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To cite this version:

E. Constant, B. Boittiaux. NON STEADY STATE CARRIER TRANSPORT IN SEMICONDUCTOR, APLICATION TO THE MODELLING OF SUBMICRON DEVICES. Journal de Physique Colloques, 1981, 42 (C7), pp.C7-73-C7-94. 10.1051/jphyscol:1981708 . jpa-00221644

HAL Id: jpa-00221644
https://hal.science/jpa-00221644

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JOURNAL DE PHYSIQUE
Colloque C7, supplément au n°10, Tome 42, octobre 1981 *page* C7-73

NON STEADY STATE CARRIER TRANSPORT IN SEMICONDUCTOR, APPLICATION TO THE MODELLING OF SUBMICRON DEVICES

E. Constant and B. Boittiaux

Centre Hyperfréquences et semiconducteurs, LA CNRS N° 287, Bât. P3, Greco micro-onde CNRS N°11, 59655 Villeneuve d'Ascq Cedex, France

Résumé. - On se propose ici, d'une part d'étudier quelles sont les nouvelles caractéristiques de la dynamique électronique dans un composant submicronique et d'autre part de décrire de nouvelles méthodes de modélisation qui permettent de les prendre en compte.

Abstract. - It is the purpose of this paper to study on the one hand, what new features characterise non steady state carrier transport in sub-micron semiconductor devices, and on the other to suggest and describe new methods of modelling which take these new features into account.

I. Introduction. - The main goal of the microelectronics industry is to make ever-increasing numbers of smaller devices on a single chip. The advent of high-resolution electron and X-ray lithographic techniques is leading toward an era in which individual features sizes might well be fabricated on the scale of 100-200 nm. It will then become feasible to develop very small device structures where size and related effects may be as important as the bulk properties of the host semiconductor material. In this type of devices, carriers are often in non stationnary conditions characterized by strong spatial non uniformity and it becomes obvious that we must now ask whether classical device modelling may be extrapolated down to the very small space and time scales usually encountered in sub-micron devices. It is the purpose of this paper to study what kind of new phenomena may occur in non steady conditions in a semiconductor and to suggest and to describe new methods which take them into account.

In the first part of this paper, the main features of carriers transport in conditions which are either non stationnary or characterized by strong spatial non uniformity, will be discussed. It will be assumed that transport physics may still be based on the Boltzmann equation but it will be shown that, even for this case, the features characterizing carrier transport can be very different from those related to steady state and bulk transport. These include the well known balistic motion and overshoot velocity phenomenon but also other ones which have not yet been studied in

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detail such as non stationnary state diffusion, and special effects due to transverse electric field in a depletion or inversion layer.

In the second part of this paper, we discuss new methods of modelling which could take all the previously described features into account. Suitable improvements can be made to the classical modelling of large devices by using the relaxation time approximations and the principle of such a method is presented. Particle models can also be used in the modelling of submicronic devices. In Monte Carlo methods, motions of the particles representative of the carriers in the device are studied simultanously in $\vec{k}$ and $\vec{r}$ space. A few examples will be given concerning this powerfull method which unfortunately involves very long computation time. As a consequence, simplified procedure will aslo be shortly discussed.

II. Basic features of non steady state carrier transport in S.C. - II.1. Theoretical background, carrier transport and physical scale. - In order to study new phenomena which may occur in sub-micron devices, it is necessary to recall briefly the basic physics of carrier transport in a semiconductor.

Transport properties are usually described by the Boltzmann transport equation (BTE) :

$$\frac{\partial f}{\partial t} + \vec{v}\,\frac{\partial f}{\partial \vec{r}} + \frac{e\vec{E}}{\hbar}\,\frac{\partial f}{\partial \vec{k}} = \int_{\vec{k}} dk[f(\vec{k}')W(\vec{k}',\vec{k}) - f(\vec{k})W(\vec{k},\vec{k}')], \qquad (1)$$

which allows us to obtain the carrier distribution $f(\vec{r},\vec{k},t)$ in k-space and geometrical r-space. In this relation, the drift velocity $\vec{v}$, can be obtained from the band structure $\varepsilon(k)$ characterising the semiconductor material through the classical equation

$$\vec{v} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}} \qquad (2)$$

Consequently the main parameters which occur in the BTE are the band structures, scattering mechanisms (represented by the functions $W(\vec{k},\vec{k}')$), and the electric field $E(r,t)$. If all these quantities are known, the BTE can be solved to obtain the distribution function from which all average quantities such as $<\varepsilon>$, $<\vec{v}>$ can be deduced. This is achieved practically using either iterative methods [1] [2] to obtain f directly, or more indirect methods such as the Monte Carlo (MC) procedure [3] [4]. The interest in this last method is not only because it is a powerful tool in the study of nonlinear transport in semiconductors, but also because it provides a clear explanation of electron dynamics in a semiconductor. In this method, the stochastic motion of the representative points of the carrier in k-space is studied numericaly in order to obtain at each time step full information on the state of the carrier (i.e.its energy and its drift velocity). Motions are calculated taking into account every time step Δt, i.e. the effect of the electric field which will modify $\vec{k}$:

$$\vec{\Delta k} = (q\vec{E}/h)\Delta t;$$

and the effect of the scattering mechanisms which may randomly change the position of the representative points with a probality

$$\lambda(k)\Delta t = \Delta t \int_{\vec{k}'} W(\vec{k}\vec{k}')\, d\vec{k}'$$

(pratically suitable random trials can be achieved to find out whether an interaction has occured during Δt, and, if so, to determine which specific scattering has occured).

Since, for each Δt, the energy and velocity are known, the average quantities $<\varepsilon>$ and $<\vec{v}>$ can be obtained : (i) by an ensemble average, studying the motion of a great number of representative points ; or (ii) by a time average, studying the motion of a single representative point over a very long period of time. In addition since $\vec{v}$ can be determined the location of the carrier in the geometrical space can also be known for each step.

Consequently, the MC method makes it possible to solve the BTE whatever the scattering mechanisms and band structure may be, and to obtain in almost all cases useful results on carrier transport in semiconductors. However, signficant results will be obtained only in cases where the BTE can be applied, and so it is necessary to point out the three main assumptions which are needed for the BTE to be valid :

(i) effective mass and band approximations hold ;

(ii) collisions are instantaneous in both space and time

(iii) scatterings are independent of the electric field.

