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High Field Transport and Advanced Modeling Techniques for Submicron Devices

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It is the purpose of this paper to study in a first part what kind of new transport phenomena may occur in sub-micron devices, to suggest and to describe in a second part new methods of modelling which take them into account.

I. INTRODUCTION

Progress in the microelectronics industry is strongly coupled with the ability 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 10-20 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. Moreover, 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 submicron devices. It is the purpose of this paper to study in a first part what kind of new phenomena may occur in submicron devices, to suggest and to describe in a second part new methods of modelling which take them into account.

II. WHAT NEW PHENOMENA OCCUR AND MUST BE TAKEN INTO ACCOUNT IN SUBMICRONIC DEVICES

The following features are gènerally observed for submicronic devices:

. because of systems requirements and also noise considerations, voltage have to be reduced much less than the size is reduced and as a result the electric field increases and hot carriers are achieved.

. because of the increasing influence of parasitic resistances since when we decrease the active region length, the impedance is reduced, high doping concentration and high carrier density are employed

. because of the high doping concentration, the thickness of the active layer is often greatly reduced and increasing influence of surface and interface is observed.

. because of the submicronic length of the active region and because of the possibility for submicronic devices to operate at very high frequencies, the electric field configuration is characterized by short spatial scale and by fast temporal variation.

All these new features give rise to new transport phenomena which have to be described and taken into account in the modelling of submicronic devices.

The most striking new phenomena result from the increasing influence of the surface and interface and from the very short time scale or/and small spatial scale characterizing the electric field.

II.1. Increasing influence of interface

With the advent of new technologies for the fabrication of semi-conductors (molecular beam epitaxy), new structure of devices have been imagined in which in particular, heterointerfaces play a predominent part. A typical example is the HEMT (or TEGFET) in which the conductive channel consist of a quasi two dimensional electron gas trapped due to size quantization in the potential well formed at the interface of a GaAlAs/GaAs heterojunction. Such a device involves to a large extent in a way similar to inversion electrons in the most usual Si MOSFET many special physical features :

- quantization of one degree of freedom (perpendicular to the wall of the well)
- existence of energy subbands in the well
- possible transfers between subbands induced by scattering

Due to these new features, electron transport characteristics can be very different from those observed in bulk materials and this difference are illustrated in Fig. 1 [1].

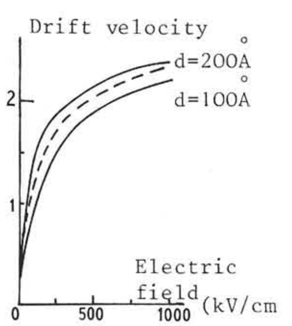

Fig.1. Monte Carlo calculations of drift velocity versus the electric field for 2D and 3D electron gaz in GaAs (T=77°K). Full line: 2D datas for two values of the quantum well width d. Dashed line : 3D datas

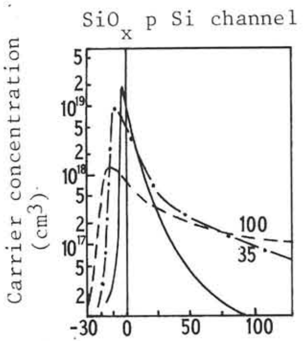

Fig. 2. Monte Carlo calculations of carrier concentration across the interface Si-SiO^2 for three values (3, 35, 100 kV/cm) of the driving field (T = 300°K Q_{ss} = 3.10^{11} cm^{-2})

Consequently this effects should be taken into account in the modelling of HEMT but also of Si MOS particulary for low temperature operation. As a matter of faċt , when the operating temperature raises and the voltage applied increases the electron energy increases and becomes greater than the difference of energy between subbands and as a result, the effect of quantization of carrier transport becomes negligible.

Other effects then become important such as the injection of the carriers through the interface in GaAlAs (HEMT) or in the oxyde (Si MOS). Such effect [2] which are illustrated in Fig. 2 can be drastic in the case of Si MOS since it may determines the adging of the device. Consequently, it must be taken into account in the design and also in the modelling of the component.

