} - \mu_n^* \mathbf{E}\nabla n - D_n^* \nabla^2 n + \frac{\delta n}{\tau^*} = \frac{t^{-\alpha_n}}{\Gamma(1-\alpha_n)}\,\delta n(\mathbf{r},0)\,, \tag{69}$$

$$\frac{\partial^{\alpha_p} p}{\partial t^{\alpha_p}} + \mu_p^* p \operatorname{div}\mathbf{E} + \mu_p^* \mathbf{E}\nabla p - D_p^* \nabla^2 p + \frac{\delta p}{\tau^*} = \frac{t^{-\alpha_p}}{\Gamma(1-\alpha_p)}\,\delta p(\mathbf{r},0)\,, \tag{70}$$

where $D_n^* = D_n \tau_{0n} c_n^{\alpha}$, and $\mu_n^* = \mu_n \tau_{0n} c_n^{\alpha}$. Discarding terms with $\operatorname{div}\mathbf{E}$ from these equations yields

$$\frac{1}{\mu_n^* n + \mu_p^* p}\left(\mu_n^* n \frac{\partial^{\alpha_p}}{\partial t^{\alpha_p}} + \mu_p^* p \frac{\partial^{\alpha_n}}{\partial t^{\alpha_n}}\right) p + \frac{\mu_p^* \mu_n^* (n-p)}{\mu_n^* n + \mu_p^* p}\,\mathbf{E}\nabla p - \frac{\mu_n^* n D_p^* + \mu_p^* p D_n}{\mu_n^* n + \mu_p^* p}\,\nabla^2 p + \frac{\delta p}{\tau^*} = \frac{1}{\mu_n^* n + \mu_p^* p}\left[\mu_n^* n \frac{t^{-\alpha_p}}{\Gamma(1-\alpha_p)} + \mu_p^* p \frac{t^{-\alpha_n}}{\Gamma(1-\alpha_n)}\right]\delta p(\mathbf{r},0)\,. \tag{71}$$

Introducing the following notations:

$$\sigma_n = \mu_n n\,, \qquad \sigma_p = \mu_p p\,, \qquad \sigma = \sigma_n + \sigma_p$$

for electron/hole conductivity and total conductivity, respectively;

$$\mu_{amb} = \frac{\mu_p^* \mu_n^* (n-p)}{\mu_n^* n + \mu_p^* p}$$

for ambipolar mobility, and

$$D_{amb} = \frac{\mu_n^* n D_p^* + \mu_p^* p D_n^*}{\mu_n^* n + \mu_p^* p}$$

for the ambipolar diffusion coefficient, we rewrite the equation of ambipolar dispersive transport with inclusion of monomolecular recombination in the form

$$\frac{\sigma_n}{\sigma}\frac{\partial^{\alpha_p} p(\mathbf{r},t)}{\partial t^{\alpha_p}} + \frac{\sigma_p}{\sigma}\frac{\partial^{\alpha_n} p(\mathbf{r},t)}{\partial t^{\alpha_n}} + \mu_{amb}\mathbf{E}\nabla p(\mathbf{r},t) - D_{amb}\nabla^2 p(\mathbf{r},t) + \frac{\delta p(\mathbf{r},t)}{\tau^*} = \left[\frac{\sigma_n}{\sigma}\frac{t^{-\alpha_p}}{\Gamma(1-\alpha_p)} + \frac{\sigma_p}{\sigma}\frac{t^{-\alpha_n}}{\Gamma(1-\alpha_n)}\right]\delta p(\mathbf{r},0)\,. \tag{72}$$

The last ambipolar transport equation contains two fractional derivatives of different orders in the general case.

12. From transient current to waiting time distribution

Waiting time distribution density is related to important physical characteristics of both the transport process and the medium wherein this transport occurs. Such characteristics comprise energy density of localized states in the case of multiple trapping and trap spatial distribution in the case of tunneling. Transport under certain physical conditions can be described using a phenomenological integral equation based on waiting time distribution density alone, even if the transport mechanism remains unknown. The question is how to deduce waiting time distribution from transient current curves.

The proposed algorithm for the retrieval of the sought-for density is applicable on the following assumptions inherent in standard time-of-flight experiments:

(1) The semiconductor is homogeneous and the transport in it is macroscopic.

(2) The external electric field is high compared with the field of nonequilibrium carriers.

(3) The carriers travel in the positive direction of the x-axis.

The transient current is determined from formulas

$$I(t) = \frac{1}{L}\int_0^L j(x,t)\,\mathrm{d}x\,, \qquad j(x,t) = eNp(t|x)\,.$$

If a sample is mentally divided into identical layers transverse to the electric field, a carrier that crosses n layers has the coordinate roughly equal to the product of the number n by elementary layer width l: $x \approx nl$. Propagation time along coordinate x is the sum of n random residence times in individual layers; in distribution terms, it is written with the help of convolution

$$p(t|x) = \psi^{*n}(t)\,,$$

where $\psi(t)$ is the residence time distribution density in each elementary layer. Substituting the latter expression into the formula for transient current gives

$$I(t) = \frac{eN}{L}\int_0^L \psi^{*n}(t)\,\mathrm{d}x\,.$$

The Fourier transform converts the convolution of functions into the product of their Fourier images and makes the integral easy to calculate:

$$\tilde{I}(\omega) = \frac{eN}{L}\int_0^L \tilde{\psi}^{x/l}(\omega)\,\mathrm{d}x = \frac{eN}{L}\int_0^L \exp\left(\frac{x}{l}\ln\tilde{\psi}(\omega)\right)\mathrm{d}x = \frac{eNl}{L\ln\tilde{\psi}(\omega)}\left[\exp\left(\frac{L}{l}\ln\tilde{\psi}(\omega)\right) - 1\right].$$

The solution of this equation is written as

$$\ln\tilde{\psi}(\omega) = -\frac{l}{L}\,W\!\left(-\frac{eN}{\tilde{I}}\exp\left(-\frac{eN}{\tilde{I}}\right)\right) - \frac{eNl}{L\tilde{I}}\,, \tag{73}$$

where $W(x)$ is the Lambert function (the solution of the transcendent equation $W\exp W = x$). Thus, by finding the Fourier transform of the transient current curve, calculating transformant $\tilde{\psi}(\omega)$ by formula (73), and inverting it, we obtain the waiting time distribution density.