The validity of such assumptions has been discussed by Ferry and Barker [5] [6] [7]

Based on this theoretical background, the influence of the size of the device and of the operating conditions on the characteristics of carrier transport will now be studied. From equation (1), it can be noted that the space and time variation of the electric field will determine values of $\frac{\partial f}{\partial t}$ and $\frac{\partial f}{\partial \vec{r}}$ In classical devices operating in usual conditions, one generally assumes that these space and time variations are so weak that in each point of the S.C. a steady state is obtained. This results from an "equilibrium" between perturbations due to the electric field and scattering mechanisms (practically this assumption means that the BTE can be used neglecting the term $\partial f/\partial t$). Then the main characteristics of carrier transport in a large device (average drift velocity $<\vec{v}>$, average energy $<\varepsilon>$ and diffusivity) will depend only on the instantaneous local electric field, regardless of the values of the electric field in the past, all around the point being studied in the semiconductor material. Such assumption will generally be valid if the variation of the electric field along a mean free path or during a mean free time between two collisions can be neglected. This is not always the case for high frequency operation (even for bulk semiconductor) and for submicronic devices (even in D.C. operations). New features then appear and in order to obtain a good understanding of this phenomena, we intend to successively study the case of a bulk semi-conductor submitted to fast temporal variations of the applied electric field, and the case of submicronic devices where the electric field applied is characterised by short spatial scales.

II.2. Phenomena due to fast temporal variations of the electric field

II.2.1 Study of the average drift velocity. - The two following cases can be investigated (note that in both cases spatial uniformity of the electric field E is assumed) :

(i) a high-frequency sinusoidal electric field superposed upon a steady state field is applied to the whole semiconductor material :

$E(t) = E_0 + E_1 \sin \omega t$;

(ii) a time pulse or a time step configuration of the electric field is applied to the whole semiconductor material.

In both cases, we have to determine the average transient drift velocity which could result from the applied electric field. In the first case, results obtained concerning the time variation drift velocity $<\Delta v(t)>$, caused by the sinusoidal electric field, can be characterised by introducing a complex differential mobility using the relation :

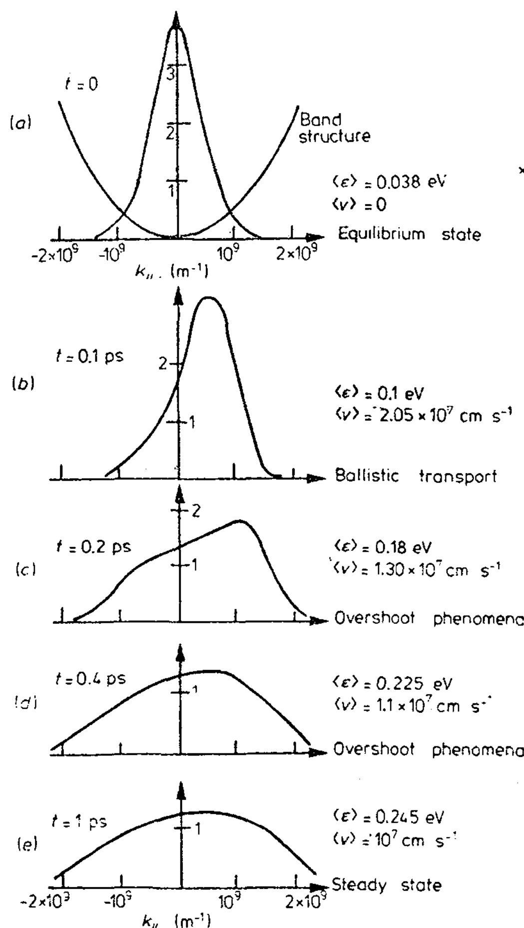
$\Delta v_\omega = \mu^* E_1$,

where Δv_ω is the Fourier transform of $(\Delta v(t))$.

The low frequency differential mobility can easily be obtained as the derivative $(\frac{dv}{dE})_{Eo}$ of the velocity field characteristics because it can be assumed that a steady state exists, resulting from a balance between the effect of the electric field and the scattering mechanisms. By contrast, that is no longer the case when V.H.F. electric field is applied to the semi-conducteur materials because the carriers can be strongly accelerated or decelerated between two successive collisions. As a result, mobility values very different from low frequency values can be achieved. This is the case even in the saturated velocity range where an extra mobility can occur [8]. Such an effect also determine the frequency limit of the negative differential mobility of most of the multi valley semi-conductors, which result from the non instantaneousness of the transferred electron effects [9] [10].

The above phenomens will occur only in microwave devices. The case where a time pulse or a time step configuration of the electric field is applied to the semiconductor material appears to be more interesting since it is the simplest way to stimulate roughly the electric field applied to a carrier when it travels through the active layer of a small device. A first example of results obtained when a time step configuration of E is applied to Si is given in figure 1 [11], where the average transient drift velocity and energy are plotted against time. It can be noted that just after the application of the step, the drift velocity increases proportionnally with time ; the motion of the carrier is uniformly accelerated - this is the classical concept of ballistic transport [12]. The drift velocity then has a maximum value which is much higher than the steady state value ; this is the well known overshoot phenomenon [13]. As time increases, the average energy of the carrier also increases progressively until a steady state value is obtained, while the drift velocity decreases and also reaches a stationary value.

In order to understand these phenomena better it is interesting to study them in k-space. In figure 2 the corresponding distribution functions obtained by MC methods are plotted



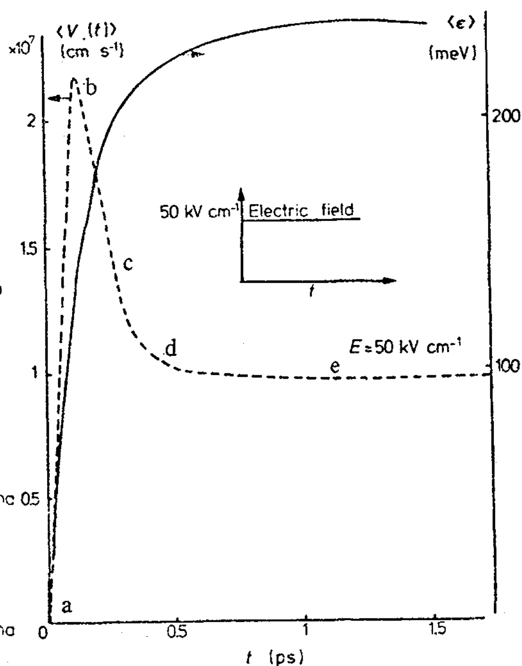


Figure 1 . Transient drift velocity ⟨v⟩ and average energy ⟨e⟩ resulting from a time step of the electric field (n-Si, E‖<111> ,T =293K)

