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A Monte Carlo study of r–$\mathcal{E}$-hopping transient currents in thin dielectric layers with a macroscopically inhomogeneous spatial distribution of hopping centres

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Abstract. In the present paper we report the results of the Monte Carlo simulation of the time-of-flight experiment for variable-range hopping transport in thin dielectric layers, which are spatially inhomogeneous on the macroscopic scale (i.e. on a scale comparable with the layer thickness). In particular, the total density of hopping centres (with Gaussian distribution in energy) is assumed to change exponentially as a function of the distance from the contacts. The results of simulations performed for various system dilutions, various widths of the Gaussian distribution in energy, and various degrees of the layer spatial non-uniformity are discussed.

1. Introduction

One of the most widely used methods for determination of the microscopic transport parameters, such as the band mobility, the concentration of traps, the trap energy distribution and the trapping cross section, is the analysis of results obtained in the classical time-of-flight (TOF) experiment (Scher and Montroll 1975, Schmidlin 1977a,b, Arkhipov and Rudenko 1982, Rudenko and Arkhipov 1982a,b). The classical theory of the TOF experiment describes transient currents in thin layers, which are assumed to be spatially homogeneous on the macroscopic scale. Having at our disposal well developed theoretical tools such as those described by Marshall (1983a), Marshall and Main (1983), Marshall *et al* (1985), Weissmüller (1985), Muller-Horsche *et al* (1987), Seynhaeve *et al* (1988) and Di Marco *et al* (1989), one can extensively analyse the measured transients. Experimentally, however, it is very difficult to prepare an exactly uniform system. A number of phenomena introduce macroscopic-scale variations in the total density of hopping centres over the layer thickness (see, e.g., Kao and Hwang (1981, p 150) and Samoć and Zboiński (1978)). Thus, the straightforward application of the theory developed for spatially uniform layers cannot be fully reliable. For the multiple-trapping transport mechanism, the influence of spatial inhomogeneity in the trap distribution on the transient currents, measured in the constant-temperature TOF experiment, as well as in the thermally stimulated TOF experiment, has been investigated by Rybicki and Chybicki (1988, 1989), Rybicki *et al* (1990, 1991b) and Tomaszewicz *et al* (1990), and some simple formulae for the determination, or at least the estimation, of the spatial distribution of multiple-trapping centres have been proposed.

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The TOF experiment is obviously not limited only to the multiple-trapping transport mechanism (band transport being interrupted by trapping acts), and transient currents are intensively studied also in materials, which reveal a hopping transport mechanism (jumps between localized states) (see, e.g., Bässler *et al* (1982), Emoto and Kotani (1983), Bässler (1984), Schein *et al* (1986), Yuh and Stolka (1988) and Abkowitz *et al* (1989)). The measurement interpretation for the hopping transport mechanism, however, is much more difficult than in the case of multiple-trapping transport. Computer experiments, and in particular Monte Carlo simulations, are often performed in order to elucidate certain features of the hopping transport in materials characterized by diagonal or/and off-diagonal disorder (see, e.g., Marshall (1978, 1981, 1983b), Marshall and Sharp (1980), Adler and Silver (1982), Ries and Bässler (1987), Pautmeier *et al* (1989) and Richert *et al* (1989)).

The shape of a current signal in the TOF experiment depends in a complicated way on both energy and positional disorder. Each individual hop depends on the local random environment of a given centre. The TOF currents will also depend strongly on variations in the centre parameters on a macroscopic scale (over distances comparable with the layer thickness). In particular, because of a very strong (exponential) dependence of hopping probabilities on the separation between hopping centres, the transient currents measured in the TOF experiment not only should depend markedly on the fluctuations in the hopping centre density on the microscopic scale (of the order of several hop lengths) but also should reveal a pronounced sensitivity to the macroscopic-scale changes in the total centre concentration over the specimen thickness. As far as the nearest-neighbour hopping (r-hopping) transport is concerned, the influence of the macroscopic spatial variation in the total density of hopping centres on the TOF transient currents has been discussed to some extent by Rybicki *et al* (1992). In the present paper we deal with the influence of a similar spatial inhomogeneity of the centre distribution on the TOF transient currents in the case of the variable-range hopping (r–$\mathcal{E}$-hopping) transport mechanism (preliminary results given by Rybicki *et al* (1991a)). In section 2 we describe briefly the Monte Carlo simulation algorithm that we have applied. The simulation results showing the dependence of the TOF transient currents on various model spatial distributions of the total density $N(x)$ of hopping centres possessing a Gaussian distribution in energy are presented and discussed in section 3. Section 4 contains concluding remarks.

