

Modeling of MODFET's

GEORGES SALMER, JACQUES ZIMMERMANN, AND RENAUD FAUQUEMBERGUE

Abstract—Accurate modeling of MODFET's and of certain novel structures recently proposed requires that a number of physical phenomena occurring in these devices be considered. Among these, some specific electron dynamic properties of the two-dimensional gas, the influence of deep levels of the doped AlGaAs layers, and the influence of the source parasitic access impedance are reviewed and discussed. The presently available models can roughly be sorted into three classes: the particle or Monte Carlo models, the two-dimensional solving methods of semiconductor equations, and the simpler one-dimensional or analytical models. After a brief review of the physical bases on which the models rely, their main capabilities and ranges of applicability are compared and discussed. Some conclusions are drawn as to the effort which must be developed in the near future in order to improve MODFET modeling. It is recommended that simulations of new devices such as SISFET's, multichannel structures, and pseudomorphic AlGaAs/InGaAs transistors be undertaken.

I. INTRODUCTION

RECENTLY, there has been considerable interest in the development of an AlGaAs/GaAs heterojunction field effect structure commonly called a modulation doped field effect transistor (MODFET), a high electron mobility field effect transistor (HEMT), or a two-dimensional electron gas field effect transistor (TEGFET). This device is very promising for both microwave and high-speed digital circuit applications. For instance, MODFET ring oscillators have demonstrated switching delay times of 10.2 ps at 1.03 mW/stage and 5.8 ps at 1.76 mW/stage at 300 K and 77 K, respectively, using 0.35 μm gate length devices [1]. On the other hand, a 2.4 dB noise figure has been measured at 60 GHz in a 0.25 μm gate MODFET [2]. This has demonstrated MODFET capability to be used at 94 GHz. MODFET's may also constitute very good candidates for power amplification in the millimeter-wave range, as has recently been shown by Saunier *et al.* [3] using multichannel structures. Moreover, a large number of very promising new heterojunction structures have been proposed, allowing a significant improvement of performance to be expected. Among these we should mention:

- the self-aligned accumulation mode GaAs MIS-like FET (SISFET) having an n^+ GaAs/undoped AlGaAs/undoped GaAs structure [4];
- the inverted GaAs/AlGaAs structure which shows a very high transconductance [5];
- a MODFET structure where the n^+ doped AlGaAs is replaced by a n^+ GaAs/AlAs superlattice [6], so as to

improve low-temperature behavior and reduce DX center formation;

- the multichannel structure [3], in which the total current and power capabilities may be strongly enhanced;
- the n^+ AlInAs/GaInAs MODFET, using lattice-matched compositions with which one profits from better carrier dynamic properties in GaInAs [7];
- the pseudomorphic GaAlAs/GaInAs MODFET, which takes advantage of both the interesting properties of GaInAs and the better channel confinement in this particular structure [8].

In order to optimize the operation of both classical MODFET's and of new structures, we must obtain an accurate understanding of their physical behavior and have a deep knowledge of the various physical phenomena occurring in these devices. In this connection, accurate simulation methods are clearly needed. In addition, models are necessary in order to substitute inexpensive, fast, and accurate simulations prior to fabrication for very expensive systematical technological studies.

In practice, however, we need several kinds of models. On the one hand, the most sophisticated and complete ones, such as Monte Carlo simulations, are used for basic studies in order to obtain a better understanding of device behavior as well as to check the validity of more elementary models. On the other hand, for the CAD of monolithic digital or microwave integrated circuits, very simple and quick models must be worked out, even though their range of validity may be limited because, for instance, adjustable fitting parameters must be assumed. Between these two extreme cases, a large number of models are used for specific applications, for example, ac or transient responses.

The earliest HEMT models ever presented were one-dimensional and analytical [9], [10], but they took into account the quantized character of the two-dimensional electron gas (2 DEG). These models used a relationship between the areal electron density n_s in the channel and the gate voltage. The external current–voltage characteristics are then computed by direct self-consistent integration of the current from source to drain. However, these models currently include a number of simplifying assumptions. These mainly concern the specific electron dynamics of the 2 DEG, hot electron effects, real space transfer or injection in the GaAlAs layer, and certain others of lesser importance. As a consequence, a large number of more sophisticated and realistic models have been conceived.

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The authors are with the Centre Hyperfréquences et Semiconducteurs, U.A. CNRS no. 287, Université des Sciences et Techniques de Lille-Flandres-Artois, 59655 Villeneuve d'Ascq Cedex, France.

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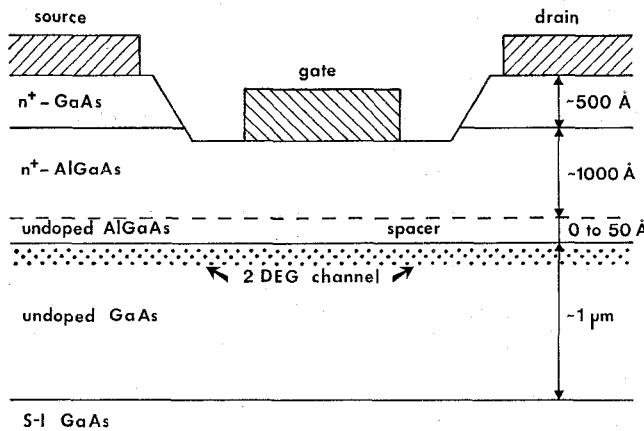


Fig. 1. The basic structure of the HEMT (or MODFET).

The purpose of the present paper is chiefly to introduce these various models. In Section II we present some physical phenomena or specific aspects which are not often taken into account and may be of particular importance, especially with certain devices (submicron gate devices, for instance). Among these, we can cite some two-dimensional aspects of electron dynamics, the influence of DX centers in doped AlGaAs layers, and the specific behavior of the source and drain access zones. In Section III we will try to give some additional information on various simulations as performed today, trying to precisely classify them and their respective advantages and domains of applicability. Finally, in Section IV various problems arising from simulations of various new structures as mentioned above will be outlined.

II. SOME PHYSICAL FEATURES PERTAINING TO HETEROJUNCTION STRUCTURES

A. Two-Dimensional Electron Gas Transport Properties

What characterizes transport in a structure including one or more heterojunctions is the possibility of quantum effects in the conduction and/or valence bands coming into play. In a simple HEMT structure with one heterojunction (see Fig. 1), the wide band gap doped material can transfer electrons to the narrow band gap undoped material where the energy levels are lower. Because of the space-charge reaction, electrons tend to accumulate near the GaAs side of the heterojunction. The concentration there is then easily controlled by the gate voltage. One advantage of heterojunctions is the possibility of using doped modulation (doping of the large band gap material only). Using a so-called spacer layer (see Fig. 1), one separates the carriers from their parent impurities and thus decreases the effect of ion Coulomb scattering. If the carrier concentration is sufficiently high, the bands may be strongly bent toward and even below the Fermi level. The width of the potential well formed in this way can be narrow enough for quantum effects to occur. The condition for this to happen is that the width of the well at energies near the Fermi level be of the order of magnitude or even smaller than the thermal wavelength of the car-

riers, that is,

$$\lambda_{th} = \frac{\hbar}{\sqrt{m^* k_B T}} < \text{well width.} \quad (1)$$

For instance, at 300 K in n-GaAs, one finds $\lambda_{th} \sim 400 \text{ \AA}$. In general, though, quantum effects manifest themselves only along the direction perpendicular to the plane of the heterojunctions, hereafter referred to as the z direction. Accordingly, one degree of freedom is bound to the quantum well, and one can write for a band

$$E_n(\vec{k}_{//}) = E_{nz} + E_{//} = E_{nz} + \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) \quad (2)$$

where n is an integer depicting which eigenenergy level a carrier with wave vector $\vec{k}_{//}$ is occupying. The E_{nz} in (2) comes from the analysis of discrete energy levels via the Schrödinger equation over the entire electron population. In writing (2), one assumes that the carrier is free along the x and y directions. In (1) and (2), m^* is an effective mass which, in general, in device simulations is taken as the bulk free carrier effective mass in the same material. Whether or not this assumption is legitimate is still a matter of controversy [11], [12]. At any rate, this has the advantage of simplicity when one computes the eigenenergies E_{nz} with the Schrödinger equation. Along with relation (2), the state of a carrier is given the form

$$\psi(x, y, z) = \phi_n(z) \exp[i(k_x x + k_y y)] \quad (3)$$

where the envelope wave function $\phi_n(z)$ is also determined by the Schrödinger equation and represents the localized part of the electron state from which the carrier density in the well can be evaluated. This is illustrated in Fig. 2.