Knowing the waiting time distribution, it is possible to write out the integral transport equation for a regular homogeneous medium controlled by trapping in localized states. As before, it is assumed that trap concentration in any region of a semiconductor is much higher than the concentration of the carriers involved in the transport. Free and localized carrier densities are related by the equation

$$n_{\rm t}(\mathbf{r},t)=\tau_0^{-1}\int_0^t n_{\rm c}(\mathbf{r},t')\,Q(t-t')\,{\rm d}t'\,, \tag{74}$$

where $Q(t)=1-\Psi(t)=P(\tau>t)$ is the additional distribution function of carrier residence time in traps. Concentration $n_{\rm t}(\mathbf{r},t)$ is independent of the localized state energy, and $Q(t)$ is the energy-averaged waiting time distribution function in localized states:

$$Q(t)=\left\langle\exp\left(-\omega_\varepsilon t\,\exp\left(-\frac{\varepsilon}{kT}\right)\right)\right\rangle$$
$$=N_{\rm t}^{-1}\int_0^{\varepsilon_g}\rho(\varepsilon)\exp\left(-\omega_\varepsilon t\,\exp\left(-\frac{\varepsilon}{kT}\right)\right){\rm d}\varepsilon\,.$$

The density of delocalized carriers can be expressed through the trapped carrier density with the help of the integral equation

$$n_{\rm c}(\mathbf{r},t)=\tau_0\int_0^t n_{\rm t}(\mathbf{r},t')\,Q^*(t-t')\,{\rm d}t'\,, \tag{75}$$

where $Q^*(t)$ is the conjugate integral kernel that can be defined in terms of the Laplace transform:

$$\hat{Q}^*(s)=\left[\hat{Q}(s)\right]^{-1}.$$

After substituting expression (74) or (75) into continuity equation (41), taking into account formula (40), we obtain transport equations for the mobile carrier concentration:

$$\frac{\partial n_{\rm c}(\mathbf{r},t)}{\partial t}+\tau_0^{-1}\,\frac{\partial}{\partial t}\int_0^t n_{\rm c}(\mathbf{r},t')\,Q(t-t')\,{\rm d}t'$$
$$+\,{\rm div}\left[\mu\mathbf{E}\,n_{\rm c}(\mathbf{r},t)-D\nabla n_{\rm c}(\mathbf{r},t)\right]=0\,,$$

and for the total concentration of nonequilibrium carriers:

$$\frac{\partial n(\mathbf{r},t)}{\partial t}+\tau_0\int_0^t{\rm d}t'\,Q^*(t-t')$$
$$\times\,{\rm div}\left[\mu\mathbf{E}\,n(\mathbf{r},t')-D\nabla n(\mathbf{r},t')\right]=0\,,\qquad n(r,t)\approx n_{\rm t}(\mathbf{r},t)\,.$$

13. Transport in structurally inhomogeneous semiconductors

Transient current relaxation in certain disordered semiconductors, for example, porous silicon [81], assumes the form

$$I(t)\propto\begin{cases}t^{-1+\alpha_i}\,, & t<t_{\rm tr}\,,\\ t^{-1-\alpha_f}\,, & t>t_{\rm tr}\,,\end{cases}\qquad 0<\alpha_i\neq\alpha_f<1\,. \tag{76}$$

The Scher–Montroll model of charge transfer in disordered semiconductors leads to the current dependence (2), where $\alpha_i=\alpha_f=\alpha$. It has been shown in Ref. [82] that the value of α found from the dependence of carrier flight time in porous silicon on the electric field strength differs from that determined from transient photocurrent curves. The authors explained this discrepancy on the assumption of additional dispersion in terms of carrier mobility in structurally inhomogeneous porous silicon samples. It is natural to further extend this idea by assuming dispersion of the parameter α. It will be shown below that this assumption is enough to substantiate dependence (76), at least for the discrete spectrum $\{\alpha_1,\alpha_2,\ldots,\alpha_m\}$.

Let k_j be the fraction of traps that capture carriers for random time τ distributed according to an asymptotically power law with exponent α_j. The averaged distribution function of a carrier residence time in the localized state has the form

$$\Psi(t)\sim 1-\sum_j k_j\,\frac{(b_j\,t)^{-\alpha_j}}{\Gamma(1-\alpha_j)}\,,$$

where b_j are the normalization constants. Substituting this function into relationship (37) leads to the equation

$$\frac{\partial n_{\rm t}(\mathbf{r},t)}{\partial t}=\frac{1}{\tau_0}\sum_j c_j^{-\alpha_j}\,\frac{\partial^{\alpha_j}n_{\rm c}(\mathbf{r},t')}{\partial t^{\alpha_j}}\,,\qquad c_j=b_j\,(k_j)^{-1/\alpha_j}\,. \tag{77}$$

Taken together with continuity equation (41), expression (77) gives the drift–diffusion equation for the concentration of delocalized carriers in the case of the discretely distributed dispersion parameter:

$$\frac{\partial n_{\rm c}(\mathbf{r},t)}{\partial t}+\frac{1}{\tau_0}\sum_j c_j^{-\alpha_j}\,\frac{\partial^{\alpha_j}n_{\rm c}(\mathbf{r},t')}{\partial t^{\alpha_j}}$$
$$+\,{\rm div}\left(\mu\mathbf{E}\,n_{\rm c}(\mathbf{r},t)-D\nabla n_{\rm c}(\mathbf{r},t)\right)=n(\mathbf{r},0)\,\delta(t)\,. \tag{78}$$

Let us calculate transient current in a structure, the transport of which is described by the last equation. To this end, we neglect diffusion, regard the electric field as being uniform, and align the x-axis along field $\mathbf{E}$. Then, equation (78) can be rewritten as

$$\frac{\partial n_{\rm c}(\mathbf{r},t)}{\partial t}+\frac{1}{\tau_0}\sum_j c_j^{-\alpha_j}\,\frac{\partial^{\alpha_j}n_{\rm c}(\mathbf{r},t)}{\partial t^{\alpha_j}}+\mu E\,\frac{\partial n_{\rm c}(\mathbf{r},t)}{\partial x}=N\delta(x)\,\delta(t)\,.$$

Laplace transform

$$\tilde{n}_{\rm c}(\mathbf{r},s)=\int_0^\infty{\rm d}t\,n(\mathbf{r},t)\exp\left(-st\right)$$

of the last equation gives

$$s\tilde{n}_{\rm c}(\mathbf{r},s)+\frac{1}{\tau_0}\sum_j\left(\frac{s}{c_j}\right)^{\alpha_j}\tilde{n}_{\rm c}(\mathbf{r},s)+\mu E\,\frac{\partial\tilde{n}_{\rm c}(\mathbf{r},s)}{\partial x}=N\delta(x)\,.$$

The solution for the case $\alpha_j<1$ has the form

$$\tilde{n}_{\rm c}(\mathbf{r},s)=\frac{N}{\mu ES}\exp\left[-\frac{x}{\mu E\tau_0}\sum_j\left(\frac{s}{c_j}\right)^{\alpha_j}\right],\qquad \mu E\tau_0=l\,,$$

where S is the sample area transverse to the electric field.