2. Simulation algorithm

We consider a thin layer of thickness L placed between two planar contacts (at $x = 0$ and $x = L$, respectively), with an x-dependent total density of hopping centres. At $t = 0$ an infinitesimally thin sheet of carriers is generated on the left contact ($x = 0$). The applied external electric field E enforces carrier motion towards the $x = L$ contact. The transport mechanism to be considered is r–$\mathcal{E}$ hopping, i.e. hopping between centres distributed at random in energy $\mathcal{E}$ according to a given distribution $f(\mathcal{E})$, and at random in space, with a total concentration $N_0S(x)$, where $S(x)$ is a rather slowly varying function of x, with $S(x = 0)$ of the order of unity. This means that we consider continuous changes (in x) of the average centre concentration, which obey the following condition: the distance over which the shape function S changes markedly is much greater than the average inter-centre distance. Thus the local environment of the centre located at x_i may be viewed as a region of random spatial distribution of hopping centres with well defined average density $N_0S(x_i)$. The energy distribution of centres $f(\mathcal{E})$ is assumed to be the normal Gaussian distribution of standard deviation σ.

By writing $f(\mathcal{E})$ and $S(x)$ we wish to point out that the energy distribution of centres is x independent, and the spatial distribution of centres of any energy $\mathcal{E}$ is the same. This means that we assume a relatively simple but, we think, a sufficiently wide class of centre distributions $N(x, \mathcal{E})$ in the factorized form

$$N(x, \mathcal{E}) = N_0 S(x) f(\mathcal{E}). \tag{1}$$

The transient currents were calculated from the time and spatial evolution of the injected carrier packet $n(x, t)$ during its motion towards $x = L$, according to the expression

$$j(t) = -\frac{1}{n_0}\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_0^L n(x,t)\,\mathrm{d}x\right) + \frac{1}{n_0 L}\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_0^L x n(x,t)\,\mathrm{d}x\right) \tag{2}$$

(see, e.g., Leal Ferreira 1977), where $j(t)$ is the particle current per carrier, n_0 is the number of injected carriers. The applied increment of $\log_{10}(t)$ was equal to 0.1 or 0.05. The carrier packets $n(x, t)$ were obtained by averaging the random walks of 10^4 individual carriers.

The random walk of each individual carrier started at $x = 0$ and $t = 0$, finished on arriving at the collecting electrode at $x = L$ and was realized numerically as follows. Let a carrier remain (at a given instant of time) in the centre located at distance x_i from the injecting contact. The neighbouring centres are assumed to be unoccupied (which corresponds to a low injection limit). The total centre concentration at x_i is equal to $N_0 S(x_i)$. The neighbouring centres of x_i are generated at random in space, with an average concentration $N_0 S(x_i)$ (as described by Rybicki *et al* (1992)), and at random in energy, according to the distribution $f(\mathcal{E})$. The neighbourhood of the centre at x_i is chosen as a sphere containing a given number n of centres, i.e. the radius $R(x)$ of the local random environment of the centre at x_i is given by the relation $\frac{4}{3}\pi N_0 S(x_i) R^3(x_i) = n + 1$. It has been checked numerically that the dependence of transient currents on the size $R(x)$ of each local environment becomes saturated for $n \geqslant 36$ for the spatial distributions that we dealt with. Thus $n = 36$ has been chosen arbitrarily for all simulations that we present below. After a hop from the centre at x_i to one of the neighbouring centres (at distance x_j from the contact) is performed, a new random environment of the centre at x_j is generated according to the local average total centre density $N_0 S(x_j)$, and the same energy distribution $f(\mathcal{E})$. If a hop from the centre at x_i near the plane $x = 0$ to the centre with $x_j < 0$ occurs, the carrier position is set to 0. The random walk of each carrier finishes when a hop from $x_i < L$ to $x_j > L$ is encountered for the first time.

