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1996 J. Phys.: Condens. Matter 8 2089

(http://iopscience.iop.org/0953-8984/8/12/021)

J. Phys.: Condens. Matter **8** (1996) 2089–2093. Printed in the UK

The thickness dependence of the hopping time-of-flight current profiles in spatially non-uniform thin dielectric layers

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Received 20 May 1995, in final form 30 August 1995

Abstract. In the previous paper by Rybicki *et al* in 1995 we presented the Monte Carlo calculations of the time-of-flight (TOF) hopping-transport current profiles in non-uniformly defected crystalline layers, and a marked influence of the spatial non-uniformity of the total hopping centre distribution has been shown in the case of extremely thin layers. In the present paper we report using a Monte Carlo simulation the dependence of the TOF transient currents on the layer thickness L, in the wide range $35a \leqslant L \leqslant 10\,000a$. The characteristic current maxima occurring in layers with hopping centre density which increases with increasing x (x is the distance from the injecting contact) just before the effective TOF, reported previously for very thin layers, persist in much thicker samples ($L = 10\,000a$). The relative height of the current peaks initially increases with increasing layer thickness and tends to a saturated value for thicker layers.

1. Introduction

One of the classical methods for the determination of the microscopic transport parameters is the analysis of the results obtained in the time-of-flight (TOF) experiment (see, e.g., Kao and Hwang (1981)). A number of phenomena can introduce macroscopic-scale variations in the total density of traps or hopping centres over the layer thickness, and understanding of the dependence of the TOF current profiles on the degree of the layer non-uniformity is of a great practical interest. Such an influence in non-uniformly defected (doped) crystalline layers has been investigated to some extent in our previous paper on the subject (Rybicki *et al* 1995, hereafter referred to as I), where a marked sensitivity of the TOF current profiles to the spatial non-uniformity of the hopping centre density (exponential decrease and increase in the function of the distance from the injecting contact) has been demonstrated. The most striking effect due to the spatial non-uniformity of the centre density was the appearance of the characteristic current maxima just before the effective TOF in the case of increasing centre density (curve b in figure 1B below), in quite a wide range of parameters. In the Monte Carlo model, calculations in I, however, the layer thickness considered was equal to $70a$ where a is the lattice constant, and one could suspect that such a strong effect of the layer non-uniformity would disappear in real-thickness layers. Thus, in the present work

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0953-8984/96/122089+05$19.50

we extend markedly the dimensions of the simulation box, arriving at more realistic layer thicknesses (up to $10\,000a$, which with $a \approx 7$ Å corresponds to a thickness of several micrometres). In section 2 we recall briefly the Monte Carlo algorithm which we have applied. The simulation results are presented and discussed in section 3.

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 $N_0 S(x)$ of hopping centres. The simulation system is similar to that used by Ries and Bassler (1987): a regular cubic lattice containing $N_x \times N_y \times N_z$ sites with periodic boundary conditions imposed in directions perpendicular to the applied field. A fraction c of the total number of the lattice nodes are chosen as hopping centres and distributed along the direction of the external field E according to the shape function $S(x)$. The energies taken from the normalized distribution $f(\epsilon)$ are then assigned to the transport sites. The remaining $1 - c$ of the lattice nodes are labelled as host sites not participating in the transport process. At $t = 0$ a charged carrier is generated at $x = 0$, and the external electric field E enforces the carrier motion towards the $x = L$ contact. The field is held uniform and constant, which means that our model corresponds to the low-injection case, and no space-charge effects are included. Individual carrier jumps are realized numerically as in the work of Ries and Bassler (1987), using the transition rates proposed by Schonherr *et al* (1981). Random walks between $x = 0$ and $x = L$ of (1–3)$\times 10^3$ carriers are averaged, giving the evolution of the carrier packet: $n(x, t)$. From the latter the current $j(t)$ in the external circuit is calculated (see, e.g., Leal Ferreira (1977)).

3. Simulation results

The simulations have been performed for the centres distributed in energy according to the normalized Gaussian distribution of standard deviation σ/kT. The value $\sigma/kT = 0.0$ (i.e. a single discrete energy level) was used for simulations of the nearest-neighbour hopping transport (r hopping), and the Gaussian distribution with $\sigma/kT = 3.5$ for the simulations of the variable-range hopping transport (r–ϵ hopping). In order to investigate qualitatively the influence of the macroscopic non-uniformity of the spatial distribution of the centres, we performed our simulations for exponential variations in the centre concentration as a function of x, the total number of centres within the sample being held constant. In particular, the results presented below were obtained for $S(x; D) = \exp(-(L - x)/D)$, where D is a concentration increase parameter.