The traps being regarded as uniformly distributed in the sample, the time transformant of the charge carrier density for $x\gg l$ (where l is the mean intertrap distance) equals

$$\tilde{n}(x,s)=\frac{N}{ls}\sum_j\left(\frac{s}{c_j}\right)^{\alpha_j}\exp\left(-\frac{x}{l}\sum_j\left(\frac{s}{c_j}\right)^{\alpha_j}\right). \tag{79}$$

Taking account of the last relationship, we have for the Laplace image of the transient current:

$$\tilde{I}(s) = \frac{eNl}{L} \frac{1 - \exp\left(-L \sum_j (s/c_j)^{\alpha_j}/l\right)}{\sum_j (s/c_j)^{\alpha_j}} . \qquad (80)$$

If parameter α_j takes on a unique value, the inverse Laplace transform of formula (80) gives expression (11).

Let us undertake asymptotic analysis of the time dependence of transient current. In accordance with the Tauberian theorem, the behavior of function $I(t)$ for $t \gg b_j^{-1}$ is determined by that of function (80) for $s \ll b_j$:

$$\tilde{I}(s) \sim \frac{eNl}{L} \frac{2L \sum_j (s/b_j)^{\alpha_j}/l - \left(-L \sum_j (s/b_j)^{\alpha_j}/l\right)^2}{2 \sum_j (s/b_j)^{\alpha_j}}$$

$$\sim eN - \frac{eNL}{2l} \left(\frac{s}{b_{\min}}\right)^{\alpha_{\min}} ,$$

where $\alpha_{\min}$ is the minimum value from the set $\{\alpha_1, \alpha_2, \ldots, \alpha_m\}$, and $b_{\min}$ is the corresponding value of the normalization constant. The inverse Laplace transform leads to

$$I(t) \propto t^{-1-\alpha_{\min}} , \qquad t \gg b_j^{-1} .$$

In the case of $s/b_j \gg (l/L)^{1/\alpha_j}$ for all j, it follows that

$$\tilde{I}(s) \sim \frac{eNl}{L \sum_j (s/b_j)^{\alpha_j}} \sim \frac{eNl}{L(s/b_{\max})^{\alpha_{\max}}} , \qquad s \gg b_j ,$$

where $\alpha_{\max}$ is the maximum value from the set $\{\alpha_1, \alpha_2, \ldots, \alpha_m\}$, and $b_{\max}$ is the corresponding value of the normalization constant. Hence follows

$$I(t) \propto t^{-1+\alpha_{\max}} , \qquad t \ll b_j .$$

Thus, if the exponent in the carrier residence time distribution in traps takes on one of the values from the ordered set $\{\alpha_1, \alpha_2, \ldots, \alpha_m\}$ (discrete spectrum), the transient current behavior is determined by the maximum value of $\alpha_{\max} = \alpha_m$ in the initial time segment, and by the minimum value of $\alpha_{\min} = \alpha_1 \neq \alpha_m$ in the terminal one, in agreement with the results of the aforementioned experiments.

14. Truncated power-law waiting time distributions

If the distribution of waiting times is governed by the truncated power law, they have finite dispersion. The central limit theorem is applicable to this case, and transport in the long-time asymptotic limit must be normal. Analysis of truncated Levy flights in Refs [83, 84] revealed that the form of distribution of the sum of such random quantities, given by the Levy stable law, turns into that consistent with Gauss's law in the limit of a very large number of terms. We shall consider below the effect of truncated power-law waiting time distribution on the properties of dispersive transport. Evidently, this influence has to manifest itself in certain scale effects. Specifically, it will be shown that the truncated power law provides a probabilistic interpretation of the transition from normal to dispersive transport and back in some disordered semiconductors upon a change in sample size and electric field strength.

The introduction of truncation actually modifies the Scher–Montroll model, altering the distribution pattern of carrier residence time in traps. One of the causes behind the truncated power law is a recombination, the model of which was described in Section 10. In this case, truncation of power-law density $\psi(t)$ is associated with the 'withdrawal' of carriers from the transport process, resulting in a decrease in their total number with time. Hereafter, we shall be interested in those situations where the number of carriers remains unaltered.

It is only natural that the power-law waiting time distribution undergoes truncation. A cause of truncation may be the constraints imposed on the exponential tail by the finite size of the mobility gap in the multiple trapping model, and on the maximum jump length in the hopping model. Moreover, truncation may be a consequence of the secondary transport mechanism operating together with the primary one.

As shown in Ref. [84], analytical results for truncated Levy flights can be obtained regarding the product of the power law by a slowly damping exponent as a limited distribution. Let waiting times be distributed according to the law

$$1 - \Psi(t) = \mathsf{P}\{\tau > t\} \sim \frac{(ct)^{-\alpha}}{\Gamma(1-\alpha)} \exp(-\gamma t) , \qquad t \gg c^{-1} . \qquad (81)$$

The corresponding distribution density has the form

$$\psi(t) \sim \exp(-\gamma t) \frac{(ct)^{-\alpha}}{\Gamma(1-\alpha)} \left(\frac{\alpha}{t} + \gamma\right) , \qquad t \gg c^{-1} . \qquad (82)$$

Distribution density of the sum of n terms, $\tau = \tau_1 + \tau_2 + \ldots + \tau_n$, is expressed through the n-fold convolution $q(t|n) = \psi^{*n}(t)$. Taking integral Laplace transformation yields $\tilde{q}(s|n) = [\tilde{\psi}(s)]^n$. Laplace image of density (82) has the form

$$\tilde{\psi}(s) \sim 1 - c^{-\alpha}\left[(s+\gamma)^{\alpha} - \gamma^{\alpha}\right] , \qquad s \ll c .$$