Figure 2 . Evolution of the distribution function when a time step of the electric field ($0-50 kVcm^{-1}$) is applied to Si (E‖<111>, T = 300 K).

for various times after the application of the pulse [11]. At time 0 the symmetrical distribution function of the equilibrium condition is observed (figure 2a). Drift velocities of the simulated carriers are proportional to the slope $\partial\varepsilon/\partial k$, corresponding to the location of representative points in the band structure (also represented in figure 2a). Obviously, in this symmetrical case, the average value of the drift velocity vanishes, while the value of the average energy corresponds to the temperature of the semiconductor material. In figure 2b is plotted the distribution function obtained when the electric field has just been applied ; scattering mechanisms have not yet occured, and consequently only the perturbation due to the electric field is

observed. Every carrier, or, more exactly, every representative point, goes in the same direction and only a shift in the distribution function (proportional to the observation time) is observed. The drift velocity of all carriers increases proportionally with time and a high value of the average drift velocity can therefore be achieved. This ballistic transport is obtained in Si at room temperature during the first tenth of a picosecond. As time increases, however, the scattering mechanisms progressively occur, the distribution function widens (figure 2c and d), and the average drift velocity decreases because, when a carrier is submitted to an interaction, the drift velocity resulting from the action of the electric field is generally reduced. Values higher than the steady state value remain (the overshoot phenomenon) until the steady state is reached (figure 2e) when there is a balance between the energy gained from the electric field and energy lost through scattering mechanisms.

Keeping these various phenomena in mind a first description of the most suitable semi-conductor, which could allow to achieve the highest value of the overshort and balistic velocity, can be given.

Firstly, for a given variation of k imposed by the electric field, the variation of the velocity of the carriers must be as large as possible. Consequently, the band structure should be characterized by the lowest value of the effective mass. In addition, this effective mass must not increase too much when the carrier energy ε increases (paralolic band is the optimum case).

Secondly, the scattering rate must remain as weak as possible regardless of the value of ε, because due to scattering mechanisms the distribution function widens and the average velocity decreases.

Taking into account these requested properties, III V semi-conductor compounds present particular interest because, in most cases, effective mass and scattering rates are very weak. However, they are multualley semi-conductors and for an energy close to the intervalley gap, scattering rates strongly increase and carriers transfer in the valley in which only very low values of the drift velocity can be achieved. Consequently semi-conductors such as Ga_{1-x} In_xAs or In AsP which have a large intervalley gap, a low effective mass appear to be the most suitable materials [14] [15].

Nevertheless, so far Ga As appears to be the most used semi-conductor material. Consequently, it seems of interest to determine the value of the maximum average transient velocity which could be realized by a carrier travelling over a distance d in this semi-conductor. First of all, let us consider the case of a time step configuration of the electric field : for every distance d, an optimum value of the electric field E_o can be choosen in order to obtain the maximum value of the average velocity over a distance d. The obtained results appear in figure 3.

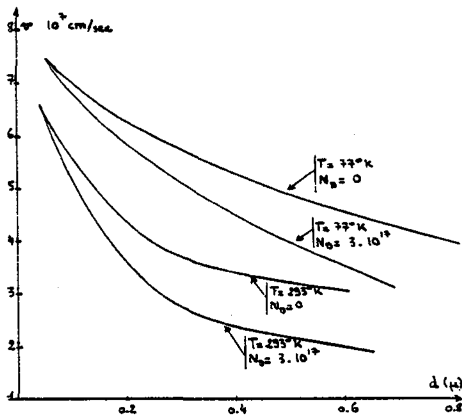


Fig. 3

Maximum average velocity of carriers submitted to a time step and tranvelling over d distanced

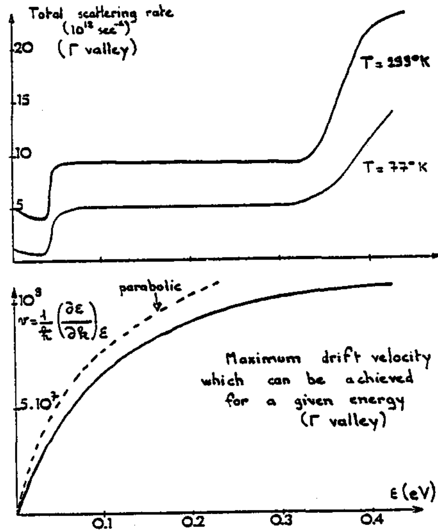


Fig. 4

Total scattering rate and maximum velocity versus the energy of the carrier (GaAs)

It can be noted that the average drift velocity can be increased by using very small submicronic distance d, low impurety concentrations and low temperature operations. However, for very small values of d, balistic and overshoot motions progressively occur regardless of the impurety concentration values and of the temperature. In addition, it should be pointed out that the optimum value of the electric field step E_0 requested in order to achieve a maximum average velocity is roughly inversely proportional to the distance d, the product E_0d being very close to the intervalley gap as it could be expected by using simple arguments [14].

One can now wonder if higher values of average velocity could be achieved by using a time configuration of the electric field different from the simple time step. The answer to this question is in figure 4. The maximum value of the velocity which can be achieved along one direction of the space (velocity distribution and velocities along the two other directions are assumed to be close to zero) has been reported versus the energy of the carriers. In the same figure, the dependence of the total scattering rate on the energy is also studied. From these results, it can be noted that it is possible to realize, for energy values slighly smaller than the intervalley gap, very high values of the instantanous drift velocity ($\#10^8$ cm/s) with reasonnable values of the scattering rates and consequently during a relatively long time. However, this can only be achieved if the energy of the carrier (close to $\Delta\varepsilon_{TL}$) is kept to a constant value during a very long time. Pratically this can be realized by using very short time pulse configuration of the electric field E characterized by

very high value of E. The pulse duration has to be choosen in order to obtain a final energy slighly smaller than the intervalley gap. For very short pulse durations (very high values of E are then requested), scattering events have no time to occur, and consequently very high drift velocity can be achieved without an important velocity distribution. However when this state is realized, the electric field has to be cancelled since ε must be kept to a value smaller than $\Delta\varepsilon_{\Gamma L}$. The electric field vanishing to zero, a really balistic motion of all the carriers is then archieved ; consequently the initial very high velocities decrease very slowly.As a result, rather long distances can be archieved during very short times. An example of results obtained by using such a balistic motion is given in figure 5.