We have investigated our hopping system in the following range of parameters: average concentrations c of hopping centres, $0.2 \leqslant c \leqslant 1.0$; spatial non-uniformity parameter L/D, $0.0 \leqslant L/D \leqslant 2.0$; the layer thickness $35a$–$10\,000a$, where a is a cubic lattice constant. The parameters common to all the simulations are (cf Ries and Bassler (1987)) the cubic lattice constant $a = 7 \times 10^{-10}$ m, the wavefunction overlap parameter $2a\alpha = 5.0$ (where α is the reciprocal Bohr radius), the temperature $T = 400$ K and the external electric field $E = 1.1 \times 10^8$ V m^{-1}. The time is normalized to $1/\nu = \tau$, where $\nu = 6\nu_0 \exp(-2a\alpha)$ and ν_0 is the frequency factor. τ is the average dwell time of a carrier located at a site of undiluted ($c = 1.0$) cubic lattice with six nearest neighbours.

In figure 1 we show several typical families of the TOF transient current profiles calculated for various layer thicknesses L. Figures 1A and 1B refer to r hopping and

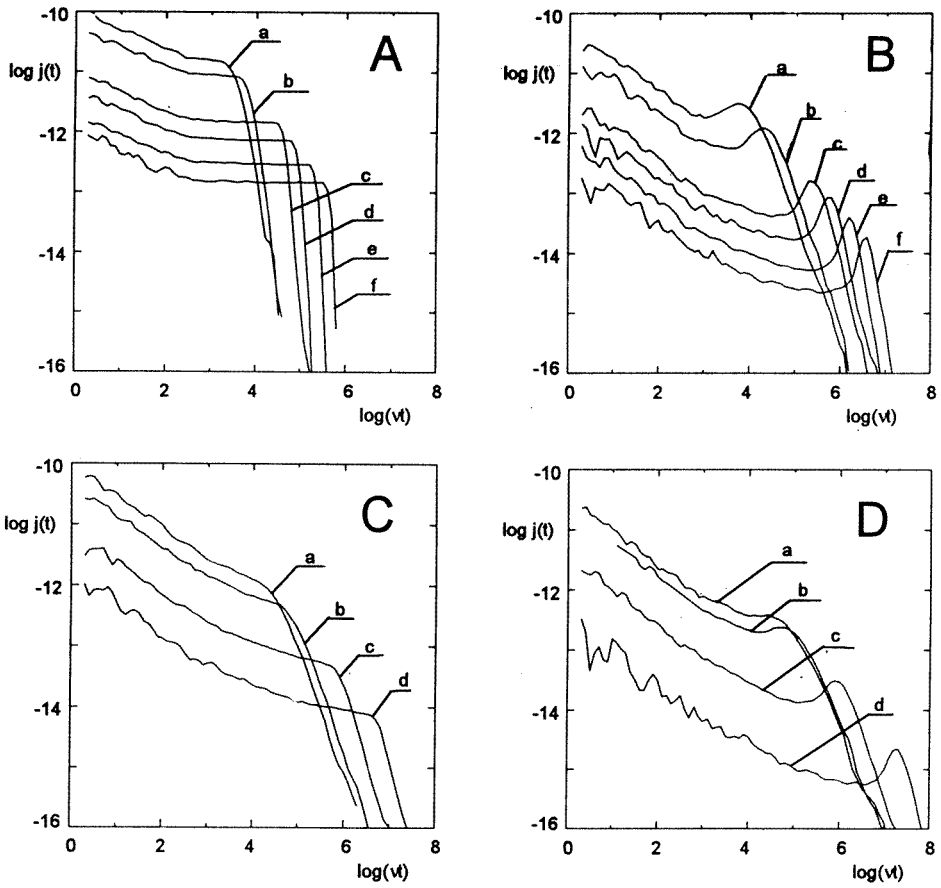

Figure 1. The dependence of the TOF current profiles on the layer thickness L for the centre concentration $c = 0.2$. A shows r-hopping transport ($\sigma = 0.0kT$), uniform centre distribution ($L/D = 0.0$): curve a, $L = 35a$, curve b, $L = 70a$; curve c, $L = 400a$; curve d, $L = 800a$, curve e, $L = 2000a$, curve f, $L = 4000a$. B shows r-hopping transport, exponentially increasing centre density with $L/D = 2.0$: curves a–f, as in A. C shows r–ϵ hopping ($\sigma = 3.5kT$), uniform centre distribution ($L/D = 0.0$): curve a, $L = 35a$; curve b, $L = 70a$, curve c, $L = 400a$; curve d, $L = 4000a$. D shows r–ϵ hopping, exponential increasing centre density with $L/D = 2.0$: curves a–d, as in C.

$c = 0.2$ with $L/D = 0.0$ and $L/D = 2.0$, respectively. Figures 1C and 1D refer to r–ϵ hopping ($\sigma = 3.5kT$) and again $c = 0.2$, with $L/D = 0.0$ and $L/D = 2.0$, respectively. In the case of r-hopping transients in uniform systems (figure 1A) the currents for thicker layers have a well defined horizontal part, which means that the equilibrium transport takes place over the major part of the effective TOF. On the other hand, r–ϵ hopping transients in even the thickest uniform layers hardly reach thermal equilibrium (figure 1C). If the total (integrated over energy) hopping centre density increases monotonically with increasing distance from the injecting electrode, the carrier packet during its drift enters regions of shorter average inter-centre distances, and the jumps become easier. This results in the appearance of the characteristic current peak just before the TOF. The current increase due to higher centre density (most pronounced just before the effective TOF) competes with

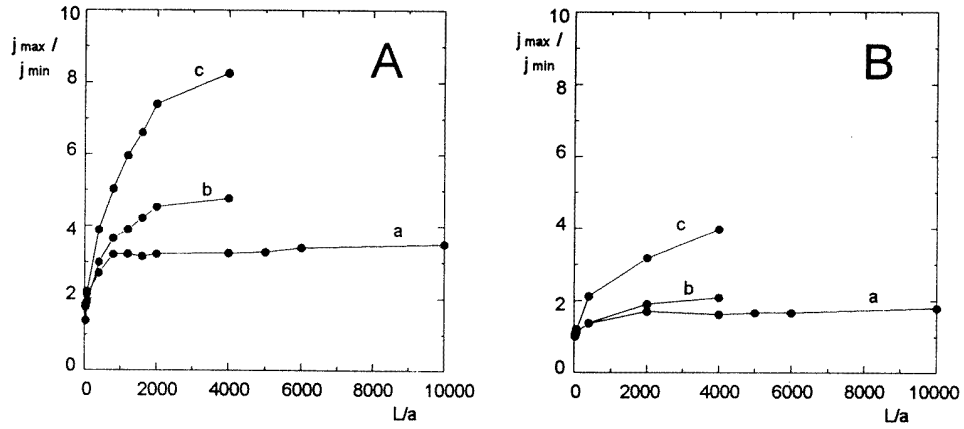

Figure 2. The ratio $r = j_{max}/j_{min}$ versus the layer thickness L for r hopping ($\sigma = 0.0kT$) in A, and for r–ϵ hopping ($\sigma = 3.5kT$) in B: curves a, $c = 0.5$, $L/D = 1.0$; curves b, $c = 0.2$, $L/D = 1.0$; curves c, $c = 0.2$, $L/D = 2.0$.