Since the electronic structure of the system is changed due to this partial quantization, the two-dimensional free charge transport properties ought to be different from bulk free charge transport. In the past few years, quite a number of papers treating this subject have been published. As far as electron dynamics in III-V heterojunctions resembles that of MOS inversion layers, the review paper by Ando *et al.* [13] is useful.

1) *Drain Voltage Influence*: In a device, though, the situation may be more complicated due, for instance, to the superposition of the drain voltage with the gate voltage. The way in which the subbands are placed and populated depends on the effective temperature of the carriers, which can be higher than the lattice temperature due to hot carrier effects. One can then easily think that the electron structure changes continuously from the source to the drain. Intuitively, one can expect that the well widens from the source to the drain. Moreover, as long as the gate length is much longer than the electron thermal wavelength, the states along the source-drain axis can be safely considered as itinerant in accordance with (3). Now since the detailed transport properties are dependent on the subband structure in the quantum well all along the channel, and the subband structure also changes all along the channel, the detailed transport properties (mobility, and so on) ought to be different from place to place.

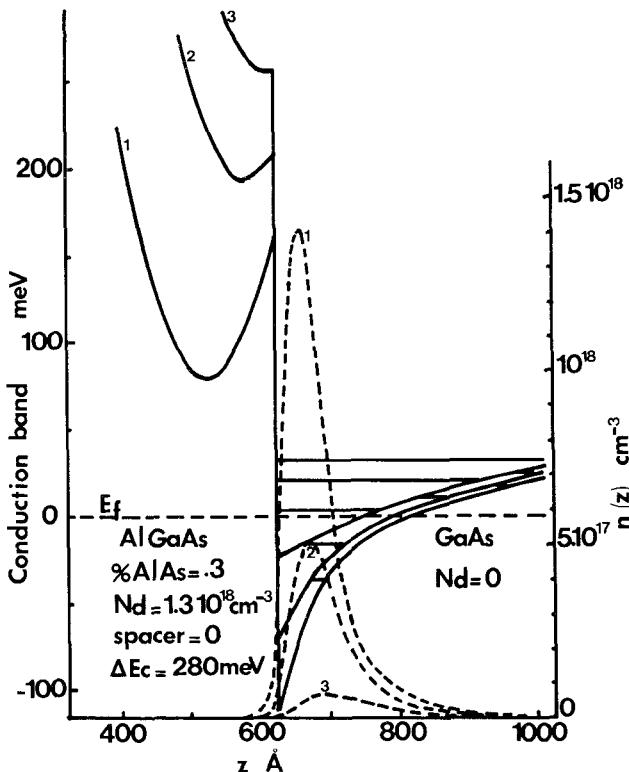


Fig. 2. Potential energy (full lines) and electron density (dashed lines) along the quantized direction z for three different bias voltages. $V_g = -1.6$ V (1); -2.3 V (2); -2.7 V (3). $T = 77$ K; the Schottky barrier height is 1 V.

2) *Collisions*: Now, because of the particular nature of the electron states, which are generally assumed to be quasi-continuous in two dimensions and discrete in one dimension, study of transport is rendered more complex than in the bulk material. Moreover since the carriers move near an interface, the nature of crystal potential there can be different from that of the bulk. Considering the lack of information on this latter point, one is obliged to assume (in the absence of a better approach) that the collisional aspects of carrier transport are similar to those of the bulk material. In particular, the matrix elements entering the scattering rates between two states, as given by the Fermi golden rule, use a three-dimensional potential, but the carrier is represented by (3) instead of a simple plane wave function. With this a S^{mn} ($\vec{k}_{\parallel}, \vec{k}'_{\parallel}$) can be defined which is the probability density (per unit time) that a carrier having the itinerant state \vec{k}_{\parallel} in subband m will transfer by a collision to another itinerant state \vec{k}'_{\parallel} in subband n [14], [15]. In general the S^{mn} have an explicit dependence on the indices m and n ; moreover one can see that a given type of collision will give rise to N^2 different S^{mn} if N subbands are included in the structure model. This of course renders the simulation more difficult to handle. Moreover the microscopic dynamic parameters are determined not only by the kind of material but also by the structure of the quantum well itself (which varies *along* the channel).

3) *Low-Field Conditions*: As far as low field mobility is concerned, one can find a great many calculations and

comparisons with experiments in the literature, especially concerning its variation with temperature and sheet carrier density n_s , [16]–[28]. Comparisons show that degenerate statistics must be included in the calculations (viz. Fermi–Dirac distribution), especially at low temperatures and/or high n_s . This may not be a difficulty at low fields, but in device simulations, the field is generally high (hot carrier phenomena) and the problem of how to deal with degeneracy in this case becomes much more difficult but more interesting, as we will see later. Secondly, it is recognized that in low temperature deformation acoustic and piezoelectric scattering, together with impurity scattering, plays the major role in limiting the mobility. Although the relative importance of acoustic phonon scattering is still controversial [29], [30], impurity scattering has received careful attention [31]. Also important in the calculations is the role of screening, which has to be considered in the potential well due to the very high carrier concentration. This may have an effect not only on carrier ion potential but also on crystal potentials. Finally, in the same spirit, collective effects may give rise to enhanced electron–electron (and electron–plasmon) interactions, of which we will say a few words.

4) *High-Field Transport*: If one considers now high-field transport in a heterojunction (in a HEMT, for instance) operated at high drain voltage, the conditions are quite different from what they are at low field. The main questions which are to be answered now are how high-field saturation velocity is approached and what is its value and how confinement in a quantum well still plays a role when high energy states can be populated. A number of theoretical simulations (using Monte Carlo methods) [32]–[34] and some recent experiments [35] have shown that i) the saturation velocity of electrons in AlGaAs/GaAs heterojunctions is not much different from bulk GaAs saturation velocity (at least between 77 and 300 K) and ii) the velocity field curve exhibits in general a negative differential mobility above a threshold field, both of which depend on the heterojunction composition. The comparison between theory and experiment is more qualitative than quantitative. Real space transfer where the electrons are able to surmount the barrier ΔE_c (quantum tunneling and thermal injection assisted by the surface field), as well as intervalley transfer in momentum space, leads to threshold fields which can be substantially lower than that of the bulk. It is quite clear that other experiments on velocity versus field like those in [35] are strongly necessary. There is no doubt that this approach is much more physical than that outlined here in Section III-C.