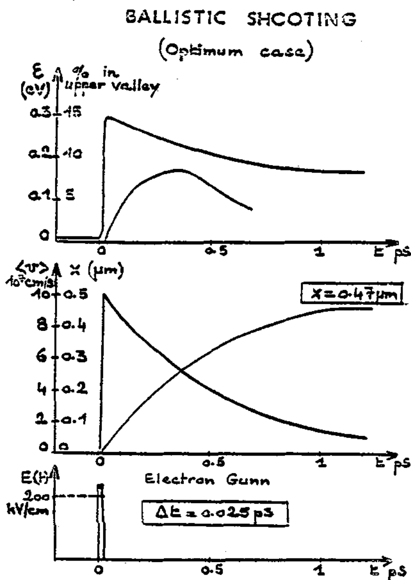


Fig. 5. : Average energy and drift velocity of the carriers resulting from a very short time pulse of Electric Field.

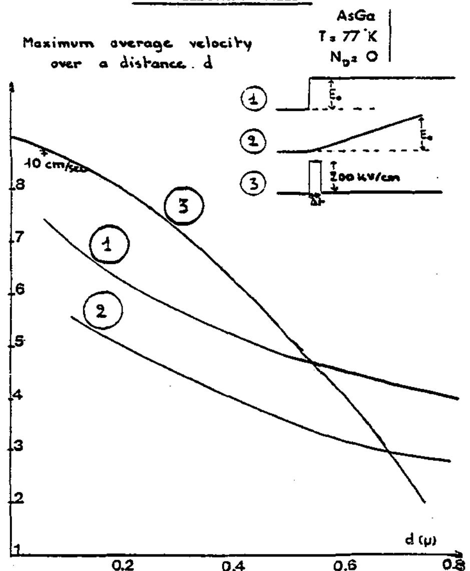


Fig. 6 : Maximum average velocity of a carrier travelling over a distance d for various time configuration of the electric field.

The pulse time duration has been choosen in order to obtain a maximum value of the distance achieved by the carrier after the application of the electric field. The corresponding maximum average velocity achieved with this type of time configuration of the electric field are given in figure 6. It can be noted that for distance smaller than 0.5μ, the average velocities are significantly greater than those obtained by using the classical time step. For comparaison, are also plotted the average velocities obtained by using a field configuration where E increases proportionnaly to the time. It must be pointed out that in this case which roughly simulates the electric field applied to the carriers when it travels through the active region of usual submicronic devices (TEC, n^+ nn^+ structures), the average drift velocities are smaller than those obtained by using a simple time step. Consequently, other devices configurations, such as balistic transistors studied by Cornell University have to be found in order to use all the possibilities of velocity of the carriers in a semiconductor.

II.2.2. Diffusion phenomena. - Depending on the phenomena we intend to study in a semiconductor, electronic concentration profile, or thermal noise, there are two main ways of defining the diffusion coefficients. In the first definition, assuming an uniform electric field in a bulk semiconductor D is given by the following relation :

$$D\ (E,T) = \frac{1}{2}\ \frac{d}{dT}\langle\Delta z^2\rangle(E,T) \qquad (3)$$

where $\langle\Delta z^2\rangle$ is the variance of the random distances parallel to the field direction travelled by the carriers during the observation time. Direct experimental determination of such D(E) can be achieved using the time-of-flight technique in which the spreading of a narrow pulse of carriers drifting in the semiconductor parallel to an applied electric field is measured by the waveform of the induced current.

In the second definition, D depends on the velocity fluctuations suffered by the cariers in the semiconductor and is proportional to the power spectral density $S_v(\omega)$ associated with these velocity fluctuations.[13] Using the Wiener-Kintchine theorem we have

$$\begin{aligned} D_{\parallel}\ (\omega,E) &= \tfrac{1}{4}S_v(\omega) \\ &= \int_0^\infty \langle\Delta v_z(o)\ \ \Delta v_z(\tau)\rangle \cos\omega\tau\ \ d\tau \qquad (4) \\ &= \int_0^\infty \langle\Delta v_z^2\rangle \phi(\tau)\cos\omega\tau\ \ d\tau \end{aligned}$$

where ϕ (τ) is the correlation function of the velocity fluctuation

Experimental determination of D, defined using Eq.4 can be achieved measuring the noise delivered by an unidimensional semiconductor submitted to a uniform electric field (this condition is not so easily achieved).

In the case of low frequency or infinite observation time T limits, the two first definition are easily shown to be identical on the contrary, if the observation time t is much smaller than the mean free time between two collisions, the carriers have no time to change during the time t and equation (i) can then be written :

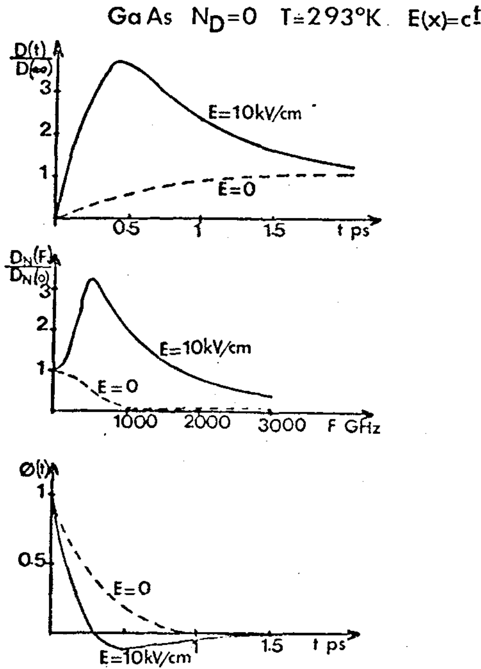
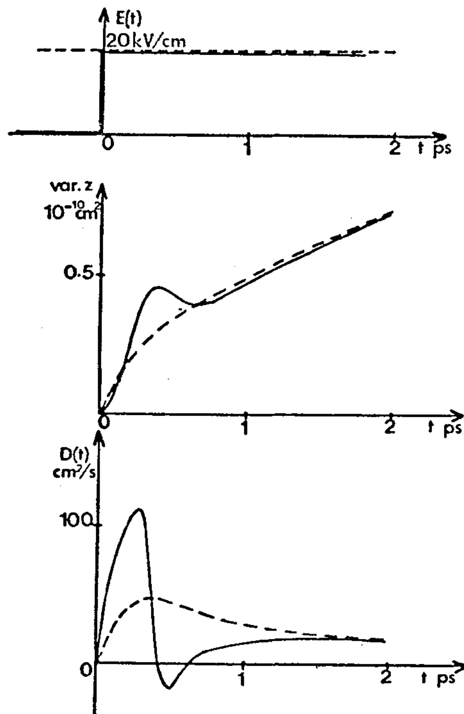


Fig. 7 : Speading diffusion coefficient versus the observation time ; Noise diffusion coefficient versus the frequency. Correlation functions of the longitudinal velocity fluctuations. The study is carried out for two values of the electric field (E = 0, E=10kV/cm) assumed to be uniform in GaAs (T = 293°K, N_D = 0).

$$D^S = < \Delta v^2 > t$$

In the high frequency limit, from relation [4] it can be noted that $D \to 0$ as $\omega \to \infty$. However, no simple relations hold in this case for D obtained using both definitions.