Let us consider a realization of an individual hop from a given occupied centre, at $\bar{r}_0$, to one of the neighbouring empty centres, located at $\bar{r}_i$, $i = 1, \ldots, n$. The probability p_{0i} of a hop from the centre at $\bar{r}_0$ to the ith neighbour at $\bar{r}_i$ is (see, e.g., Ries and Bässler (1987))

$$p_{0i} = \nu_{0i} \Big/ \sum_{i=1}^{n} \nu_{0i} \tag{3}$$

where the jump rate ν_{0i} is given by

$$\nu_{0i} = \begin{cases} \nu \exp(-2\alpha|\bar{r}_0 - \bar{r}_i|)\exp(-\Delta U_{0i}/kT) & \Delta U_{0i} > 0 \\ \nu \exp(-2\alpha|\bar{r}_0 - \bar{r}_i|) & \Delta U_{0i} \leqslant 0 \end{cases} \tag{4}$$

and

$$\Delta U_{0i} = \mathcal{E}_i - \mathcal{E}_0 - qE(x_i - x_0). \tag{5}$$

In equations (3)–(5), α is the reciprocal Bohr radius, $\mathcal{E}_0$ and $\mathcal{E}_i$ are the energies of the actually occupied centre and the ith neighbouring unoccupied centre, respectively, E is the applied external field, ν is the frequency factor and q is the elementary charge. According to the probabilities p_{0i} (equation (3)), a corresponding length in random-number space is given to each site in the environment of the site at $\bar{r}_0$. A random number from the uniform distribution serves then to select a site j (at $\bar{r}_j$), into which the carrier remaining at $\bar{r}_0$ jumps. The time for the jump is given by

$$t_{0j} = \left(1 \Big/ \sum_k \nu_{0k}\right) X \tag{6}$$

where X is a random number from an exponential distribution (Schönherr *et al* 1981). The procedure is then repeated for a new random environment generated as a neighbourhood of $\bar{r}_j$.

3. Simulation results

Simulations have been performed for systems of various dilutions, various standard deviations of the Gaussian distributions of the hopping centre energies and various degrees of spatial inhomogeneity of centre total density, always for $qEN_0^{-1/3}/kT = 1.0$ and $L = 150N_0^{-1/3}$ (as results from the construction of the simulation algorithm, in the directions perpendicular to E the computer sample is not limited in any way). Prior to presenting the influence of the spatial macroscopic-scale inhomogeneity of the total centre concentration on the TOF transient currents, we shall show separately the pure effect of increasing the system dilution and increasing the width of the energy distribution of centres, assuming the total hopping centre density to be constant over the layer thickness.

In figure 1 we show several transient currents calculated from (2) for an x-independent (constant over the layer thickness) average centre density for an extremely narrow energy spread of centres, i.e. for the limiting case of $\sigma = 0$, which corresponds to nearest-neighbour hopping (r hopping). The parameter being changed here is the system dilution α', where $\alpha' = N_0^{-1/3}/r_B$ and r_B is the Bohr radius of the localized state. Figure 2 shows histograms of the total numbers of jumps performed by the carriers during their walk from $x = 0$ to $x = L$. As is seen, dispersion of the total numbers of hops increases rapidly with increasing dilution of the system, in accordance with increasing dispersive character of the transients in figure 1. The slopes of the final current decay decrease from about -6 to -2 in the range of α' from 3.0 to 8.0.

The pure effect of increasing the width σ of the Gaussian distribution of site energies is shown in figure 3, where the system dilution is kept constant ($\alpha' = 5$), and the layer has a constant x-independent average total centre density. On increase in the energy distribution width σ, the transients become more dispersive, in a similar way as occurred for increasing dilution a'. With increasing α', however, the slopes for times greater than the effective TOF change (in particular decrease), whereas in the case of increasing σ they remain approximately constant, only weakly decreasing with increasing σ (from -2.25 to -1.75 for σ in the range from 0 to 5.0). The histograms of the total numbers of hops performed during the walk from $x = 0$ to $x = L$ (figure 4) show almost the same dispersion for all values of σ. One can also see that a wider energy distribution of the centres lowers the average number of hops necessary to reach $x = L$.