5) *Electron Transfer*: The possibility that electrons transfer from the partially quantized electron states to other states in three dimensions, and vice versa, raises a theoretical problem which is not easy to solve. However, inasmuch as the electron states are sufficiently well known on each side of the structure, it should be possible to handle the problem starting from the Fermi golden rule [36], together with the usual requirements on energy and momentum conservation principles, as far as the collisions

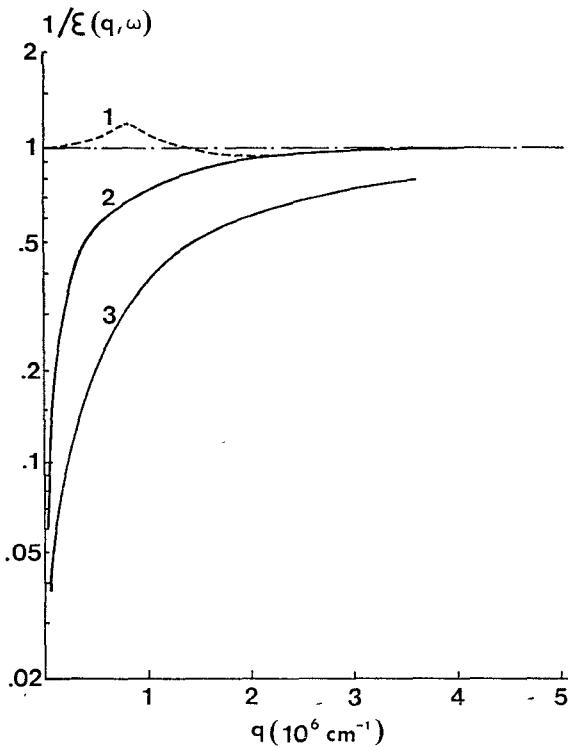


Fig. 3. Screening factor of two-dimensional matrix elements of scattering potentials. 1: $\hbar\omega_0 = 0.0354$ eV (polar optical phonon frequency $\omega_0 = 8544$ GHz) and $T = 300$ K. 2. $\hbar\omega_0 = 0$ (nearly elastic deformation and piezoelectric phonon frequency $\omega_0 \sim 0$) and $T = 300$ K. 3: same as 2, but $T = 10$ K. Case of a square-well potential with width 100 Å and $n_s = 10^{11} \text{ cm}^{-2}$.

can be considered instantaneous in space and time. As mentioned earlier, real-space transfer may also constitute a way of connection between 2-D states and 3-D states, especially in the region where the electrons are hot and their energy is near or higher than the barrier height ΔE_c . Simulations show that this occurs generally on the drain side of the gate in a HEMT [37].

6) *Screening*: Screening in two-dimensional systems has been studied by Price [38] based on the usual approach of random phase approximation and Linhard formula, with which the electron dielectric function can be evaluated as a function of wave vector and frequency (linear response regime in general). The screened matrix elements of the various scattering potentials can then be calculated as $M = M_0/\epsilon(q, \omega)$, where M_0 are the same unscreened matrix elements. Note, however, that the q dependence of $\epsilon(q, \omega)$ in two dimensions is, in general, different from what it is in three dimensions [39].

By way of illustration, we show the dielectric function in Fig. 3 for an electron system trapped in a square potential well at $\omega = 0$ (for quasi-elastic collisions) and at $\omega_0 = 0.0354$ eV/ \hbar (which corresponds to the bulk GaAs polar optical phonon frequency) as a function of q (we recall that q is a phonon wave vector modulus). As expected, dynamical screening is strongly damped at high frequency and the dielectric function is almost flat around 1. Note that below 10^6 cm^{-1} , there exists a slight antiscreening, where $1/\epsilon(q, \omega_0) > 1$, which may lead to an enhancement

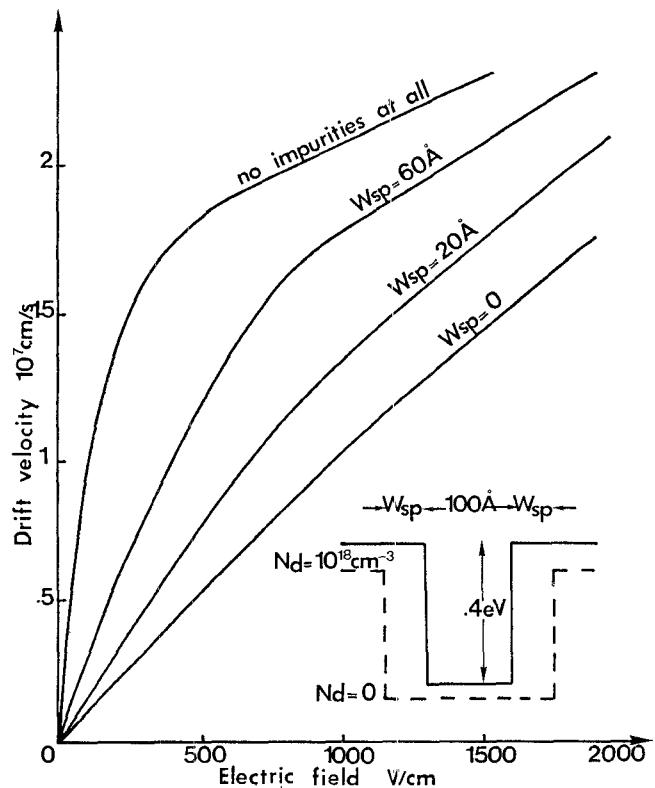


Fig. 4. Drift velocity of the 2DEG as a function of the electric field and spacer width. $T = 77$ K and $n_s = 10^{11} \text{ cm}^{-2}$. Two subbands are taken into account in the square potential well (all electrons are in the Γ valley of GaAs).

of the scattering probability. Otherwise, screening is very weak. On the contrary, the dielectric function evaluated at $\omega = 0$, the case which concerns elastic collisions, varies strongly over the entire q range. In this case screening must be taken into account, especially where it affects small angle scatterings or small q . As far as nearly elastic scattering dominates mobility at low temperature, screening must be taken into account [40]. At ambient temperature, however, mobility is dominated by polar optical phonon scattering, on which screening effect is weak, and by impurity scattering, on which it may be strong. Thus, screening should be taken into account also at high temperature [41].

7) *Impurity Scattering*: Doping modulation is used to separate the 2 DEG from their parent donors so that the influence of the Coulomb interaction potential on mobile carriers is minimized. However, a significant concentration of electrons in the conductive channel of the HEMT is needed to form a 2 DEG. This requires a high concentration of donors in the AlGaAs layer and a spacer which is not too wide so that substantial transfer of electrons to GaAs is maintained. The balance which must be found between these two conflicting effects makes impurity scattering and its effect on mobility one of the key points of device modeling.

The way in which the problem is formally treated can be found in the early work of Stern on MOS inversion layers [13] and in [31] for III-V heterostructures. By way of illustration, we show in Fig. 4 the variation of the drift

velocity (as a function of the longitudinal field applied parallel to the heterojunctions) of a 2 DEG trapped in a square potential well for various widths of the spacer layer. One can see that the absence of a spacer can cut down the mobility by a factor of 10. This shows the importance of this effect, which below 77 K dominates transport. At ambient temperature in the same structure, the factor is still about 2, which shows that this kind of interaction should be correctly treated in simulation.

Two other effects which we have mentioned above, namely collective effects and degeneracy, are not easy to incorporate in a transport theory. But an efficient way to study them, especially when hot carrier regimes are involved, is by use of Monte Carlo simulations.

8) *Collective Effects*: Collective effects incorporate electron-electron interactions and electron-plasmon interactions. This has already been implemented in the Monte Carlo simulation in three dimensions [42]–[44]. By nature, an ensemble of particles to be simulated simultaneously is required. Each kind of interaction is characterized by a collision probability where the distribution of the entire population is involved. The effect of the electron-electron interaction will be to randomize the energy and the momentum of the carriers among themselves.

It is not easy to tell at which electron concentration this interaction begins to come into play. If it is assumed, for instance, that this limit concentration is the one at which the screening distance of the mutual Coulomb potential is comparable to the electron mean free path due to all the other interactions, one arrives at a value of a few 10^{16} cm^{-3} for GaAs at room temperature. Thus at densities higher than $5 \times 10^{17} \text{ cm}^{-3}$, where this interaction should be really effective, degeneracy effects might equally well come into play since for GaAs at 300 K, N_c is in the range $\sim 5 \times 10^{17} \text{ cm}^{-3}$.

For instance, Ferry [43] has shown that electron-electron interaction may lead to a substantial reduction of ballistic effects. This point may affect the expected performances of devices using non-steady-state transport properties, such as submicron FET's. Recently electron-electron interaction has been implemented in a 2 DEG Monte Carlo simulation of heterojunction structures by Al-Mudares *et al.* [45].