Typical variations of the speading diffusion with the observation time and of the noise diffusion with the frequency are given in figure 7 in the case of GaAs[33] Two main cases occur. The first one is obtained when scattering between non equivalent valley is negligible, i.e. when the electric field is much smaller than the critical field. In this case, the noise diffusion coefficient is a monotonous decreasing function as ω increases and the spreading diffusion coefficient increases monotonously as t increases. This corresponds (figure 7) to velocity correlation functions close to an exponential form. The second case is observed at high electric fields when intervalley scatterings increase to a great extent. The frequency or time evolution of the diffusion coefficient presents a maximum and this behavour corresponds to



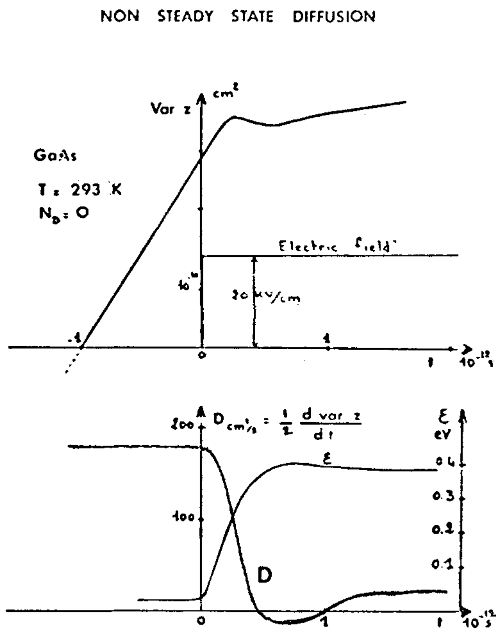


Fig. 8a

Fig.8b

Variance of the random distances travelled by the carrier and transient diffusion coefficient versus time.
Fig. 8a. : The electric field step is applied just at the beginning of the observation time (full lines); a static electric field is applied to the semi-conductor in order to realize a steady state (dashed lines).
Fig. 8b. : The electric field step is applied a long time after the beginning of the observation time.

correlation functions of velocity fluctuations which reach negative values and then vanish. These phenomena can be explained in the following way. In the higher velocity valley (i.e. the central valley for n-GaAs), the lifetime of electrons with positive velocity fluctuations is very short since they are highly likely to transfer to other valleys. Consequently, we should mainly observe the long flight in k-space accross the central valley of electrons characterized by initial negative velocity fluctuations. For such an electron, the z component of velocity should vary roughly linearly with time.

As a result, the frequency or the time which correspond to the diffusion coefficient peak or to the minimum negative value of the correlation function should be related to time period of this phenomena[33] [34].
All the above results have been obtained in steady state when a constant electric field is applied to the whole semi-conductor. Nevertheless, it seems interesting to study the behavior of the S.C. materials submitted to a time step configuration of the electric field because such a situation roughly occurs in submicronic devices.

In figure 8 are reported the variations of the mean square displacement of the carriers versus time when a time step of electric field is applied. Two cases are investigated. In the first case (figure 8a) the time step is applied at the beginning of the observation time. In the second case (figure 8b) the time step is applied a long time after the beginning of the sampling time.

In both cases, one can note that, a small time after the application of the electric field, the mean square displacement saturates, and then, slightly decreases. The spreading diffusion coefficient which can still be defined by using equation (3) are ploted versus time in figure 8.

The following remarks can be pointed out :

. the transient diffusion coefficient presents negative values during a small time
. a very long time (more than 1pS) is needed for the steady value of the diffusion coefficient to be obtained.

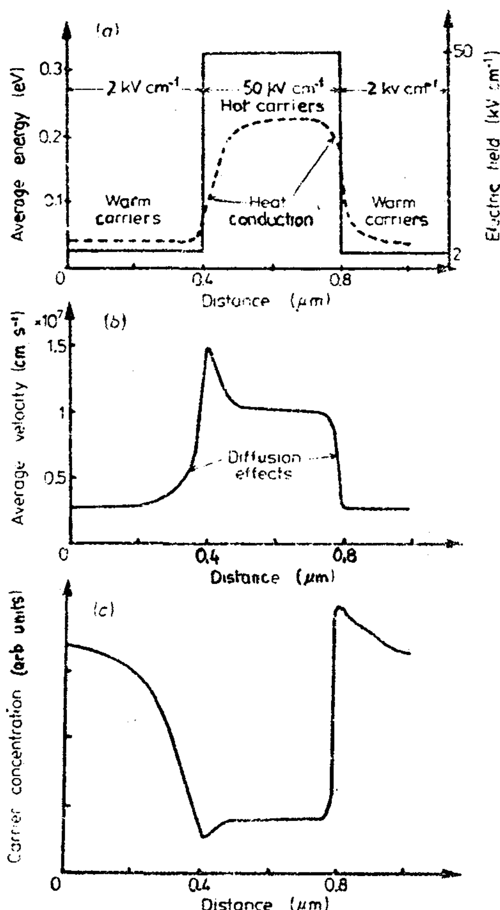
Consequently, it seems to be necessary to take account of such transient phenomena in most of the submicronic devices.

II.3. Phenomena observed when the electric field applied to the semiconductor is characterised by short spatial scales.- Because sub-micron devices are always characterised by short spatial scales of the electric field, this case is particularly interesting. Some of the characteristics of carrier transport in this case can be deduced from the results obtained when a time pulse configuration of $\vec{E}$ is applied to a uniform semiconductor by using the following relation :

$$d\vec{r} = \langle\vec{v}\rangle \, dr \qquad (5)$$

However, it is very important to note that additional phenomena caused by the spatial non-uniformity of the free-carrier concentration, of the energy and of the distribution function occur simultaneously. The most important are (16) :

(i) a diffusion current due to the non-uniformity of n
(ii) heat conduction due to the non-uniformity of ε
(iii) a thermoelectronic current due to the non-uniformity of v^2.