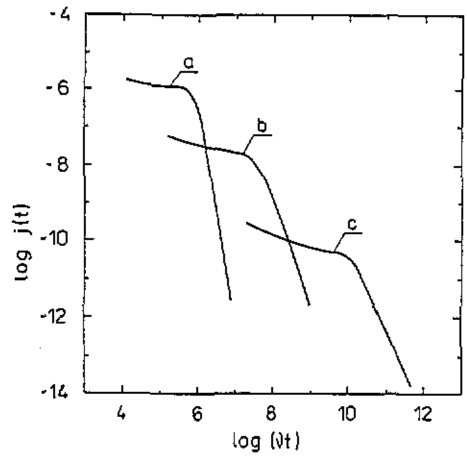

Figure 1. Dependence of r–$\mathcal{E}$-hopping transient currents for $\sigma = 0$ against spatially uniform average centre concentration on the system dilution α': curve a, $\alpha' = 3.0$; curve b, $\alpha' = 5.0$; curve c, $\alpha' = 8.0$.

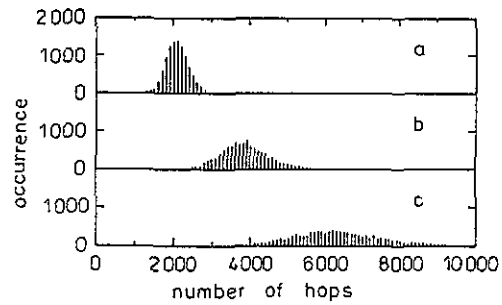

Figure 2. Histograms of the total numbers of jumps performed by the carriers during their walk from $x = 0$ to $x = L$: (a) $\alpha' = 3.0$; (b) $\alpha' = 5.0$; (c) $\alpha = 8.0$. The heights of the vertical lines are proportional to the number of carriers that performed a given number of hops. The histogram resolution is 100 hops. $\sigma = 0$; the average hopping centre density is uniform over the layer thickness.

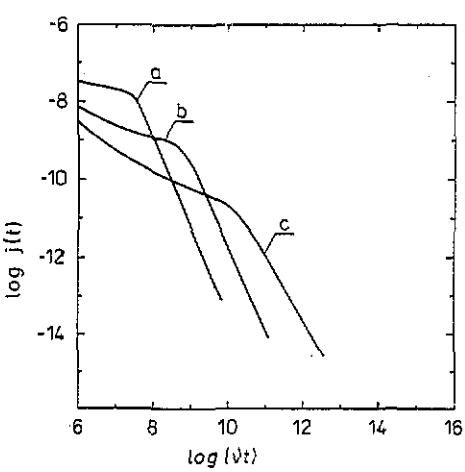

Figure 3. Dependence of r–$\mathcal{E}$-hopping transient currents for dilution $\alpha' = 5.0$ against spacially uniform average total centre concentration on the standard deviation σ of the Gaussian energy distribution of centres: curve a, $\sigma = 0.0$; curve b, $\sigma = 3.0kT$; curve c, $\sigma = 5.0kT$.

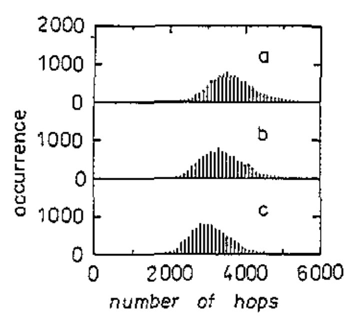

Figure 4. Histograms of the total numbers of jumps performed by the carriers during their walk from $x = 0$ to $x = L$: (a) $\sigma = 1.0kT$; (b) $\sigma = 3.0kT$; (c) $\sigma = 5.0kT$. The heights of the vertical lines are proportional to the number of carriers that performed a given number of hops. The histogram resolution is 100 hops. The system dilution $\alpha' = 5.0$; the average hopping centre density is uniform over the layer thickness.

In order to investigate qualitatively the influence of the macroscopic inhomogeneity of the r–$\mathcal{E}$-hopping centre spatial distribution, we performed our simulations for exponential variations in the total centre concentration as a function of x. In particular, the results presented below in figures 5–10 were obtained for

$$S(x) = \exp(-x/D) \tag{7}$$

and

$$S(x) = \exp[-(L-x)/D] \tag{8}$$

where D is a concentration decay (increase) parameter. For distribution (7) the hopping carriers moving towards $x = L$ enter the region of lower centre density and thus are slowed down. For distribution (8), the increasing centre density makes the carrier motion easier. Figure 5 shows spatial distributions $n(x,t)$ of hopping carriers at the same time ($\nu t = 10^8$) after injection into the layer of given α' and σ, for the total centre concentration increasing and decreasing e^2 times over the layer thickness, and also for a homogeneous spatial distribution. For distribution (7) we see a well developed carrier packet, whereas for (8) the carriers still remain in the immediate proximity of the injecting contact. For a homogeneous spatial centre distribution, the considered time $\nu t = 10^8$ is greater than the effective TOF, and only a few carriers (note the logarithmic scale on the vertical axis) remain within the sample and distributed almost uniformly in space.