The transformant of the density distribution of the sum of n independent random times,

$$\tilde{p}(s|n) \sim \exp\left[n\left(\frac{\gamma}{c}\right)^{\alpha} - n\left(\frac{s+\gamma}{c}\right)^{\alpha}\right] , \qquad s \ll c , \qquad (83)$$

is the Laplace image of the truncated stable density:

$$p(t|n) \sim \exp\left[n\left(\frac{\gamma}{c}\right)^{\alpha} - \gamma t\right] cn^{-1/\alpha} g^{(\alpha)}(ctn^{-1/\alpha}) . \qquad (84)$$

Function (83) satisfies the relation

$$\frac{\partial \tilde{p}(s|n)}{\partial n} = \gamma^{\alpha} c^{-\alpha} \tilde{p}(s|n) - c^{-\alpha}(s+\gamma)^{\alpha} \tilde{p}(s|n) + \delta(n) ,$$

the inverse Laplace transform of which leads to the fractional differential equation

$$\frac{\partial p(t|n)}{\partial n} = \gamma^{\alpha} c^{-\alpha} p(t|n)$$

$$- c^{-\alpha} \exp(-\gamma t) \frac{\partial^{\alpha}}{\partial t^{\alpha}} \exp(\gamma t)\, p(t|n) + \delta(n)\delta(t) . \qquad (85)$$

All moments of independent, identically distributed random waiting times being finite, the central limit theorem holds true. Using the formula for the kth-order moments of the random quantity τ:

$$m_k = (-1)^k \left[\frac{\mathrm{d}^k}{\mathrm{d}s^k} \tilde{p}(s|n) \right]_{s=0},$$

we shall find mathematical expectation M_n of the sum of n independent waiting times:

$$M_n = \frac{\alpha n}{c} \left(\frac{\gamma}{c} \right)^{\alpha-1},$$

and the corresponding dispersion

$$D_n = \frac{\alpha(1-\alpha)n}{c^2} \left(\frac{\gamma}{c} \right)^{\alpha-2}.$$

Then, in accordance with the central limit theorem for times $t \gg \gamma^{-1}$, one finds

$$p_\tau(t) \sim D_n^{-1/2} \, \varphi\left(\frac{t - M_n}{\sqrt{D_n}} \right),$$

where $\varphi(t) = (2\pi)^{-1/2} \exp(-t^2/2)$ is the normal (Gaussian) distribution density.

This means that stable distributions are intermediate asymptotics for the sums of random quantities being considered. For a sufficiently large number of terms, the stable limiting distribution with the exponent $\alpha < 1$ is transformed into the Gaussian one.

Let us now compose an equation for describing the transport process with truncated power waiting time distributions. The relationship between free and localized carrier concentrations is given by

$$n_\mathrm{t}(\mathbf{r}, t) = \int_0^t \tau_0^{-1} n_\mathrm{c}(\mathbf{r}, t') \left[1 - \Psi(t - t') \right] \mathrm{d}t'.$$

Going over to the Laplace transformants, we obtain

$$\begin{aligned} \tilde{n}_\mathrm{t}(\mathbf{r}, s) &= \tau_0^{-1} (s+\gamma)^{\alpha-1} \, \tilde{n}_\mathrm{c}(\mathbf{r}, s) \mapsto (s+\gamma) \, \tilde{n}_\mathrm{t}(\mathbf{r}, s) \\ &= \tau_0^{-1} (s+\gamma)^{\alpha} \, \tilde{n}_\mathrm{c}(\mathbf{r}, s). \end{aligned}$$

The inverse Laplace transform of this relation yields the following equation

$$\frac{\partial n_\mathrm{t}(\mathbf{r}, t)}{\partial t} + \gamma n_\mathrm{t}(\mathbf{r}, t) = \tau_0^{-\alpha} \exp(-\gamma t) \, \frac{\partial^\alpha}{\partial t^\alpha} \exp(\gamma t) \, n_\mathrm{c}(\mathbf{r}, t).$$

Its rewriting in the form

$$n_\mathrm{c}(\mathbf{r}, t) = \tau_0^\alpha \exp(-\gamma t) \, \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \exp(\gamma t) \, n_\mathrm{t}(\mathbf{r}, t)$$

and substitution into the continuity equation result in

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} + \operatorname{div} \left(\mu \mathbf{E} \, n_\mathrm{c}(\mathbf{r}, t) - D \nabla n_\mathrm{c}(\mathbf{r}, t) \right) = 0.$$

In the dispersive transport case, most carriers are captured in traps, i.e., $n(\mathbf{r}, t) \approx n_\mathrm{t}(\mathbf{r}, t)$; hence, it follows that

$$\begin{aligned} \frac{\partial n(\mathbf{r}, t)}{\partial t} + \operatorname{div} \Bigg[& \exp(-\gamma t) \, \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \exp(\gamma t) \\ & \times \left(\mathbf{K} \, n(\mathbf{r}, t) - C \nabla n(\mathbf{r}, t) \right) \Bigg] = 0. \end{aligned} \tag{86}$$

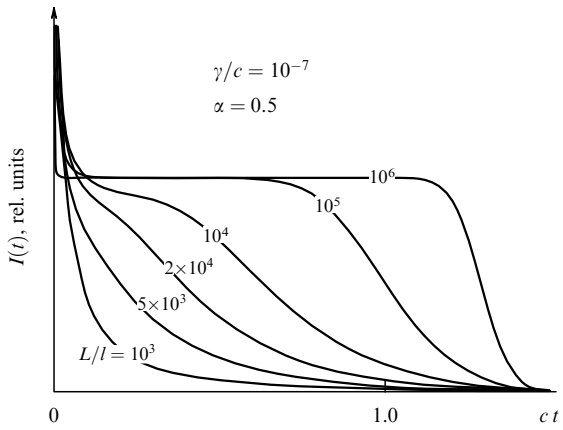

Figure 12. Transient photocurrent in the case of truncated power-law waiting time distributions for different L/l ratios.

Constants K and C are defined in the same way as in equation (43). By turning α to unity, the above equation goes over into the ordinary Fokker–Planck equation. At $\gamma = 0$, this equation coincides with equation (43) for the nontruncated power-law waiting time distribution.

As follows from formula (84), conduction current density in pulsed injection for the case of truncated power-law waiting time distributions is expressed as

$$j(x, t) = eN \exp\left[\frac{x}{l} \left(\frac{\gamma}{c} \right)^\alpha - \gamma t \right] c \left(\frac{x}{l} \right)^{-1/\alpha} g^{(\alpha)} \left(ct \left(\frac{x}{l} \right)^{-1/\alpha} \right). \tag{87}$$

Transient current density is found by substituting this expression into formula (5).