9) *Degeneracy*: The effect of degeneracy on electron transport has been recently studied in detail by Ferry *et al.* [46]. The usual Monte Carlo method assumes that the state reached by a carrier after completing a collision is always available. This may be true for nondegenerate systems where the occupation density $f(k)$ of a state k is always very weak. When one is to simulate degeneracy effects, one has to introduce the Pauli exclusion principle, for which $f(k) \neq 0$. This in principle requires $f(k)$ to be known, thus introducing a new kind of iteration in the Monte Carlo process since the occupation density is built up by the process itself. Of course, $f(k)$ is not known *a priori*. With an ensemble Monte Carlo technique of the type suggested in [46] and using an idea formerly proposed by Jacoboni [47], the problem is rendered more tractable. A

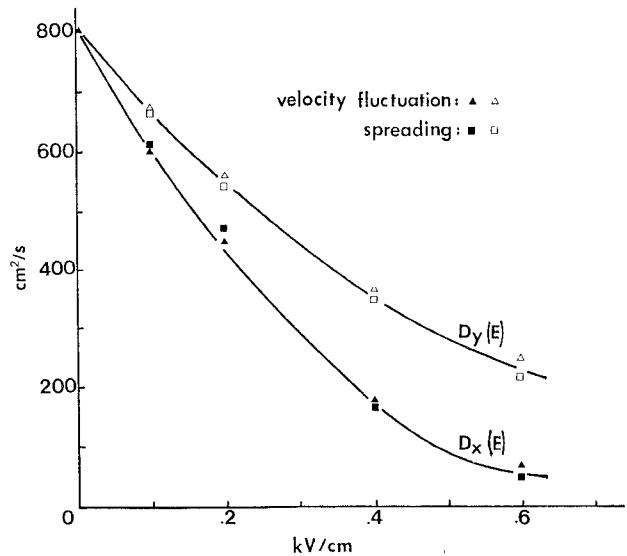


Fig. 5. Parallel (D_x) and transverse (D_y). Diffusion coefficients of a 2DEG in a basic HEMT structure. The electric field is along x , the direction of the channel. $T = 77 \text{ K}$ and $n_s = 10^{11} \text{ cm}^{-2}$.

cubic cell Ω_c of k space will never accept a new electron when it already contains two electrons (Pauli's exclusion principle). Any further interaction sending an electron k vector in this cell will thus be forbidden and the electron will pursue its route as if the interaction had never occurred. The size of the cell Ω_c is simply obtained from the number of simulated carriers and from the density of the system under study by virtue of Heisenberg's principle.

In a two-dimensional carrier system, the general scheme will be the same, except that the system will evolve in a multifold two-dimensional k space, and in each subband the partition of k vectors will be made of squares rather than cubes. Ultimately, one expects this model to tell us what kind of distribution the carriers can achieve in case of high fields or how this distribution departs from the equilibrium Fermi-Dirac distribution. This point seems to be out of the reach of analytical physical analyses. Here, once again, the Monte Carlo approach seems to be the safest way to tackle the problem. Also, further work is needed on this subject in order to see how far degeneracy has a critical role at high fields.

10) *Diffusion*: This is a problem which can be studied with the MC method, which has received almost no attention till now. Since one of the major advantages of the HEMT is its good noise figure at high frequency, a good knowledge of diffusion coefficients is necessary [48]. The way in which a diffusion coefficient can be computed in the MC method in the case of a 2 DEG is quite similar to what was formerly done in bulk materials [49]–[51]. We illustrate this point in Fig. 5, where we show the diffusion coefficients parallel and transverse to the driving electric field applied along the heterojunction. This figure only concerns purely 2-D electrons, however. The contribution of intervalley and/or real-space transfer to diffusion coefficients is still unknown, although it constitutes a key parameter in noise evaluation of devices.

In conclusion, and rigorously speaking, all these phenomena should be taken into account in an accurate simulation of the device. Thus, it is very likely that only a Monte Carlo method would permit this to be done in spite of the extraordinary complexity of the model. However this work is essential as long as safe physical bases are necessary to undertake simplified simulations of any other kind (see Section III).

B. Effects of Shallow and Deep Donors in AlGaAs

Most of the time, it is assumed that only a single discrete donor level due to Si or any other doping species exists in a heavily doped AlGaAs. The activation energy of this level is chosen according to the case which is considered. The early models [52], [53] assumed a shallow level, located a few meV below the conduction band edge. As a consequence, the doping atoms could be easily ionized and free carrier concentration might equal the doping concentration N_D in the undepleted zone. Accordingly, no freeze-out was observed above nitrogen temperature, for instance. Finally, in the depleted zone, the resulting fixed charge concentration N_D^+ would always equal the doping level N_D .

Under these assumptions, a number of experimental results pertaining to devices and AlGaAs layers with Al content in the range $0.2 < x < 0.4$ remain unexplained. Hall electron density measurements in dark show that at any temperature the free electron concentration remains smaller than the dopant density N_D . This has been clearly shown by Chand *et al.* [54], Schubert and Ploog [55], and Ishikawa *et al.* [56]. This fact is embarrassing since the Al content range and doping densities in question correspond exactly to what is commonly used in MODFET fabrication.

In general one observes that n/N_D , which is less than one at room temperature, rapidly decreases with temperature (freeze-out) until, below ~ 140 K, it remains almost constant. Moreover, below 140 K, a strong persistent photoconductivity (PPC) is observed [57]. Additionally, experience shows that n/N_D is a function of N_D and the Al content x [56].

In reality, it seems very well established by several experiments [54]–[56], [58], [59] and first of all by Watanabe [58] that when introduced in the AlGaAs ($x \sim 0.3$) a Si doping atom creates two or three donor levels: one is shallow and the others are deep. The shallow level is bound to the Γ valley, with an activation energy of about 6 meV as a result of the hydrogen atom model for GaAs. Its ground-state energy becomes slightly deeper when the Al mole fraction is increased, due to the small change of the effective mass in the Γ valley [55].

The properties of deep donors in AlGaAs responsible for the PPC effects were first studied by Lang *et al.* [60]. The donor level was called a DX center, suggesting that it might be a complex formed by an ordinary donor and another defect, probably an As vacancy. Lang suggested a model where the center has a strong coupling between an electronic and a vibronic system. This is illustrated in Fig.

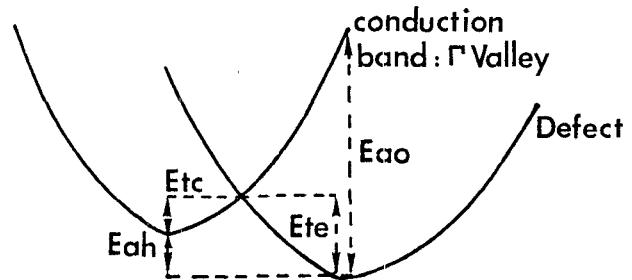


Fig. 6. Deep donor in AlGaAs: electronic energy and vibrational energy as functions of the defect coordinate.

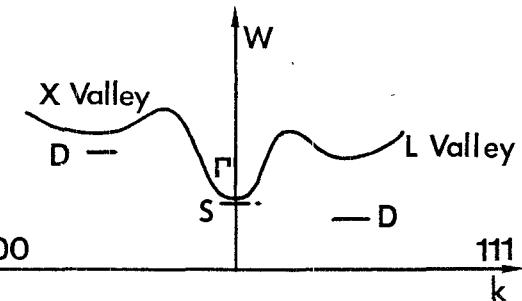


Fig. 7. Electron energy diagram: Γ , L , X conduction bands, shallow S and deep donors D levels.

6, where the sum of the electronic energy and the defect energy is plotted as a function of the defect coordinate. The large differences between the optical activation energy E_{ao} , the Hall activation energy E_{ah} , and the thermal emission and capture energy E_{te} and E_{tc} can be explained when this diagram is considered. More recently a model was proposed by Mizuta *et al.* [59] in order to explain experiments realized with GaAs, and AlGaAs layers subjected to hydrostatic pressure. Mizuta pointed out that the deep levels are attached to each of the L and X conduction band minima as shown in Fig. 7: they are located at 140–160 meV and 40–50 meV below the L and X minima, respectively. The model of Mizuta *et al.* gives a consistent picture of the behavior of AlGaAs layers: it was recently used with success for evaluating the 2 DEG density in MODFET's at 10 K [61].