II.2. Short spatial and fast time scale characterizing the electric field

In the usual case of large devices, the time and space variation of the electric field during the carrier mean free time and along the carrier mean free path can be neglected : carrier transport can then be considered as in steady state conditions since there is a balance between the determinist effect of the electric field which generally increases the carrier velocity and the stochastic effect of the scattering mechanisms which randomizes the velocity. As a result, all the average values characterizing the dynamics of the carrier such as the average value of ε $\bar{\varepsilon}$ and of the drift velocity $\bar{v}$ depend only on the instantaneous local electric field regardless of the values of the electric field in the past and around the point being studied in the semi-conductor material. In this case, classical current equations and methods of modelling can be used assuming that all quantities only depend on the electric field.

"Non steady state carrier transport" will be achieved either when very high frequency or fast transient voltages are applied to large devices or when submicronic devices are used (even in steady state regime). In these cases, the variation of the electric field during either a mean free time between two collisions or along a mean free path cannot be neglected and new features will characterize electron transport and must be taken into account in the modelling of the devices.

Most of the phenomena involved are due to the specific characteristics of electron dynamic in usual semi-conductor where in most cases, when the energy increases, the scattering rates and the effective mass also increase. As a result, cold carriers submitted to high electric field will be able to reach very high value of the drift velocity since the electric field effect on the drift velocity is much higher (the effective mass is reduced) and the scattering rates is strongly reduced. But obviously such a phenomenon will only be observed during the short while necessary for the electron energy to increase and reach a steady value. This is the well known overshoot phenomenon which can be observed [3] in the channel of submicronic gate FET (see for example on Fig. 3). On the contrary very hot carriers submitted to low value of the

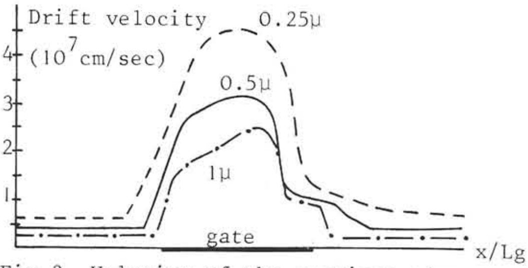

Fig.3. Velocity of the carriers along the source to drain axis of GaAs FET's for three values of the gate length.

electric field will be characterized by low values of the drift velocity since for this type of carriers, the effective mass is very high and the increase of the velocity due to the electric field is very small while the randomization of the velocity due to the scattering mechanisms strongly occurs. This is the undershoot phenomena which can be observed at the output of the channel (Fig3).

Other phenomena such as ballistic motion can also be observed. This type of motion can be achieved by using the internal electric field due to the alloy composition variation in gradual heterojunctions such as GaAlAs-GaAs. In this type of junction very high electric fields occur over a very small distance (smaller than the mean free path) and such fields can be used to strongly accelerate the carriers while scattering events do not occur. When the carriers cross the heterojunction, only the effect of electric field is observed and a result, very high drift velocity can be achieved without an important velocity distribution (Fig 4).

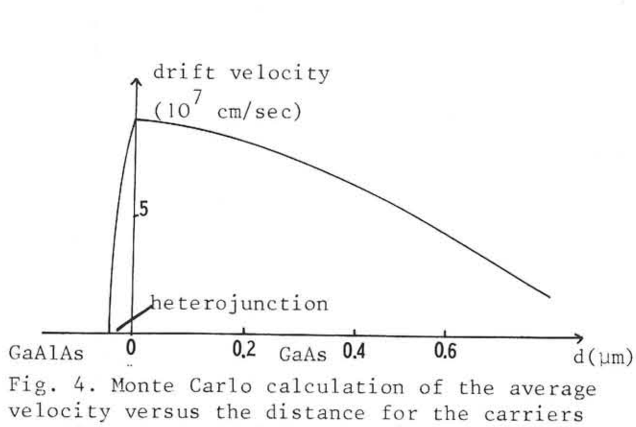

Fig. 4. Monte Carlo calculation of the average velocity versus the distance for the carriers crossing the heterojunction $Ga_{1-x}Al_xAs/GaAs$. The initial carrier energy in GaAlAs is assumed to be the thermal lattice energy
(x = 0.3, T = 77°K)