If $\alpha = 1/2$, the expression for transient current takes the form

$$\begin{aligned} I(t) = \frac{eNl\sqrt{c}}{L} \Bigg\{ & \frac{\exp(-\gamma t) - \exp\left[-\left(\sqrt{\gamma t} - 1/(2\sqrt{\tau}) \right)^2 \right]}{\sqrt{\pi t}} \\ & + \sqrt{\gamma} \left[\operatorname{erf}\left(\sqrt{\gamma t} \right) - \operatorname{erf}\left(\sqrt{\gamma t} - \frac{1}{2\sqrt{\tau}} \right) \right] \Bigg\}. \end{aligned} \tag{88}$$

Figure 12 illustrates transformation of transient current curves with an increasing L/l ratio. When the flight time of carriers is much smaller than the truncation time γ^{-1}, the transport remains dispersive and does not pass to Gaussian asymptotics. If t_tr is compared with γ^{-1}, the shape of the transient current curves undergoes modification, and they become inconsistent with the curves for normal and dispersive transport. For $t_\mathrm{tr} \gg \gamma^{-1}$, transport in the long-time asymptotic regime becomes normal.

15. Frequency dependence of conductivity

The frequency dependence of the real component of conductivity in disordered semiconductors is usually fairly well described by the power law

$$\operatorname{Re} \sigma(\omega) = A \omega^\gamma, \tag{89}$$

where the exponent γ normally takes on values from 0.7 to 1 [85]. As mentioned in book [2], the dependence of type (89) "is characteristic of a very broad class of materials."

Conductivity is related to mobility by the expression

$$\sigma(\omega) = e\eta\mu(\omega)\,.$$

Here, η is the concentration of effective carriers. The Nyquist formula (generalized Einstein relation) linking mobility with the diffusion coefficient at nonzero frequencies has the form

$$\mu(\omega) = \frac{e}{kT}\,D(\omega)\,,$$

where the noise spectrum according the Wiener–Khintchin theorem is expressed through the Fourier transform of the velocity autocorrelation function [86]:

$$\operatorname{Re} D(\omega) = \int_0^\infty \cos(\omega t)\,\langle v(t)v(0)\rangle\,\mathrm{d}t\,. \tag{90}$$

As emphasized by Scher and Lax [87], formula (90) is important in that "a knowledge of the fluctuations of the equilibrium ensemble in the *absence of the electric field* permits a calculation of the *linear response* of the system (mobility)." The authors of Ref. [87] showed that relation (90) can be written out as

$$D(\omega) = -\frac{1}{6}\,\omega^2 \int_0^\infty \mathrm{d}t\,\exp(-\mathrm{i}\omega t)\big\langle\big[\mathbf{r}(t) - \mathbf{r}(0)\big]^2\big\rangle\,. \tag{91}$$

The last relation is possible to rewrite in the form

$$D(\omega) = -\omega^2 \int_0^\infty \mathrm{d}x\,x^2\big[\tilde{n}(x,s)\big]_{s=\mathrm{i}\omega}\,, \tag{92}$$

where $\tilde{n}(x,s)$ is the Laplace image in time of the solution to the diffusion equation.

Equation (86) for a one-dimensional case with coordinate-independent coefficient C in the absence of a field assumes the form

$$\frac{\partial n(x,t)}{\partial t} = C\exp(-\gamma t)\,\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\exp(\gamma t)\,\frac{\partial^2 n(x,t)}{\partial x^2}\,.$$

The Laplace transform of this equation yields

$$s\,\tilde{n}(x,s) = C\,(s+\gamma)^{1-\alpha}\,\frac{\partial^2\tilde{n}(x,s)}{\partial x^2} + \delta(x)\,.$$

Substituting the solution of this equation, viz.

$$\tilde{n}(x,s) = \frac{s^{-1/2}(s+\gamma)^{(\alpha-1)/2}}{\sqrt{C}}\exp\left(-\frac{|x|}{\sqrt{C}}\,\sqrt{s(s+\gamma)^{\alpha-1}}\right),$$

into relation (92) gives

$$D(\omega) = 2C\,(\gamma + \mathrm{i}\omega)^{1-\alpha}\,.$$

Hence follows

$$\begin{aligned}\operatorname{Re}\sigma(\omega) &= \frac{e^2\eta}{kT}\operatorname{Re} D(\omega)\\ &= 2C\,\frac{e^2\eta}{kT}\,(\gamma^2+\omega^2)^{(1-\alpha)/2}\cos\left((1-\alpha)\arctan\frac{\omega}{\gamma}\right).\end{aligned} \tag{93}$$

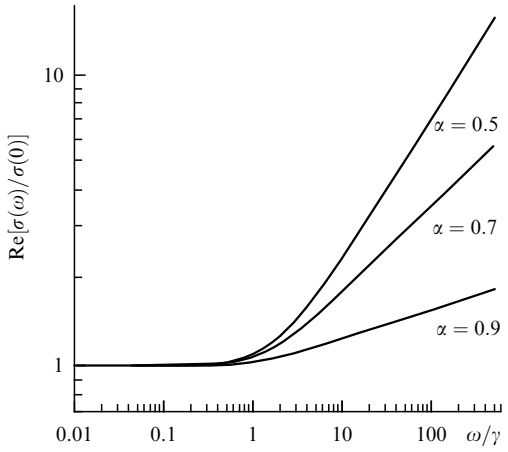

Figure 13. Frequency dependence of conductivity for different α values.

For frequencies $\omega \gg \gamma$, it is easily shown that

$$\operatorname{Re}\sigma(\omega) = 2C\,\frac{e^2\eta}{kT}\,\omega^{1-\alpha}\sin\frac{\pi\alpha}{2}\,.$$

Figure 13 presents frequency-dependent conductivity curves calculated from Eqn (93). Formula (93) predicts the power-law dependence of conductivity on ω at high frequencies in the dispersive transport case. The exponent may acquire values from 0 to 1; in normal transport ($\alpha \to 1$), conductivity is totally frequency independent. In transport driven by the multiple trapping mechanism, exponent α grows linearly with temperature. Consequently, exponent $s = 1 - \alpha$ in the frequency dependence of conductivity in the case of alternating current must linearly decrease with increasing temperature. Such temperature behavior has been reported for a variety of semiconductors (see, for instance, Ref. [88]).