Figures 6 and 7 show the influence of the degree of the layer spatial inhomogeneity for $\alpha' = 3$ (relatively dense system), figures 8 and 9 show the same influence for $\alpha' = 5$, and figure 10 for $\alpha' = 8$ (relatively diluted system). Let us consider first the case of the decreasing (in x) total concentration of hopping centres (7). The initial value of the current obviously does not depend on the ratio L/D, because the centre concentration at $x = 0$ always remains the same. With increasing degree of inhomogeneity L/D, the slopes before the effective TOF increase, whereas after the effective TOF they decrease. The σ dependence of the latter becomes weaker (cf curves d in figures 6 and 7). For a high degree of spatial non-uniformity ($L/D \simeq 5.0$) the effective TOF is difficult to determine, the whole transient being the current decay of slope close to -1 independently of σ. Thus the increase in L/D acts qualitatively as the increase in the system dilution, and the overall shape of the transient is governed by the minimum-density region.

For the increasing (in x) total centre density (8) the effect of spatial inhomogeneity is more interesting. Here the initial current values depend on the ratio L/D. The characteristic feature is the occurrence of current maxima immediately before the final current decay for relatively dense systems, with a rather narrow energy distribution of centres and mild spatial non-uniformity of the layer. The current peaks become the current plateaux for a sufficiently wide energy distribution of centres (cf. curves c of figures 6 and 7, and figures 8 and 9), and/or for a sufficiently diluted system (cf. curves c of figures 6, 8 and 10). For more inhomogeneous samples ($L/D = 5.0$ curves) only low-α' and/or low-σ transients reveal a plateau before the effective TOF; for higher α' and/or σ a structureless current decay (with a slope of the order of -1) is observed.

Comparison of the curves for the same L/D ratio and spatial centre distributions (7) and (8) (and the same α' and σ) shows a marked polarity dependence of transient currents. Note that the slope of the final current decay does not depend on the polarity (the final parts of curves b and c and curves d and e in figures 6–10 are parallel).

Figures 11 and 12 show several transients calculated for the layers with enhanced centre density at both contacts, i.e. for the centre spatial distribution of the form

$$S(x) = \exp(-x/D_1) + \exp[-(L-x)/D_2]. \tag{9}$$

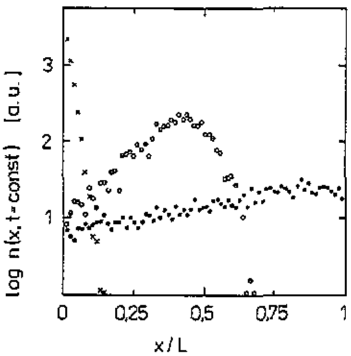

Figure 5. Spatial distributions of the carrier packets at the same time after injection ($\nu t = 10^8$) for different spatial distributions of hopping centres (a.u., arbitrary units): ●, $L/D = 0.0$ (uniform distribution); ○, distribution (7), $L/D = 2.0$; ×, distribution (8), $L/D = 2.0$. In all cases, $\alpha' = 5.0$ and $\sigma = 1.0kT$.

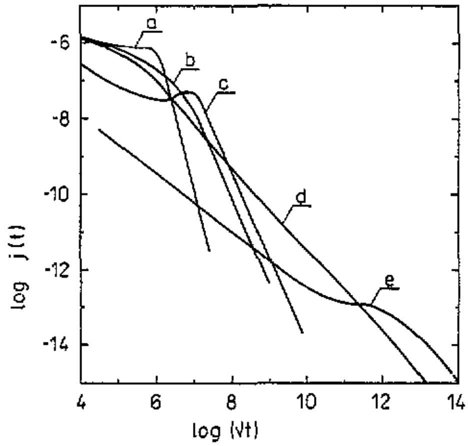

Figure 6. r–$\mathcal{E}$-hopping transient currents for $\alpha' = 3.0$ and $\sigma = 1.0kT$ for the exponential spatial centre distributions (7) and (8): curve a, $L/D = 0$ (x-independent average total centre concentration); curve b, distribution (7), $L/D = 2.0$; curve c, distribution (8), $L/D = 2.0$; curve d, distribution (7), $L/D = 5.0$; curve e, distribution (8), $L/D = 5.0$.