When the heterojunction has been crossed, the internal electric field vanishes and the initial very high velocity decreases very slowly since scattering mechanism are needed to randomize the drift velocity. The electric field vanishing to zero in GaAs a really ballistic motion of all the carriers is then achieved a little like a ballistic rocket where all the motion is carried out without driving field i.e when the engine stopped and with this type of motion quite long distances can be achieved over very short time [4]. ★

From all the results previously described, it clearly appears that the main characteristics of carrier dynamics in submicronic devices depend not only on the electric field but also on the instantaneous average energy of carriers. Such features cannot be taken into account using classical approximations and electrokinetic equations. The modelling of such devices requires either the elaboration of new methods which will be more suitable for submicron devices, or the improvements of the methods presently used for large device and low frequency operation. In the second part of this paper, we will study these two types of methods.

III. HOW TO MODEL SUBMICRONIC DEVICES

III.1. Monte Carlo particle models : the process and its basic features

Monte Carlo (M.C.) particle models appear to be the most powerfull methods for modelling, and will therefore be described first. 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) M.C. simulation of the scattering process in three-dimensional k-space, and (ii) a space (one, two, or three dimensional) description of the electric field of the device (obtained from Poisson's equation).

The M.C. 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

★ In non steady state transport diffusion phenomena can also be very different from those achieved in steady conditions [5] and obviously these features have also to be taken into account in the modelling of submicronic devices.

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 M.C. simulations.

The main application of M.C. methods were to FET's [6] and an example of results obtained are given in Fig. 5 [7]

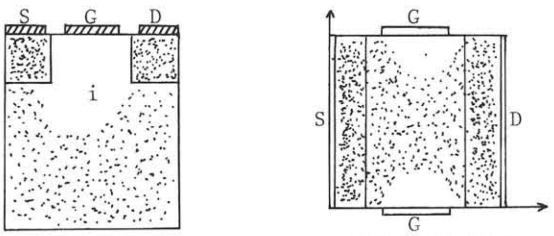

Fig. 5. Monte Carlo simulation of space charge injection FET's, i.e FET's using a non doped active layer. Instantaneous locations of the electrons in the device.

In view of the importance of this 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 Boltzmann transport equation and the band structure approximation must be valid

(3) Surface and interface scattering, effect due to heterostructure and heterojunction (for example 2D transport) can be taken into account without too many complications

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

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

(6) Bipolar devices can be studied without greatly increasing the computation time [8].

On the other hand, a few serious problems are generally encountered using M.C. 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 (i.e. thermal noise) of the calculated parameters. 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.

III.2. Improvement of classical methods : the relaxation time approximation ; basic features

It has been shown that it is very difficult to obtain by M.C. methods very accurate numerical results due to the stochastic motion of the simulated carriers. If when studying static properties of a device, these random fluctuation can be almost cancelled by a suitable time integration this is not the case when time dependent properties of the device have to be studied. In this case more macroscopic and classical methods which dont take into account thermal noise seem more useful. The basic equations usually employed in these methods to calculate the density current in large unipolar devices are as follows

$$\vec{J} = q\, n\, \vec{v}(E) + q\, D_n(E)\, \vec{\nabla} n$$

It can be noted that the least accurate and also the main assumptions in these equations are that the average drift velocity (and also the diffusion coefficient D) are instantaneous functions of the electric field since it can be noted that these two quantities also depend on the instantanous average energy of the carrier. Consequently, suitable equations have to be found in order to obtain the energy of the carriers and then to determine the drift velocity.