16. Diode frequency properties in dispersive transport

To illustrate the application of equations with fractional derivatives, here is a calculation of the frequency dependence of semiconductor diode conduction governed by dispersive transport. To this end, an expression is needed for the density of alternating current flowing through a diode to the n-type base of which the constant displacement U is applied in the direction of transmission and weak variable signal $u_1\exp(\mathrm{i}\omega t)$ with the amplitude $u_1 \ll U$ and $u_1 \ll kT/e$, i.e.

$$u(t) = U + u_1\exp(\mathrm{i}\omega t)\,. \tag{94}$$

The total hole concentration in the diode base can be presented as the sum of constant $[p_\mathrm{c}^-(x)]$ and variable $[p_\mathrm{c}^\sim(x,t)]$ components, i.e., $p_\mathrm{c}(x,t) = p_\mathrm{c}^-(x) + p_\mathrm{c}^\sim(x,t)$.

The solution to this problem for a crystalline semiconductor diode can be found in Refs [89, 90]. The case of a low injection level is considered, in which alternating current density across the p–n junction is given by $J^\sim = -eD_\mathrm{p}\,\partial p_\mathrm{c}^\sim/\partial x\big|_{x=0}$. The expression for $p_\mathrm{c}^\sim(x,t)$ is obtained by solving the generalized diffusion equation, taking into account linear recombination [see Eqn (57)]:

$$\frac{\partial p_\mathrm{c}(x,t)}{\partial t} + \frac{1}{\tau_{0\mathrm{p}}c_\mathrm{p}^\alpha}\,\frac{\partial^\alpha p_\mathrm{c}(x,t)}{\partial t^\alpha} = D_\mathrm{p}\,\frac{\partial^2 p_\mathrm{c}(x,t)}{\partial x^2} - \frac{\Delta p_\mathrm{c}(x,t)}{\tau_\mathrm{p}}\,,$$

where $p_c(x,t)$ is the concentration of delocalized nonequilibrium carriers, and τ_0 is the mean time of a single capture on localized band tail states. Expansion of the total concentration of nonequilibrium holes into constant and variable constituents yields

$$\frac{\partial p_c^{\sim}(x,t)}{\partial t}+\frac{1}{\tau_{0p}c_p^{\alpha}}\frac{\partial^{\alpha}p_c^{\sim}(x,t)}{\partial t^{\alpha}}$$
$$=D_p\frac{\partial^2 p_c^{-}(x,t)}{\partial x^2}+D_p\frac{\partial^2 p_c^{\sim}(x,t)}{\partial x^2}-\frac{p_c^{-}(x)+p_c^{\sim}(x,t)-p_n}{\tau_p},$$

where p_n is the equilibrium concentration of delocalized holes in the n-region.

Because expression

$$D_p\frac{\partial^2 p_c^{-}(x)}{\partial x^2}=\frac{p_c^{-}(x)-p_n}{\tau_p}$$

holds for the constant constituent, the variable one satisfies the equation

$$\frac{\partial p_c^{\sim}(x,t)}{\partial t}+\frac{1}{\tau_{0p}c_p^{\alpha}}\frac{\partial^{\alpha}p_c^{\sim}(x,t)}{\partial t^{\alpha}}=D_p\frac{\partial^2 p_c^{\sim}(x,t)}{\partial x^2}-\frac{p_c^{\sim}(x,t)}{\tau_p}. \tag{95}$$

Applying the Laplace transform over time,

$$L_{p_c^{\sim}}(x,s)=\int_0^{\infty}p_c^{\sim}(x,t)\exp(-st)\,\mathrm{d}t,$$

to diffusion equation (95), we obtain

$$D_p\frac{\partial^2 L_{p_c^{\sim}}(x,s)}{\partial x^2}=\left(s+\frac{1}{\tau_{0p}c_p^{\alpha}}s^{\alpha}+\frac{1}{\tau_p}\right)L_{p_c^{\sim}}(x,s). \tag{96}$$

Let us formulate boundary conditions regarding the variable signal with frequencies at which the carrier flight time through a spatial charge region of the p–n junction is smaller than ω^{-1}. Then, it is possible to write out, by analogy with the stationary problem, the following relationships:

$$p_c^{-}(0)+p_c^{\sim}(0,t)=p_n\exp\left(\frac{e}{kT}\left(U+u_1\exp(\mathrm{i}\omega t)\right)\right)$$
$$\approx p_n\exp\left(\frac{eU}{kT}\right)+\frac{ep_n}{kT}\exp\left(\frac{eU}{kT}\right)u_1\exp(\mathrm{i}\omega t).$$

Hence, one obtains

$$p_c^{\sim}(0,t)=\frac{ep_n}{kT}\exp\left(\frac{eU}{kT}\right)u_1\exp(\mathrm{i}\omega t).$$

The second boundary condition is $p_c^{\sim}(x\to\infty,t)=0$. Taking account of boundary conditions for the solution of Eqn (96) gives

$$L_{p_c^{\sim}}(x,s)=L_{p_c^{\sim}}(0,s)\exp\left[-x\sqrt{D_p^{-1}\left(s+\frac{1}{\tau_{0p}c_p^{\alpha}}s^{\alpha}+\frac{1}{\tau_p}\right)}\right]. \tag{97}$$

Function $\exp\left\{-x[D_p^{-1}(s+1/(\tau_{0p}c_p^{\alpha})s^{\alpha}+1/\tau_p)]^{1/2}\right\}$ is the Laplace image of a certain function $y(x,t)$. It follows from formulas (94), (97) that

$$p_c^{\sim}(x,t)=\int_0^{\infty}p_c^{\sim}(0,t-t')\,y(x,t')\,\mathrm{d}t'$$
$$=\frac{ep_n}{kT}\exp\left(\frac{eU}{kT}\right)u_1\exp(\mathrm{i}\omega t)$$
$$\times\exp\left[-x\sqrt{D_p^{-1}\left(\mathrm{i}\omega+\frac{1}{\tau_{0p}c_p^{\alpha}}(\mathrm{i}\omega)^{\alpha}+\frac{1}{\tau_p}\right)}\right].$$