However, considering this model as granted, one cannot directly answer an important question concerning the reasons why according to the Al content one can experimentally observe very different behavior. To illustrate this point, we have represented the energy positions of the edges of the Γ , L , and X , conduction bands as a function of the alloy composition (Fig. 8). Moreover, we have included the donor levels below the respective minima. Following the opinion of Mizuta [59] and Subramanian [61], the distribution of electrons among the three levels $E_{d\Gamma}$, E_{dL} , and E_{dX} is governed by Boltzmann statistics. Therefore the lowest is dominant for the electron occupation and consequently the dominant donor level changes when the Al content changes. At low Al mole fraction ($x < 0.15$) $E_{d\Gamma}$ is the lowest-lying donor level, so that only a shallow donor is observed in these materials. As x increases, the E_{dL} level becomes the lowest; the donor

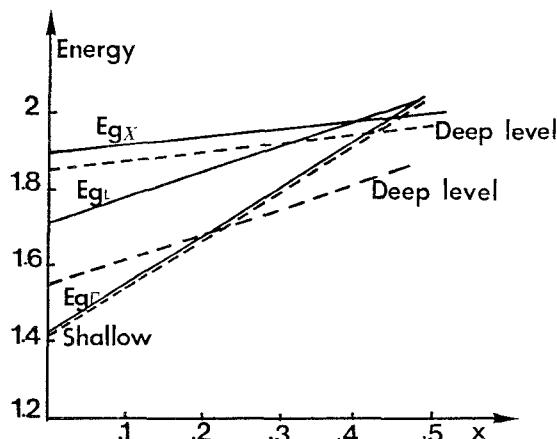


Fig. 8. Energies of the Γ , L , and X valleys, shallow and deep donors levels in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ versus Al mole fraction x .

level becomes the deep one (DX center) although the absolute conduction band minimum remains at Γ . The electronic occupation for these levels E_{dL} and $E_{d\Gamma}$ changes very rapidly according to, as a first assumption, a Boltzmann factor.

In order to account for these effects, several authors, first of all, Schubert and Ploog [55], have introduced the concept of an apparent thermal activation energy “ E_d ,” which is an increasing function of x .

In this approach one can explain why the ratio of free electron concentration over doping level concentration n/N_D in bulk GaAlAs at 300 K or below decreases as the Al content increases. Moreover, this theory also explains why the ratio n/N_D decreases when the doping density N_D increases. As the doping density may approach or sometimes be higher than N_c (the effective number of states in the Γ valley) $N_c \sim 5 \cdot 10^{17} \text{ cm}^{-3}$ at $x = 0.2$), the Fermi level may be located above the conduction band minimum. Increasing the doping concentration raises the Fermi level, thus allowing much deeper donor levels to come into play.

Introducing directly the exact positions of the donor levels, as was done by Subramanian [61] at 10 K and Constant *et al.* [62], is a better approach. These authors also took into account the fact that shallow donor levels broaden into a narrow band which overlaps with the conduction band when the donor concentration is brought up to $5 \cdot 10^{18} \text{ at/cm}^3$. They also consider carrier degeneracy effects and a Fermi distribution for the free electrons in the AlGaAs layer and the 2 DEG. In Fig. 9(a) and (b), typical results one can obtain [62] are presented. The variations of the 2 DEG concentration n_s at 300 K as a function of the Al mole fraction x using the most probable position of the deep donor level or, on the other hand, simply using a single hydrogenoid shallow donor level are calculated. As has been said before, the differences between the different curves and the subsequent errors introduced by the usual assumption at a single level become increasingly important as the Al content and the doping level increase. In practice ($x = 0.3$ and $N_D = 5 \cdot 10^{18} \text{ at/cm}^3$ in AlGaAs), this error may reach 50 percent. In addition,

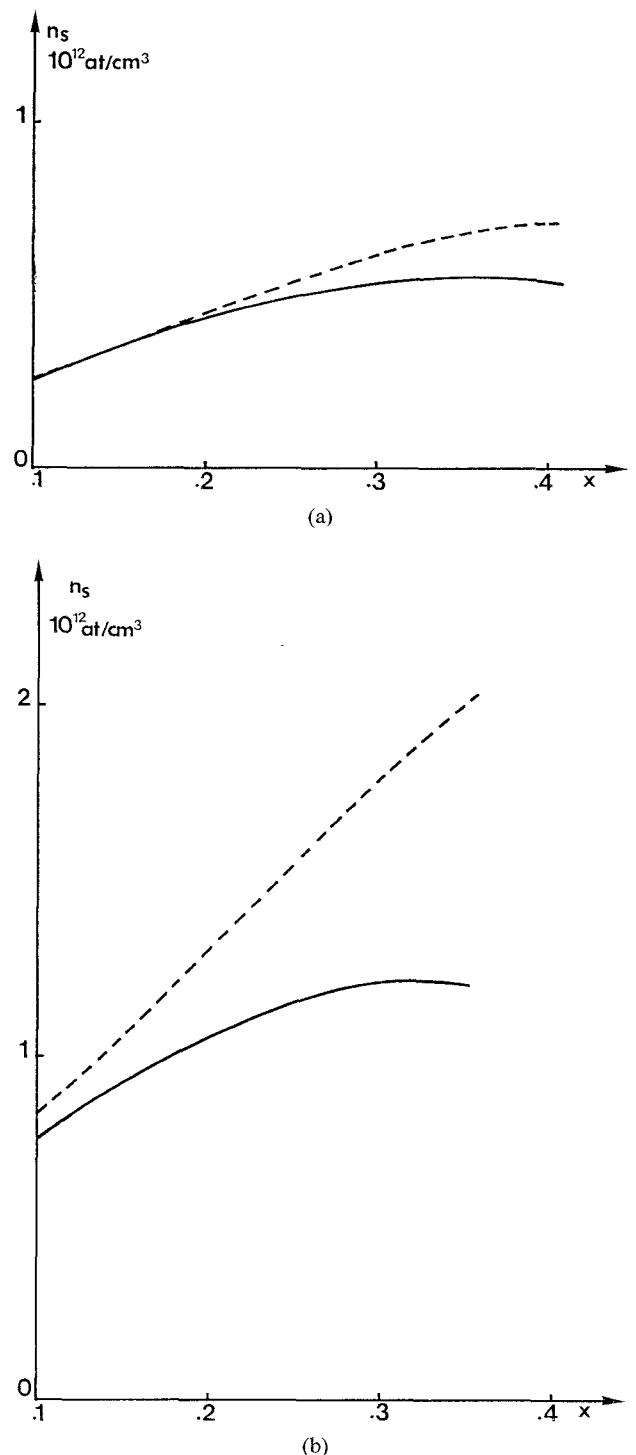


Fig. 9. Dependences of the carriers concentration n_s in the 2DEG on Al mole fraction x . (a) $N_D = 2 \cdot 10^{17} \text{ at/cm}^3$ (b) $N_D = 5 \cdot 10^{18} \text{ at/cm}^3$. — the exact positions of donor levels are taken into account. --- All the donor levels are considered to be shallow.

these figures clearly show that n_s does not increase continuously with x , but rather saturates when x approaches 0.3.

As a conclusion, it seems necessary to take into account the exact positions of donor levels in AlGaAs layers if an accurate and reliable simulation of MODFET's is to be performed.