Balance equations obtained by integration of the Boltzmann equation over the $\vec{k}$ space taking into account the space variation of all quantities appear to be very usefull. Using suitable assumptions [9], the following equation are obtained

$$\frac{\partial n}{\partial t} + \vec{\nabla}\,\vec{J} = 0 \qquad (1)$$

$$\frac{\partial (n\bar{\varepsilon})}{\partial t} + \vec{\nabla}\,\vec{J}\,\varepsilon = \vec{J}\,\vec{E} - \vec{\nabla}\,(\vec{J}\;k\;T\;(\varepsilon)) - \frac{n(\bar{\varepsilon} - \varepsilon_o)}{\tau_\varepsilon(\bar{\varepsilon})} \qquad (2)$$

$$J = \frac{q\tau_m(\bar{\varepsilon})}{m^*(\bar{\varepsilon})}\; n\;\vec{E} - \vec{\nabla}\;(n\;kT(\bar{\varepsilon})) \qquad (3)$$

where T is the electronic temperature, $\bar{\varepsilon}$ the average instantanous energy and m^* the average effective mass. The momentum and energy relaxation time τ_m and τ_ε are introduced in order to take into account the scattering mechanisms. In these 3 equation, τ_m, τ_ε T, and m^* are assumed to only depend on the average energy of the carriers and one of the main problem to be solved when we want to use equations (1)-(3) is to obtain the dependence of τ_m, τ_ε and m^* against $\bar{\varepsilon}$. This can be achieved practically by using the static characteristics $v_s(E_s)$, $\varepsilon_s(E_s)$ and $m^*(E_s)$ relating stationary average drift velocity, energy and effective mass to the electric field (obtained for example by M.C. methods in steady state conditions and in an uniform semiconductor). In the modelling of any practical device, obviously, these equations have to be solved together with the Poisson's equation.

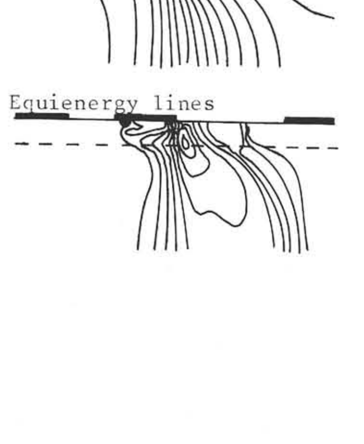

Figure 6

Simulation of FET using equations (1-3). The doping concentration of the active layer is

$N_D = 2.10^{17}$

$V_D = 2$ volts

$V_G = 0$ volt

An example of results which can be obtained are illustrated Fig. 6. Such method allows to obtain with a good accuracy the time properties of submicronic devices. Unfortunately, in C.A.D. applications, the computer time which is needed might still be too long. Consequently very fast simplified models based on one dimensional description of equations (1)-(3) can also sucessfully be used [10].

IV. CONCLUSION

The main new transport phenomena occuring in submicron devices result from the increasing influence of interfaces and from "non steady states" due to the short time and small spacial scale characterizing the electric field configuration. Among the advanced methods of modelling which can be used to take these phenomena into account M.C. methods appear to be very powerfull but unfortunately is not very accurate and requires very long computation time. Consequently suitable methods based on the relaxation time approximation and using the M.C. method for the determination of this relaxation times appear to be the most promising and usefool tools in the design of submicron devices.

REFERENCES

[1] ZIMMERMANN, 14th ESSDERC Conference, Lille 1984
[2] CHU HAO, Phys Stat Sol(a) 81 569 (1984)
[3] CARNEZ, J. Appl. Phys. 51(1) (1980)
[4] GHIS, J. Appl. Phys. 54(1) (1983)
[5] BOITTIAUX, Appl. Phys. Lett 40(5) 407 (1982)
[6] REES, Electron. Lett. 156 (1977)
[7] FAUQUEMBERGUE et all, Electron. Lett Vol 18 n° 15 p 670 (1982)
[8] VATERKOWSKI, Solid State Elect. Vol. 27 n° 2 pp. 207-209 (1984)
[9] EL GHAZALY et all, 13th ESSDERC 1983 CANTERBURY (U.K.)
[10] CAPPY, Revue Phys. Appl. 18 (1983) 719-726

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