The density of alternating current flowing through the p–n junction is given by

$$J^{\sim}=-eD_p\left.\frac{\partial p_c^{\sim}(x,t)}{\partial x}\right|_{x=0}=\frac{e^2p_nD_p}{kT}\exp\left(\frac{eU}{kT}\right)$$
$$\times\sqrt{D_p^{-1}\left(\mathrm{i}\omega+\frac{1}{\tau_{0p}c_p^{\alpha}}(\mathrm{i}\omega)^{\alpha}+\frac{1}{\tau_p}\right)}\,u_1\exp(\mathrm{i}\omega t).$$

Complex p–n-junction conductivity is

$$Y=S_{p-n}\frac{e^2p_nD_p}{kT}\exp\left(\frac{eU}{kT}\right)\sqrt{D_p^{-1}\left(\mathrm{i}\omega+\frac{1}{\tau_{0p}c_p^{\alpha}}(\mathrm{i}\omega)^{\alpha}+\frac{1}{\tau_p}\right)},$$

where S_{p-n} is the p–n junction area. Separating out the real and imaginary parts brings Y to the form

$$Y=G_{p-n}+\mathrm{i}\omega C_{dif},$$

where G_{p-n} is the total conductivity, and C_{dif} is the diffusion capacity of the p–n junction.

For total p–n-junction conductivity, one has

$$G_{p-n}=S_{p-n}\sqrt{\frac{D_p}{2}}\frac{e^2p_n}{kT}\exp\left(\frac{eU}{kT}\right)$$
$$\times\left\{\frac{1}{\tau_p}+\frac{1}{\tau_{0p}c_p^{\alpha}}\cos\frac{\pi\alpha}{2}\,\omega^{\alpha}+\left[\left(\frac{1}{\tau_p}+\frac{1}{\tau_{0p}c_p^{\alpha}}\cos\frac{\pi\alpha}{2}\,\omega^{\alpha}\right)^2\right.\right.$$
$$\left.\left.+\left(\omega+\frac{1}{\tau_{0p}c_p^{\alpha}}\sin\frac{\pi\alpha}{2}\,\omega^{\alpha}\right)^2\right]^{1/2}\right\}^{1/2}.$$

Graphs of the conductivity frequency dependences, based on this formula, are shown in Fig. 14. Here, $\omega_0=(\tau_0c^{\alpha})^{-1/(1-\alpha)}$ and $A=S_{p-n}\sqrt{D_p/2}(e^2p_n/kT)\exp(eU/kT)\omega_0^{-1}$.

By tending α to unity ($\alpha\to1$), we come to the classical expression for a crystalline semiconductor-based diode (such as presented in Refs [89, 90]):

$$G_{p-n}^{cryst}=S_{p-n}\sqrt{\frac{D_p}{2}}\frac{e^2p_n}{kT}\exp\left(\frac{eU}{kT}\right)\sqrt{\tau_p^{-1}+\sqrt{\tau_p^{-2}+\omega^2}}.$$

Tending $\omega\to0$ leads to a differential conductivity of the p–n junction in an alternating current:

$$G_{p-n}^{0}=S_{p-n}\sqrt{\frac{D_p}{2\tau_p}}\frac{e^2p_n}{kT}\exp\left(\frac{eU}{kT}\right).$$

In the high-frequency region for which $\omega\gg(1/(\tau_{0p}c_p^{\alpha}))\omega^{\alpha}$ and $\omega\gg1/\tau_p$ hold true, we have

$$G_{p-n}=S_{p-n}\sqrt{\frac{D_p}{2}}\frac{e^2p_n}{kT}\exp\left(\frac{eU}{kT}\right)\sqrt{\omega};$$

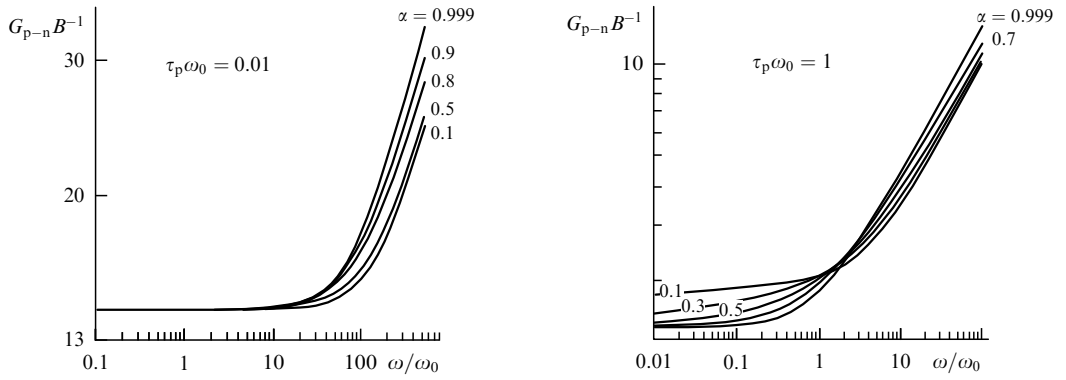

Figure 14. Frequency dependence of diode conductivity for different α values.

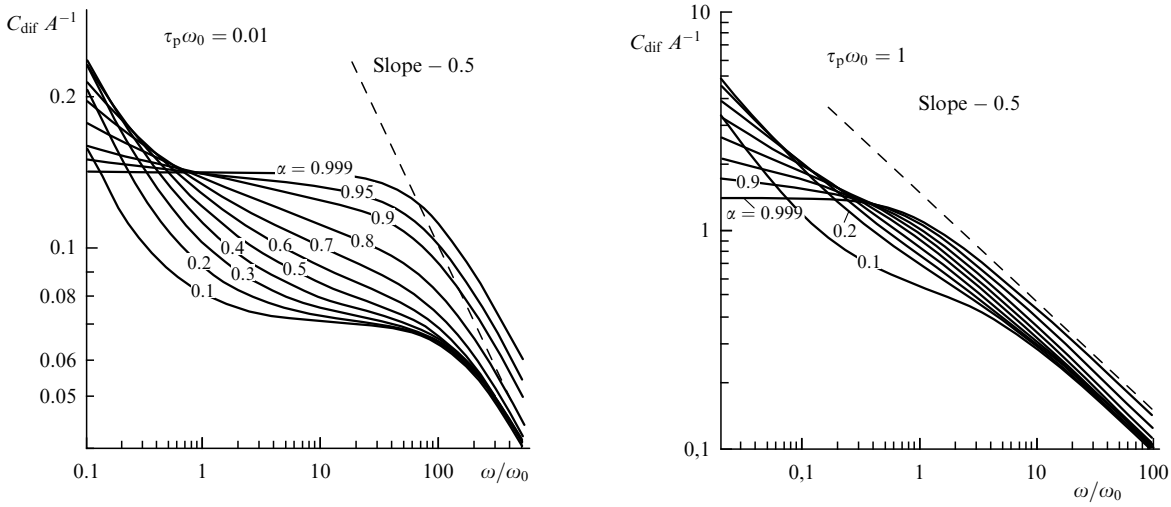

Figure 15. Frequency dependence of diffusion capacity.

in other words, neither carrier capture in localized band tail states nor carrier recombination via deep centers affects conductivity in the high-frequency region.