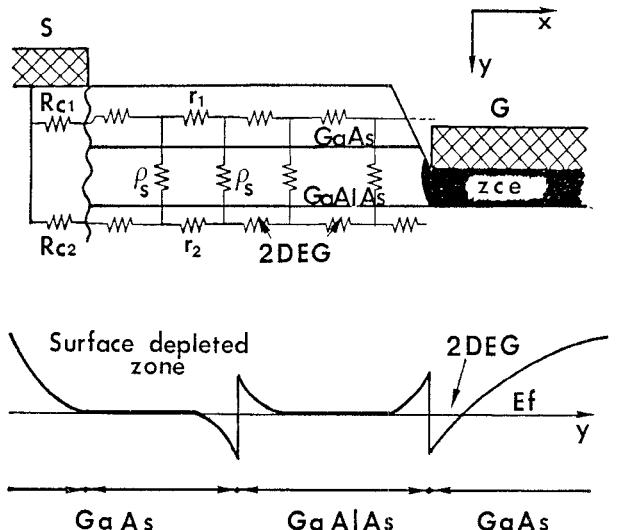


Fig. 10. Equivalent scheme of the access source zone at low frequencies.

C. Parasitic Access Impedance

In order to predict accurately the behavior of the entire device, it is necessary to describe exactly the access zones to the intrinsic active part of the device. Usually, these are represented by a source as well as a drain access resistance R_s and R_d , respectively. Due to the very high intrinsic transconductance obtained today ($g_{mi} \sim 300$ to 500 mS/mm), the access resistance value (0.3 to 1 Ω /mm) mainly governs the extrinsic transconductance given by $g_{me} = g_{mi}/(1 + g_{mi} R_s)$ and then the expected performance.

In MESFET's the behavior of this access zone is purely resistive and modeling of access resistances can be easily performed. On the contrary, the basic HEMT structure is more complicated. In the access zone, three layers must be considered: the n^+ -GaAs cap layer, the n^+ GaAlAs, and the 2 DEG layer. Fig. 10 presents a cross section of the source access zone of a typical HEMT and the band diagram along the direction perpendicular to the surface.

The sheet resistance presented by the very highly doped cap layer R_1 is usually about $200 \Omega/\square$. Since the AlGaAs zone is completely depleted throughout the heterointerface and carrier mobility is very small, the square resistance is usually higher than $3000 \Omega/\square$. Then, the sheet square resistance R_2 is typically close to $1000 \Omega/\square$. The behavior of this kind of structure has been studied by Feuer [63], Lee and Crowell [64], and Cappy [65]. Taking into account the high value of the resistance presented by the AlGaAs layer, they evaluated the equivalent access resistance by neglecting the parallel conduction in this zone and using the equivalent scheme shown in Fig. 10. In this scheme, ρ_s is the equivalent transverse resistance of the two heterojunctions in series, which is calculated taking into account electron tunnel currents [64].

Such a theory gives predicted values which are in good agreement with experimental data and explains the very high values of series resistance usually obtained. For in-

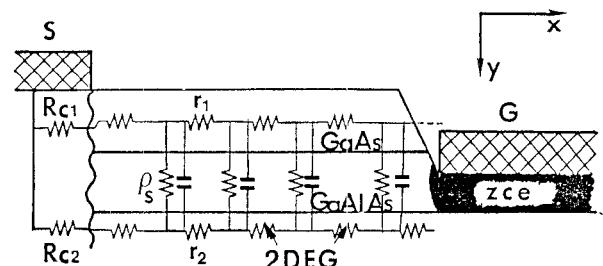


Fig. 11. Equivalent scheme of the access source taking into account displacement currents.

stance, for very small gate source distance L_{sg} , the minimum value of R_s is close to the contact resistance R_{c2} , which is often very high (1 to $1.5 \Omega/\text{mm}$).

This analysis, however, is only valid under dc or low-frequency operation. In microwave or in transient regimes, we have to account for displacement currents passing through the two depleted zones on both sides of the AlGaAs layer. The equivalent scheme is then modified, as indicated in Fig. 11, by introducing distributed heterojunction capacitances. As a consequence, the apparent source resistance now decreases as the frequency increases, with a critical frequency given by

$$f_c = \frac{1}{2\pi\rho_s \cdot C_p}.$$

In usual structures, this critical frequency lies between 5 and 20 GHz. At very high frequencies, the transverse resistance ρ_s is short-circuited by the capacitance, and R_s is then given by

$$R_s = \frac{R_{cl}R_{c2}}{R_{cl} + R_{c2}} + \frac{\Omega_1\Omega_2}{\Omega_1 + \Omega_2} L_{sg}.$$

This equivalent source resistance law has been experimentally observed by Versnaeyen *et al.* [66] by studying the evolution of the Z_{12} impedance parameter of various HEMT structures as a function of frequency.

By using these formulas, the source resistance values can be calculated and their dependence upon gate source distance, cap layer resistance R_1 , transverse resistance ρ_s , and frequency can be studied [65]. These dependences are illustrated in Fig. 12 and are compared with those obtained from a standard structure. From these comparisons, we can note that:

- i) There exists a very important decrease of the source resistance as the frequency is increased.
- ii) The cap layer has a strong influence, mainly at high frequency.
- iii) The dependence of source resistance on gate-to-source distance is weak.

In all cases and especially at high frequency, the source resistance is found to be very much smaller than $R_{c2} = R_2 L_{sg}$, the value delivered by usual theories.

In conclusion, an accurate HEMT simulation *must* take into account the distributed character of the source access

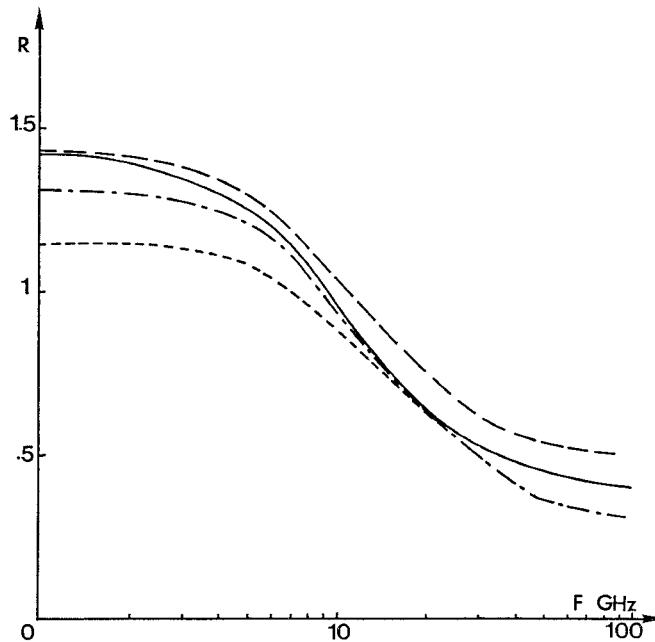


Fig. 12. Frequency variations of the MODFET equivalent source resistance $Z = 300 \mu\text{m}$ —standard structures: $r_1 = 200 \Omega/\square$; $r_2 = 1000 \Omega/\square$; $R_{c1} = 0.2 \Omega/\text{mm}$; $R_{c2} = 1.2 \Omega/\text{mm}$; $\rho_s = 2 \cdot 10^{-5} \Omega\text{cm}^2$; $C_p = 1.4 \cdot 10^{-6} \text{ F/cm}^2$; $L_{sg} = 1 \mu\text{m}$ —same values but $r_1 = 400 \Omega/\square$; —·— same values but $L_{sg} = 0.5 \mu\text{m}$; ····· same values but $\rho_s = 10^{-5} \Omega\text{cm}^2$.

resistance and the influence of displacement currents through the heterojunctions.

III. SURVEY OF MODFET SIMULATION TODAY

A. Monte Carlo Simulations

The basic principle of Monte Carlo (MC) simulations is to follow the motion of the carrier representative point in reciprocal space, simultaneously taking account of the deterministic effect of the driving electric field and of the stochastic effect of the various kinds of scatterings the carrier may undergo, as well as their respective probabilities. Carrier velocity is then obtained from its location in reciprocal space. Then carrier position in real space is obtained via the integral of velocity over time. Using this method requires knowledge of the band structure of the semiconductor material in which the carriers move and all relevant parameters necessary to exactly evaluate the various scattering probabilities. In this way, the simulation exactly accounts for any microscopic process involved in charge transport. So, MC simulations are suitable for studying many effects due to transport properties and have been widely used for this purpose [67]–[71].