Note that these additional effects are not taken into account in the modelling of a device if equation (5) is used to obtain the spatial characteristics of carrier transport. Figure 9 shows an example of results obtained by MC methods when a space pulse configuration of the electric field is applied to the semiconductor (11). Compared with the phenomena which occur when a time pulse of the electric field is applied, two additional features are also observed. Due to the spatial non-uniformity of the carrier concentration (in figure 9c), diffusion currents cannot be neglected and are "automatically" taken into account in the calculation (using MC procedures) of the average carrier velocity (figure 9b). In addition, the spatial non-uniformity of the average energy (represented in figure 9a) gives rise to heat conduction phenomena since the increase in the average energy of the carrier is

Fig. 9 : Variations of the average energy, drift velocity and free-carrier concentration with distance when a strong spatial variation of the electric field is assumed in a semiconductor. (n-Si, T = 293 K, E (111)). Calculations were carried out using MC methods.

observed in front of the space step of the electric field. It can also be noted that overshoot velocity phenomena are still observed because the maximum value of the drift velocity given in figure (b) is much higher than the steady state saturated value.

Let us now study other unusual features of carrier transport in sub-micron FET devices. The active region thickness is often comparable to a few Debye lengths, and the transition region between the fully depleted layer and the quasi-neutral region cannot be neglected. Consequently we have to determine the characteristics of electron dynamics in this transition region where carriers are not only submitted to a driving field E_X along the axis of the conducting channel, but also to a transverse one (a value often comparable to E_X). This is particularly the case in nearly pinched off GaAs FET operations and, as an example, the characteristics of the carrier dynamic in an incremental section of a symmetrical FET will be shown for gate voltages close to the pinch-off value. Such a study can be easily achieved using MC procedures (17) ; typical results obtained by this method are given in figure 11, in which are plotted along the O_y axis (perpendicular to the gate), variations in the transverse electric field E_y, the free-carrier concentration, the average energy and the average longitudinal drift velocity (v_X). It can be noted from figure(10 b) that most of the carriers are submitted not only to a longitudinal electric field (in this case E_X = 30kVcm^{-1}), but also to a non-negligible transverse electric field. It is therefore necessary to take into account as exactly as possible the influence of this transverse electric field on the carrier dynamics in the active regions of the FET. In classical models, it is assumed that both the drift velocity and the average energy depend on the magnitude of the local electric field E_T acting on the carrier, in addition the drift velocity is assumed to be isotropic (i.e. always to have the same direction as the local electric field). With these assumptions the longitudinal drift velocity along the channel is then given by

$$v_X = v_{Bulk}(E_T)\ E_X/E_T \qquad (6)$$

It is interesting to compare the values obtained using this classical equation with those obtained more exactly by MC procedures. This is achieved in figure(10 b and c) for the drift velocity, and also for the average energy of the carriers. It can be seen that in both cases classical methods using relation (6) give results which are quite different from those obtained by MC procedures, and consequently their application to the theoretical treatment of FET is inadequate and gives unreliable results.

III. Méthods of modelling sub-micron devices.- III.1. Improvement of classical methods : the relaxation time approximation : basic features.- Let us first consider whether suitable improvements can be made to the classical methods of modelling large devices in order for them to become useable for sub-micron devices. The basic equations usually employed to calculate the properties of large unipolar devices are as follows :

continuity equation : $G_n + U_n + \partial n/\partial t = \mathrm{div}\ \vec{J}$

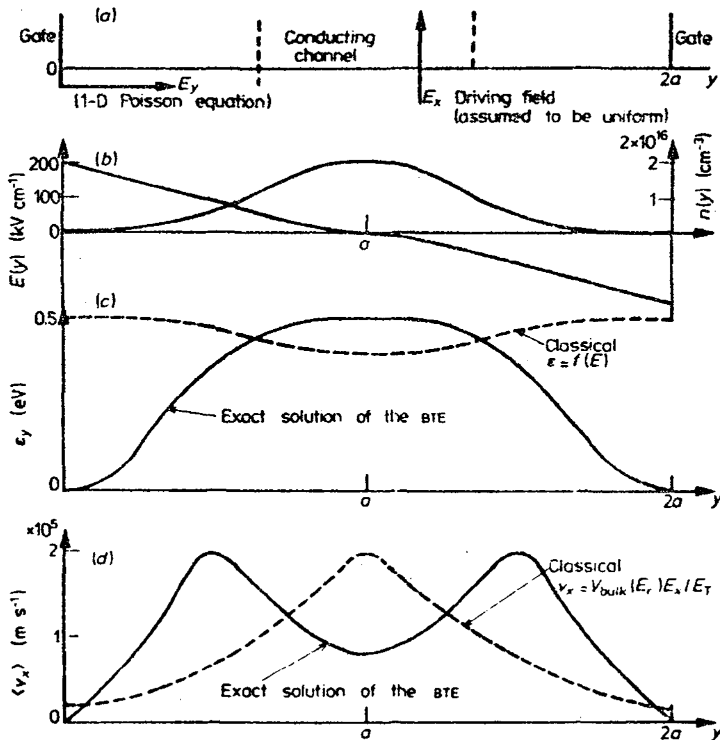


Fig. 10: (a) Representation of a section of a symmetrical FET, (b) Variation of the transverse electric field E_y and the free-carrier concentration along the Oy axis. (c) Variation of the average energy along O_y ; full curve, calculated using MC procedures ; broken curve, using classical bulk data. (d) Variation of the longitudinal average drift velocity $< v_x >$ along O_y ; full curve, calculated using MC procedures ; broken curve, using relation (3). MC simulation is achieved assuming a uniform driving field E_x, while E_y is obtained by integration Poisson's equation along O_y(E_x = 30 kVcm^{-1}, a = 0.13 µm impurity concentration of the active layer $N_D = 10^{17}$ cm^{-3}, and $|V_G + V_B|/W_{oo}$ = 0.93).