In the medium-frequency region, where $\omega^{1-\alpha} \ll 1/(\tau_{0p}c_p^{\alpha})$ but $\omega^{1-\alpha} \gg 1/\tau_p$, we have p–n-junction conductivity for dispersive transport in disordered semiconductors:

$$G_{p-n} = S_{p-n}\sqrt{D_p}\,\frac{e^2 p_n}{kT}\exp\left(\frac{eU}{kT}\right)\frac{1}{\sqrt{\tau_{0p}c_p^{\alpha}}}\cos\left(\frac{\pi\alpha}{4}\right)\omega^{\alpha/2}.$$

A similar expression was obtained for diffusion capacity [91]. By tending α to unity ($\alpha \to 1$), we come to the expression reported for crystalline semiconductor diodes in Refs [89, 90]:

$$C_{dif} = S_{p-n}\sqrt{\frac{D_p}{2}}\,\frac{e^2 p_n}{kT}\exp\left(\frac{eU}{kT}\right)\left[\frac{1}{\tau_p} + \sqrt{\frac{1}{\tau_p^2} + \omega^2}\right]^{-1/2}.$$

In the high-frequency region for which $\omega \gg (1/(\tau_{0p}c_p^{\alpha}))\omega^{\alpha}$ and $\omega \gg 1/\tau_p$ hold true, we have

$$C_{dif} = S_{p-n}\sqrt{\frac{D_p}{2}}\,\frac{e^2 p_n}{kT}\exp\left(\frac{eU}{kT}\right)\frac{1}{\omega}.$$

The frequency dependences of diode diffusion capacity in the given coordinates are shown in Fig. 15.

Analogous relations can be obtained for tunneling recombination.

The aim of the above consideration was to illustrate the convenience of fractional differential equations for the analysis of frequency characteristics of devices based on disordered semiconductors, compared to the Arkhipov–Rudenko equation (21). The last equation incorporates the time-dependent diffusion coefficient, and the Fourier transform converts it into the equation containing an integral convolution of the Fourier image of time-dependence of the diffusion coefficient with the transformant of carrier concentration. In other words, we arrive at an integral equation which is much more difficult to solve than the algebraic equation we obtained by Fourier transformation of a fractional differential equation.

17. Conclusions

Let us turn back to the logical motives that prompted us to develop the dispersive transport model based on equations with fractional derivatives. Dispersive transport is a non-Gaussian one, while Gaussian (normal) distribution belongs to the class of Levy stable laws, i.e., it is a particular case of the more general class of limiting distributions. The relationship between dispersive transport and Levy stable statistics was demonstrated by Scher and Montroll in 1975; it is underlain by scaling characteristic of transport processes in disordered semiconductors. Levy stable distributions satisfy equations with fractional derivatives,

whereas normal transport is described by the standard drift–diffusion equation with integer-order derivatives. It is well known that the standard drift–diffusion equation is a special case of fractional differential equations of anomalous diffusion [49].

These facts indicate that a formalism based on equations with fractional derivatives permits describing normal and dispersive transport in disordered semiconductors in the framework of a unified mathematical approach. This gave a major incentive to the development of the fractional differential method.

To conclude, here are the main results of this work to judge how plausible the said motives are.

(1) It necessarily follows from experimentally established facts (the shape universality of transient current curves and power-law dependence of the transient time on sample thickness) that concentrations of nonequilibrium charge carriers in dispersive transport are expressed through stable densities and satisfy drift–diffusion equations with fractional derivatives.

(2) A system of fractional differential equations was proposed that comprises drift–diffusion equations of unipolar dispersive transport for localized and delocalized carrier concentrations, taking into account monomolecular and tunnel recombinations; fractional differential equations of ambipolar dispersive transport; drift–diffusion equations with the distributed dispersion parameter for the description of transport in inhomogeneously disordered media, and the equation for truncated power-law waiting time distributions. Such a system provides a phenomenological basis for the description of dispersive transport in disordered semiconductors.

(3) The fractional differential approach is consistent with the Scher–Montroll theory and the multiple trapping model, but allows normal and dispersive transport to be described in the framework of an integrated formalism. Unlike solutions obtained with the use of the Arkhipov–Rudenko master DT equation, solutions of fractional differential equations satisfy the correspondence principle. In other words, they turn into solutions for normal transition when the dispersion parameter tends to unity. Moreover, the equations themselves undergo transformation into the ordinary Fokker–Planck equation. Equations with fractional derivatives describe transient current curves in disordered semiconductors more accurately than the Arkhipov–Rudenko nonequilibrium transport equation at the dispersion parameter values close to unity.

(4) The description of dispersive transport in disordered semiconductors by equations with fractional derivatives requires fewer adjustable parameters than the Scher–Montroll model and the multiple trapping model.

(5) Application of the generalized limiting theorem yielded the following dispersive transport conditions:

• in the case of multiple trapping, dispersive transport is observed when the mean square of energy fluctuations of localized states is greater than the mean energy trap depth multiplied by the Boltzmann temperature kT;

• in the case of hopping conductivity, the transport is dispersive if intertrap distance fluctuations squared exceed the average jump length multiplied by the half-radius of wave function localization.

(6) For the case of truncated power-law waiting time distributions, fractional differential equations predict a transition from dispersive to normal transport with increasing the sample size and/or lowering the external electric field strength.

(7) If the exponent in the carrier residence time distribution in traps takes on one of the values from an ordered set (discrete spectrum), the transient current behavior in the initial time interval is determined by the maximum value, and in the terminal time interval by the minimum one. This accounts for the discrepancy between dispersion parameters at the initial and terminal segments of transient current curves in certain disordered semiconductors.

(8) Fractional differential equations are convenient for the analysis of frequency characteristics of semiconductor devices in which dispersive transport occurs, because their Fourier transforms give rise to algebraic equations that are much simpler to solve than integral equations derived from equations with variable diffusion coefficient and mobility.

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