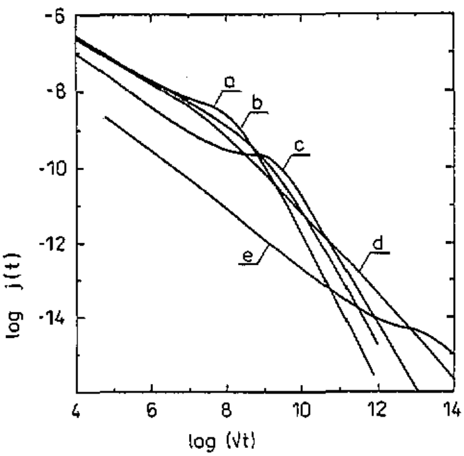

Figure 7. r–$\mathcal{E}$-hopping transient currents for $\alpha' = 3.0$ and $\sigma = 5.0kT$ for the exponential spatial centre distributions (7) and (8): curve a, $L/D = 0$ (x-independent average total centre concentration); curve b, distribution (7), $L/D = 2.0$; curve c, distribution (8), $L/D = 2.0$; curve d, distribution (7), $L/D = 5.0$; curve e, distribution (8), $L/D = 5.0$.

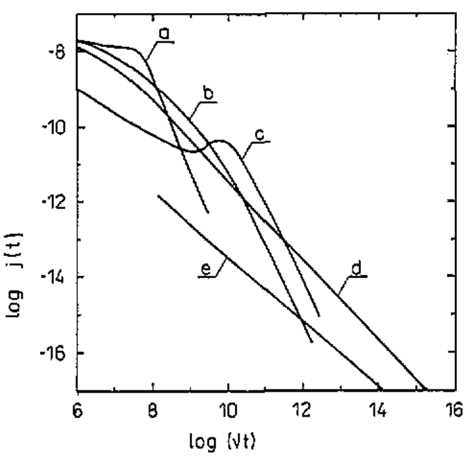

Figure 8. r–$\mathcal{E}$-hopping transient currents for $\alpha' = 5.0$ and $\sigma = 1.0kT$ for the exponential spatial centre distributions (7) and (8): curve a, $L/D = 0$ (x-independent average total centre concentration); curve b, distribution (7), $L/D = 2.0$; curve c, distribution (8), $L/D = 2.0$; curve d, distribution (7), $L/D = 5.0$; curve e, distribution (8), $L/D = 5.0$.

The curves in figure 11 have been calculated for a rather strongly non-uniform dense system ($L/D_1 = L/D_2 = 5.0$; $\alpha' = 3.0$), for various widths σ of the energy distribution of centres. One can see that the expected current minimum, related to the low centre concentration in the

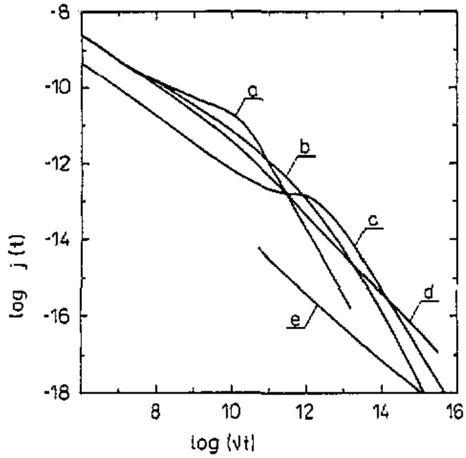

Figure 9. r–$\mathcal{E}$-hopping transient currents for $\alpha' = 5.0$ and $\sigma = 5.0kT$ for the exponential spatial centre distributions (7) and (8): curve a, $L/D = 0$ (x-independent average total centre concentration); curve b, distribution (7), $L/D = 2.0$; curve c, distribution (8), $L/D = 2.0$; curve d, distribution (7), $L/D = 5.0$; curve e, distribution (8), $L/D = 5.0$.