current equation : $J = qnv_n(E) + qD_n(E)\ \mathrm{grad}\ n$

Poisson's equation : $\mathrm{div}\ E = q/\varepsilon\ (n - N_D)$

thermal noise equation : $< \Delta i^2 > = 4\ qn\ D_n(E)\ dx$

It can be noted that the least accurate, and also the main assumptions employed in these equations are that the average drift velocity v_n and the diffusion coefficient D are instantaneous functions of the local electric field. However, a considerable improvement could be achieved by using the relaxation time approximation in order to obtain the average energy ε of the carrier from which the drift velocity v_n and the diffusion coefficient D_n can be deduced. These approximations are based in the simplest case of a time dependent uniform field on the following equations:

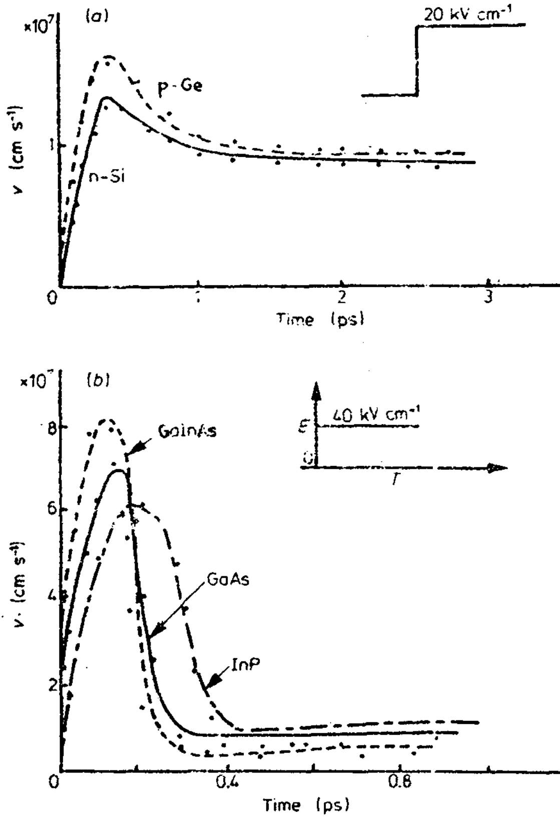


Fig. 11 : Transient drift velocity against time when a time step of the electric field is applied to a semiconductor. (a) p-Ge and n-Si Curves correspond to the relaxation time description, and dots to MC calculations (n-Si), or results obtained from iterative methods (p-Ge). (b) n-GaInAs, n-GaAs and n-InP. Curves correspond to the relaxation time description, and dots to MC calculations.

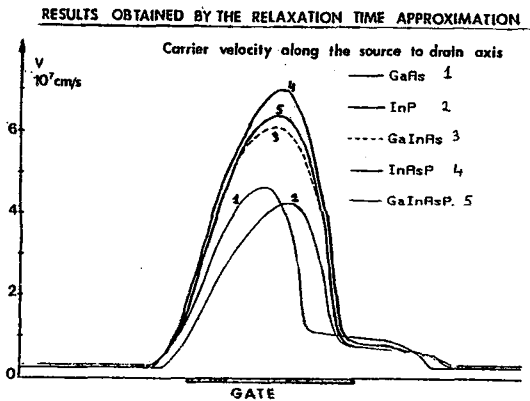


Fig. 12 : Example of results obtained with a FET model based on the relaxation time approximation: velocity of the carriers along source to drain axis for 0.25 μ gate FET realized various semi-conductor material only the alloy composition lattice matched on InP are considered.

$$\frac{d(m^*(\bar{\varepsilon})v_n)}{dt} = qE - \frac{m^*(\bar{\varepsilon})v_n}{\tau_m(\bar{\varepsilon})}$$

$$\frac{d\varepsilon}{dt} = qEv_n - \frac{\bar{\varepsilon} - \bar{\varepsilon}_o}{\tau_\varepsilon(\bar{\varepsilon})} \qquad (6)$$

These relations can be roughly justified taking into account the conservation of momentum and energy, but can also be deduced more rigorously from the BTE under certain conditions, as discussed by Nougier et al (18). In these two relations, scattering mechanisms are taken into account by introducing momentum and energy relaxation times which depend on the energy of the carrier. Consequently, in relations (6) the three quantities τ_m, τ_ε and m^* will depend on the average energy of the carrier, and the main problem to be solved when we want to use them is to obtain the corresponding dependence against $\langle\varepsilon\rangle$ This can be achieved practically by using the static characteristics $v_S(E_S)$, $\varepsilon_S(E_S)$ and $m^*(E_S)$ (obtained for example by MC methods in steady state conditions), since in this case very simple relations between drift velocity, average energy, momentum and energy relaxation times are obtained. Such methods have already been employed successfully by Shur (12), Carnez et al (19) and Cappy et al (14), and it can be noted that good agreement with a more exact calculation is generally observed.

This is clearly shown in figure 11, where a comparison between the relaxation time description and the transient response obtained by MC or by iterative methods has been carried out. It can be seen that for the five semiconductor materials studied, results obtained on the drift velocity by the relaxation time method agree very well with the more exact calculation. Consequently, the relaxation time approximation appears to be very useful for the modelling of sub-micron devices, and this method is now often employed (19) (20) (21) (32).

Compared with classical modelling, the basic feature of a model using the relaxation time approximation is the use of additional equations to obtain the average energy of the carriers in each part of the semiconductor material, from which the drift velocity and a few other quantities (for example diffusivity (22) or ionization rate (23) can be deduced.

An example of results obtained with a FET model based on the relaxation time approximation is given in figure 12.

III.2. New methods of modelling sub-micron devices : the particle model.- Monte Carlo particle models appear to be the most promising methods for modelling, and will therefore be described. In such a model, the motion of particles representative of the carriers in the device is studied simultaneously in k- and r-space using (i) an MC simulation of the scattering process in three-dimensional k-space, (ii) a space (one-, two-, or three dimensional description of the electric field of the device (obtained from Poisson's equation).

An MC simulation is first used to obtain the drift velocity of all the simulated carriers from which the instantaneous positions of carriers in the device are deduced. The carrier density can then be obtained and used to solve Poisson's equation and to determine the electric field required at each point of the device to carry out further MC simulations. Two main methods can be employed to determine the carrier density when the positions of the particles have been obtained. In the single-carrier method, the motion of only one particle is studied and the carrier density is determined progressively from the time Δt spent by the particle in an elementary volume Δr of the device

$$n(r) = \frac{K\,\Delta t}{T\Delta^3 r} \qquad (7)$$

where T is the observation time during which the motion has been studied, and K is a normalisation constant determined from the total number of carriers in the device. Such a method does not allow one to obtain the time dependence of n because, by using relation (7), the integration of n over time is carried out automatically. This method can therefore only be used to obtain stationary values of the various parameters of the device. In the multi-carrier method, the carrier density is determined from the number of simulated carriers observed at an instant t in an elementary volume $\Delta^3 r$. The time dependence of the carrier density can be obtained, and the high-frequency behaviour of the device can then be studied.