The application of MC methods to device modeling requires defining the geometry of the device boundary conditions. These are specular reflection of carriers at semiconductor-air surfaces and Schottky contacts and absorption and injection of carriers at ohmic contacts. The Monte Carlo simulation of a large number of particles (ensemble Monte Carlo method) is used, usually with a constant time step discretization scheme which allows carrier density as a function of space and time to be determined. Then, the 1-D or 2-D Poisson's equation can be

solved, including relevant electrical boundary conditions, in order to obtain and update the self-consistent electric field throughout the device. Then, this electric field is applied to the carriers for the next time step and the process is repeated until a stationary regime is eventually reached.

The main advantages of the MC method are:

- i) it is a quasi-exact method since it is able to take into account almost all kinds of microscopic processes to which carriers are subjected. As a result, for instance, nonstationary dynamic effects (velocity overshoot, ballistic phenomena) may be described.
- ii) Current and continuity equations are automatically solved in the simulation itself.
- iii) Bipolar devices can also be studied; noise properties can also be deduced from the carrier velocity fluctuations [72].

The main disadvantages are:

- i) The MC method is rather computer time consuming and needs very powerful computers.
- ii) Study of dynamic regimes is difficult.
- iii) The results may not be very accurate. Due to the statistical nature of the process, a desired accuracy can only be obtained by increasing the computation time.

Nevertheless, MC simulation is a very powerful tool for the study of devices. This is because, on one hand, it gives full information about the physics of carrier transport and, on the other, it can predict the performances of the device. For example, when studying a MESFET, MC simulation makes it possible to determine not only the position of carriers in the device, their velocity and energy, and their location in the Γ , L or X valleys, but also static characteristics, transconductance values, and the cutoff frequency of the device.

For example, Figs. 13 and 14 present some MC simulation of a AlGaAs/GaAs HEMT. Fig. 13 represents the variations of the transverse electric field in the channel of the device, along the source-to-drain axis, for various gate biases. These curves show channel pinch-off under the gate and a very strong negative electric field giving rise to real-space transfer from GaAs to AlGaAs near the drain edge of the gate. Fig. 14 represents the variation of the expected performances for a quarter-micron gate HEMT as a function of the AlGaAs doping level N_D or layer thickness a ; these parameters are chosen such that $N_D a^2$ is a constant.

So, the MC method has been widely used for studying various kinds of devices, among them 1-D GaAs n^+ - i (n)- n^+ diodes [73], GaAs MESFET's [74], [75], MOSFET's [76], [77], MISFET's [78], GaAs injection FET's [79], 1-D heterojunction ballistic structures [80], 1-D heterojunction bipolar transistors [81], and bipolar structures [82].

Using MC simulations for studying HEMT's may present some difficulties due to the specificity of these de-

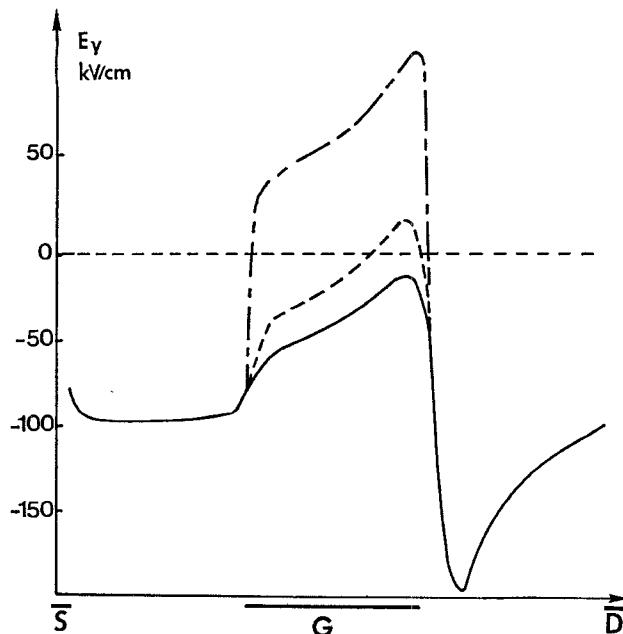


Fig. 13. Transverse electric field in the channel of a GaAlAs/GaAs HEMT for different gate bias (—: $V_{gs} - V_{bt} = -0.9$ V; - - -: $V_{gs} - V_{bt} = -1.1$ V; - · -: $V_{gs} - V_{bt} = -1.7$ V).

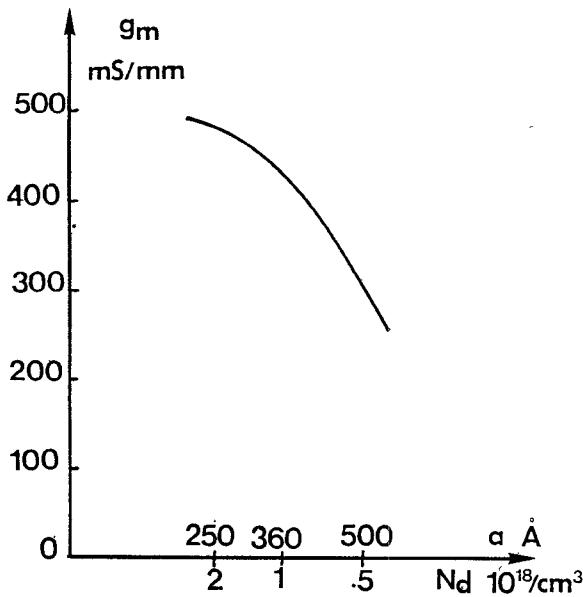


Fig. 14. Transconductance values obtained for an $0.25 \mu\text{m}$ gate length HEMT as a function of the AlGaAs doping level N_D (or thickness a) with $N_D a^2 = \text{constant}$.

vices. This is mainly due to the 2DEG induced at the heterointerface. A complete Monte Carlo simulation would have to simultaneously take into account the two-dimensional nature of electron charge transport in the conduction channel and the three-dimensional nature of transport everywhere else in the device. So, a knowledge of three-dimensional scattering rates and two-dimensional scattering rates, together with the position of the conduction energy subbands in the channel, is necessary, as discussed in Section II-A. It is also necessary to know the probabilities for electrons to transfer between the various subbands

or from a subband to three-dimensional states. In addition, in a real MODFET, the AlGaAs layer is usually highly doped, making electron density in the undoped GaAs channel very high. So, modeling these structures might require consideration of the effect of degeneracy and electron-electron and remote impurity scatterings (see Section II-A). But the difficulty which is encountered when modeling MODFET's is that the density of electrons in the channel is nonuniform, so subband levels and channel width change all along the device. As a result, two-dimensional scattering rates would have to be continuously updated in the course of the simulation at each point of the 2 DEG channel.

Only a few MC models are presently able to take into account almost all of these phenomena [83]. A number of MC simulations use instead a three-dimensional approach, thus neglecting pure quantum effects [37], [84]. A more complete MC model [85] has been developed which uses two-dimensional scattering rates for electrons in the 2DEG channel region and three-dimensional rates in the other regions; the width of the 2DEG channel is assumed to be a simple function of the transverse electric field at the heterojunction. Another sophisticated MC model [36] includes quantization in the conducting channel, using a two subband triangular well approximation for the subbands and variational wave functions for evaluation of scattering probabilities.

It is clear that the application of MC method to HEMT (or even more complicated structures) simulations is still in its infancy. The interest shown in it derives from the fact that it is almost the only method which is able to take all (or nearly all) the physics in the device into account in a systematic way. At a lower stage, Monte Carlo simulations are necessary in order to determine as accurately as possible a number of parameters which are needed in many simulation models. These are the drift velocity of 2-DEG, the relative populations of the subbands as they change under the influence of the bias fields [32], [33], the average energy of the carriers since the electron system is out of equilibrium, and as far as fluctuations and noise are concerned, the diffusion coefficients.