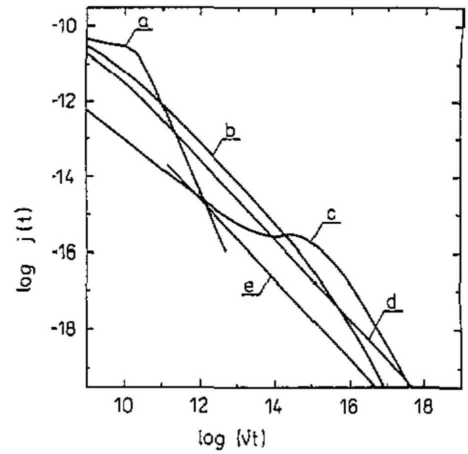

Figure 10. r–$\mathcal{E}$-hopping transient currents for $\alpha' = 8.0$ and $\sigma = 1.0kT$ for the exponential spatial centre distributions (7) and (8): curve a, $L/D = 0$ (x-independent average total centre concentration); curve b, distribution (7), $L/D = 2.0$; curve c, distribution (8), $L/D = 2.0$; curve d, distribution (7), $L/D = 5.0$; curve e, distribution (8), $L/D = 5.0$.

middle of the layer thickness, is hardly evidenced in the case of nearest-neighbour hopping (curve a) and completely disappears for wider energy distributions of centres. Figure 12 shows a very weak dependence of the TOF transient currents on the details of the spatial distribution, and in particular on the layer polarity, in the case of $\sigma = 5.0$. For a very narrow energy distribution the effect is more pronounced.

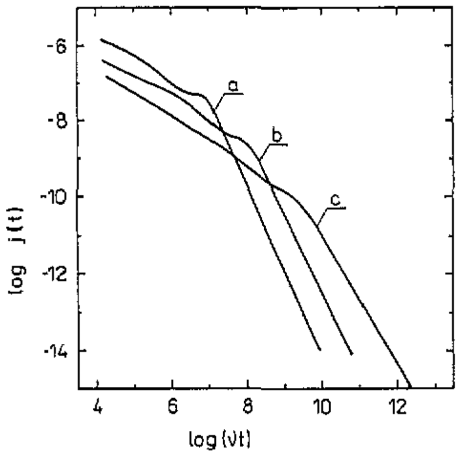

Figure 11. r–$\mathcal{E}$-hopping transient currents for the spacial centre distribution (9): curve a, $\sigma = 0$; curve b, $\sigma = 3.0kT$; curve c, $\sigma = 5.0kT$. In all the cases, $L/D_1 = L/D_2 = 5.0$ and $\alpha' = 3.0$.

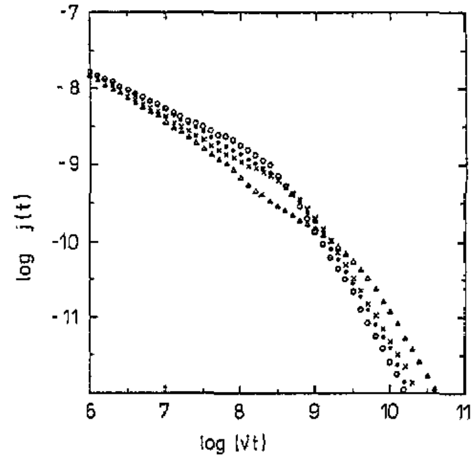

Figure 12. r–$\mathcal{E}$-hopping transient currents for the spacial centre distribution (9): ○, $L/D_1 = L/D_2 = 2.0$; △, $L/D_1 = L/D_2 = 5.0$; ●, $L/D_1 = 2.0$, $L/D_2 = 5.0$; ×, $L/D_1 = 5.0$, $L/D_2 = 2.0$. In all cases, $\alpha' = 3.0$ and $\sigma = 5.0kT$.

4. Concluding remarks

r–$\mathcal{E}$-hopping transient currents measured in the classical TOF experiment are highly sensitive to spatial macroscopic-scale variations in the total centre concentration, as has been shown above for the special case of a Gaussian distribution of the centre energies. The detailed shape of the transients depends in a complicated way on the system dilution, the width of the energy distribution of the centres and spatial variations in the total centre concentration. It seems that, even having at our disposal analytical expressions for the currents, it would be very difficult to determine reliably the spatial centre distribution from the measurement results obtainable with the TOF experiment. However, the existence of spatial non-uniformity of the layer could be recognized by observation of the qualitative changes in the current shape with increasing temperature, which leads to lower dispersion, and thus more pronounced characteristic features of the x-dependent total centre density, as the polarity dependence, or the presence of the current maxima or plateaux.

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