The first application of MC methods was to FETS (26), and further work has been done at Reading University on the modelling of FETS (27) (28) as well as Gunn devices (28) by the multi-carrier method. An example of results recently obtained (28) is given in figure 13. The device studied is a new type of transistor (space charge injection transistor) where no impurety concentration is used in the active part of the device .

In view of the importance of this new method of modelling, it is interesting to highlight the main features of MC methods in relation to other more classical methods. Its main advantages appear to be :

(1) The continuity and current equations (including the diffusivity effect) are automatically taken into account when carrying out the simulation process. Consequently the computer has to solve only one differential equation (Poisson's) and this remains true even if complex devices (such as bipolars) are studied.

(2) All the characteristics of carrier transport (for example, non-stationary features) which occur in sub-micron devices are taken into account exactly. The only condition is that the BTE and the band structure approximation must be valid.

(3) Surface and interface scattering can be taken into account without major complications (29)

(4) Additional phenomena (such as IMPATT ionisation, electron-electron interactions) can be described, and preliminary results have already been obtained (11) (30).

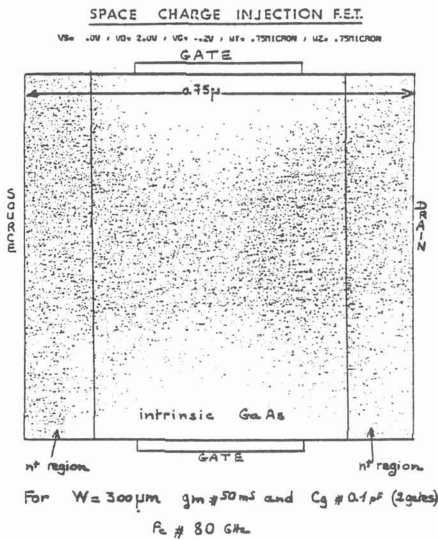
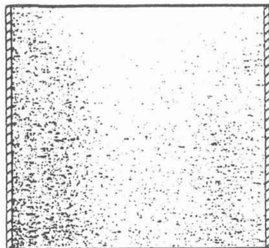


Fig. 13 : Modeling by MC methods
Location of the electrons in a space charge injection FET
Drain voltage = 1 V, gate source voltage = + 0,2 volt.
Gain bandwith close to 80 GHz can be achieved.

Without laser excitation

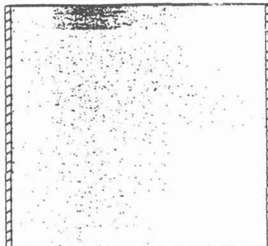


Location of electrons

Fig. 14 : Example of results obtained with a 2D. bipolar Monte Carlo simulation concerning optical detection in submicronic n^+in^+ device (surface states are taken into account V_S = 0.5 volt).

Location of electron

Location of holes



With laser excitation

(5) The MC method can be used to determine all the device properties, including noise (31).

(6) Bipolar devices can be studied without greatly increasing the computation time. The motion of a large number of particle is then studied simultaneously in k space of both the valence band (hole) and the conduction band (electron) taking into account the specific scattering mechanisms in each band. The location of all the particles can be deduced and Poisson's equation may then be solved taking into account the density of both types of particles. An example of the results obtained is given figure 14 (28).

On the other hand, a few serious problems are generally encountered using MC particle methods ; the main ones are as follows.

(1) The method requires very long computation times and consequently needs a very powerful computer.

(2) The numerical results obtained by this method cannot be very accurate due to the stochastic motion of the simulated carriers and to the resulting random fluctuation of the calculated parameters (the physical meaning of these fluctuations resulting from thermal noise can be pointed out). Concerning this point, it should be noted that the accuracy achieved is inversely proportional to the square root of the number of simulated carriers and/or the observation time ; very expensive calculations are therefore needed if highly accurate results are to be obtained.

(3) Taking into account that the computation time is roughly proportional to the observation time, the study of phenomena over a very long period will be particularly expensive and so some physical phenomena such as trapping or generation and recombination effects are very difficult to investigate.

The first two problems appear to be the most difficult features of MC particle methods, but it should be noted that by using single-carrier methods some improvement can be achieved. Since only one carrier has to be studied, computer time and memory occupation can be reduced. In addition, due to the time-integration of all quantities, thermal noise and random fluctuations of the calculated parameters are greatly reduced. Unfortunately only the stationary state can then be studied, and effects such as those due to microwave or optical fields cannot be investigated.

IV. Conclusion.- This paper has been devoted mainly to the study of non steady state carrier transport which occur in sub-micron devices. In this type of device, carrier transport can in most cases be studied using the Boltzmann transport equation. However, new features, such as overshoot and undershoot phenomena, ballistic transport, transient diffusivity and wider distribution of the carrier energy in a depletion layer then characterise the carrier dynamics.

The relaxation time approximation appears to be a successful method for taking into account (at least partly) these new features and for setting up simple models which could be used in industrial laboratories. So far, however, only Monte Carlo particle models make it possible to obtain "exact" results taking into account all

the features of carrier dynamics in medium-small devices. This procedure is therefore the most promising for modelling sub-micron devices, and could be used in the future to study all the properties of practically all types of device. Obviously at present such a method needs very long computation times, although it should be noted (i) that this disadvantage will gradually be diminished as faster computers are realised ; and (ii) that at the present time, simplified particle models such as single carrier method or diffusive model (32) are useful in solving many problems.

Finally, it should be pointed out that the characteristics of the carrier dynamic which occurs in very small devices (active region smaller than 0.1 μ) has not been studied in this paper because suitable theoretical work on carrier transport in this type of device is only just beginning. Many interesting new features (such as synergetic effects and quantum transport) will occur in very small devices, and their study will require a great deal of interdisciplinary work. This appears to be an interesting goal for the future.

Acknowledgments

The authors wish to thank Prof. Nougier, Castagne, Salmer, Dr. R. Fauquembergue, J.L. Vaterkosky, M. Pernisek, A. Cappy, P. Rolland, M. Deblock, A. Kaszynski, who have realized some part of the works presented in this paper. This work has partly been supported by the DRET and D.G.R.S.T.

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