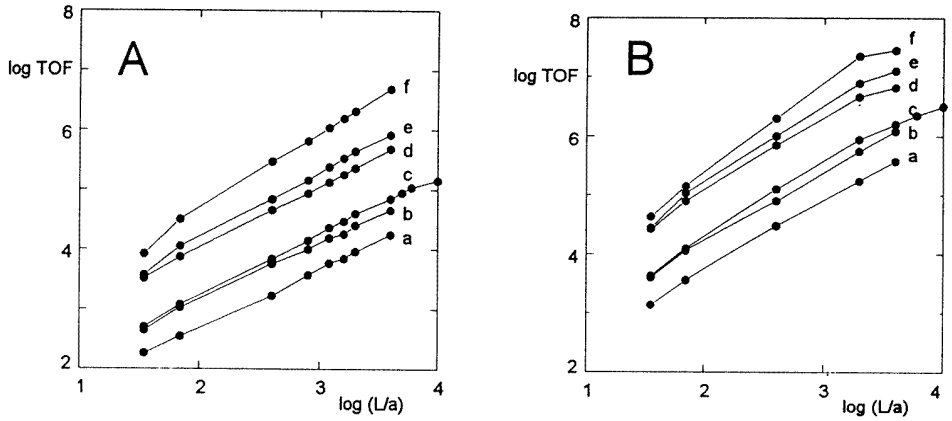

Figure 3. The dependence of the effective TOF on the layer thickness L for r hopping in A, and for r–ϵ hopping in B; curves a, $c = 1.0$, $L/D = 0.0$; curves b, $c = 0.5$, $L/D = 0.0$, curves c, $c = 0.5$, $L/D = 1$; curves d, $c = 0.2$, $L/D = 0.0$; curves e, $c = 0.2$, $L/D = 1.0$; curves f, $c = 0.2$, $L/D = 2.0$.

the current decrease due to the thermalization (most pronounced at the initial stage of the transient). As a result, the relative height r of the current peak, defined simply as the ratio of the maximum to the minimum current values, is larger for thicker layers (figures 1B and 1D). The effect is illustrated in figure 2. Figure 2A refers to r-hopping transport and shows $r = j_{max}/j_{min}$ versus layer thickness L for various concentrations c and various non-uniformity parameters L/D. The ratios r tend evidently to their saturated values, which depend on both c and L/D; for a constant value of the layer non-uniformity L/D, r is higher for lower concentration c whereas, for constant c, the higher value of r occurs obviously for more non-uniform samples. Similar tendencies are present in the case of r–ϵ hopping transport (figure 2B); however, within the considered range of layer thicknesses, saturation

is not achieved for more dispersive transients (curve c), in accordance with the lack of the thermal equilibrium.

Let us consider briefly the thickness dependence of the effective TOF (figures 3A, and 3B for r and r–ϵ hopping, respectively). Despite use of the thinnest layers ($L = 35a$), the thickness dependence of the effective TOF is well described by the linear relation $\log(\mathrm{TOF}) = A + B \log L$. The values of the parameters A and B are summarized in table 1. For uniform systems ($L/D = 0$), the coefficient B only slightly increases with decreasing centre concentration c, and the effective TOFs are approximately proportional to L and to $L^{1.2}$, for $\sigma = 0.0kT$ and $\sigma = 3.5kT$, respectively. On the other hand, for fixed c, the exponent B is an increasing function of the non-uniformity parameter L/D. Because of extremely long CPU time necessary to perform the simulations for thick layers, no systematic research on the c and L/D dependences of the exponent B and the pre-factor A has been undertaken.

Table 1. Coefficients A and B of the linear fitting $\log(\mathrm{TOF}) = A + B \log L$ for $L \geqslant 70a$.

	r hopping		r–ϵ hopping	
	A	B	A	B
$c = 1.0$, $L/D = 0.0$	0.76	0.96	1.35	1.16
$c = 0.5$, $L/D = 0.0$	1.24	0.98	1.87	1.17
$c = 0.5$, $L/D = 1.0$	1.28	0.99	1.73	1.27
$c = 0.2$, $L/D = 0.0$	1.93	1.03	2.63[a]	1.21[a]
$c = 0.2$, $L/D = 1.0$	2.05	1.07	2.68[a]	1.27[a]
$c = 0.2$, $L/D = 2.0$	2.24	1.22	2.35[a]	1.50[a]

[a] Determined for $70a \leqslant L \leqslant 2000a$; because of very long CPU times these simulations were performed for few hundred carriers only, and due to poor statistics the $L = 4000a$ points were rejected.

In conclusion we would like to emphasize that the effects due to the spatial non-uniformity in the hopping centre distribution, described previously in I in the case of very thin layers, do persist in real-thickness layers. The characteristic features of the current profiles become more evident on increasing L and tend to saturation for layers thick enough to permit thermally equilibrated transport.

Acknowledgments

The work has been partially sponsored by KBN under grant 2P 302 16004. The possibility of performing our calculations at the Computer Centre of the Camerino University (Italy), and at the TASK Computer Centre in Gdańsk (Poland) is kindly acknowledged.

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