B. Two-Dimensional Numerical Models

We consider in this subsection those simulation models which make use of current continuity and drift diffusion equations in one form or another. Many efforts have been made in order to develop other modeling methods which remain accurate but need less computation time and are usable under transient or dynamic conditions. This concerns mainly, as for MESFET's, the two-dimensional solution of the fundamental semiconductor equations [86]–[90]. Then, it is useful to point out what are the main limitations of the models presently available in order to show in which direction efforts must be made to overcome the main difficulties encountered.

First of all, most of the models use the electrical potential, the carrier concentration, and the current density as the fundamental set of variables. This choice introduces

some problems, mainly due to band discontinuities which exist in the plane of one heterojunction for instance. In the model proposed by Tang [89], the electron and hole quasi Fermi levels are used. Among the most interesting features are that:

- i) these quantities do not suffer any discontinuity when passing through the heterojunction;
- ii) boundary conditions are easy.

The main problem rests on the validity of this approach in the presence of hot electrons. It has, however, been proved accurate for n^+nn^+ GaAs structures [91], by comparison with results deduced from a one-dimensional solution of MC model and relaxation equations.

Next, another question arises from the introduction of nonstationary electron dynamic effects. This requires solving the energy relaxation equation in the manner of Widiger [88] or Loret [90]. The basic idea is similar to that used in MESFET simulations [92]–[94], and can be implemented in various ways. It was clearly shown that for submicronic gate MESFET's ($L_g < 0.5 \mu\text{m}$, for instance), these effects *must* be taken into account, and it is not possible to give an accurate prediction of the device behavior by using only a bulk $v(E)$ relationship. We think that the situation is quite similar in MODFET's, and the use of an empirical $v(E)$ relationship depending on the gate length, for instance, would not constitute an appropriate solution. Only an adequate formulation of the energy relaxation equations, as in the models quoted above, seems to be the correct approach.

Another problem concerns the possibility of treating a MODFET structure by neglecting the specific quantal nature of the 2DEG, thus assuming that the carriers obey Boltzmann statistics and 3-D electron dynamics. As it has been shown by Ravaioli *et al.* [36] with MC simulations and by Widiger and Hess [87], [88], the carriers never remain in the ground subband during the main part of their drift under the gate at usual dc bias conditions. On the other hand, Yoshida [95] has clearly demonstrated that the variation of the sheet electron density n_s with gate voltage, treated by a classical approach using Boltzmann statistics, may give similar results as compared to comprehensive quantum calculations. Next, as has been shown by MC simulations [96], carrier dynamics of the 2DEG under high-field transport may sometimes be similar to what is usually met in bulk material. As a consequence, in such simulations it seems unnecessary to account for the 2-D character of carriers. However, using Fermi statistics would be of great benefit, as it automatically accounts also for carrier degeneracy in the AlGaAs and the GaAs layers where the carrier concentration may exceed the density of states in the Γ valley. Our opinion may be quite different if we want to simulate the behavior of other kinds of heterojunction structures, for instance multichannel or superlattice structures. In these, solving the problem with a classical 3-D approach is much more questionable.

Although the current saturation parasitic conduction in the AlGaAs under the gate may be rather weak [90],

accounting for the influence of this layer in the total current is indispensable. When the gate is forward biased, conduction in the AlGaAs layer takes an important place via the gate current, and charge control of the 2DEG is completely modified [65]. Of course, as mentioned already in Section II-B, an accurate simulation of the AlGaAs contribution to the total current must also include the influence of deep donor levels (DX centers).

Another problem concerns the accurate treatment of the heterojunction. It has been suggested by several authors [97], [98] who work on one-dimensional structures (TED or HBT) that this effect can be accounted for by introducing a fictitious electric field over a few lattice meshes at the heterojunction, thus giving an equivalent variation $\langle \Delta W \rangle$ of the average energy for an electron drifting perpendicular to the interface. This method gave good results in millimeter-wave range TED's [97]. It may constitute an appropriate way for obtaining a self-consistent calculation of MODFET's.

From the point of view of numerical efficiency and considering the respective dimensions of the active zone (mainly the quantum well) as compared to the other parts of the device, an accurate simulation necessitates, as in MC models, the use of variable mesh spacings. At the present time, finite difference methods [90] give the most promising results, but it may be interesting to consider finite element methods which may constitute another possible approach.

As a conclusion, it seems that some effort must be made in order to develop and improve the two-dimensional solutions of basic semiconductor equations in MODFET's in order to correctly include:

- i) nonstationary electron dynamic effects by means of relaxation equations;
- ii) the influence of AlGaAs layer;
- iii) the influence of the band discontinuities at the heterojunction on carrier average energy.

These simulation models are essential if we have to improve our understanding of MODFET behavior and obtain accurate predictions of its performance. They need less computational effort than MC models, and consequently they can be used more easily for a systematic study of technological parameter influences. Moreover, they can be used under dynamic as well as transient conditions, which is still not possible with Monte Carlo. On the other hand, they cannot be used for the computer-aided design of complex circuits. This is the reason why even more simplified models have been imagined.

C. One-Dimensional Numerical Models for HEMT

One-dimensional numerical models of HEMT's, although less rigorous than two-dimensional or Monte Carlo models, have the clear advantage of being more simple to handle. This is especially true when the HEMT characteristics can be derived in closed forms or at least in semianalytical forms. These models therefore save computer time and memory and can be carried out and exploited on

microcomputers. This point is essential for device CAD where the model can be used to control fabrication processes. The accuracy of any model would depend of course on the number of physical effects which are taken into account and on how they are dealt with, for instance, charge control by the gate, access resistances, transconductance compression, and possibly non-steady-state transport. Next, the accuracy of a model rests on the validity of the parameters which control all the physical effects.

The most common assumption which is made in simple one-dimensional models is the gradual channel approximation along the source-drain direction x parallel to the interface. The current is simply written as $qn_s(x)ZE(x)\mu(E(x))$ in a slice cut perpendicularly to the gate plane, where Z is the width of the gate. This expression, thereby, most often relies on a local dependence of the carrier drift velocity as a function of the local electric field $E(x)$. Several expressions may be used, of which the former is the so-called Trofimenkoff relation [99]–[101] or modified form [102], whose essential advantage is that the function and its derivative are continuous over the entire field range of interest. The Trofimenkoff relation, however, is a silicon-type relation. Other relations are also often used [103]–[105]. Yokoyama *et al.* have reviewed the problem [106] recently and pointed out that the low-field $v-E$ behavior is of crucial importance. They showed that, using comparisons with Monte Carlo simulation, a GaAs-type $v-E$ relation [32], [33], [107] can be used which can lead to essentially the same quality of final results, but with a more physical assumption for the $v-E$ dependence. As a matter of fact the fit of simple one-dimensional models with experimental data of submicron structures always leads to very high saturation velocity, v_s , in the range $1.5-3 \times 10^7$ cm/s for the Trofimenkoff relation, although it is well known that in GaAs at 300 K, v_s is in the range $6-8 \times 10^6$ cm/s. But at low and medium fields the drift velocity in GaAs easily reaches $1.5-2 \times 10^7$ cm/s, and as is well known, low and medium fields are involved all along the current path beneath the gate except near the drain-end side.

In this connection, we can stress the fact (see Section III-B) that non-steady-state transport may affect carrier dynamics, especially on the submicron scale, where the gate length may no longer be considered much larger than the electron mean free path in the 2DEG channel. This is especially true at low temperature, where carrier dynamics is no longer dominated by polar optical phonon scattering and is almost free of impurity scattering, as discussed in Section II-A. Non-steady-state transport may be included [65] when one considers the carrier drift velocity $v[E(x)]$ not a local function of the electric field but rather a function of the local mean energy, and the local mean energy a function of position as the distribution function of carriers in k -space evolves gradually from the source to the drain under the gate. When this is included in the calculations, it may lead to local velocities largely in excess of saturation velocity values. This is illustrated in Fig. 15, where 1-D simulation results of a standard HEMT [65] are

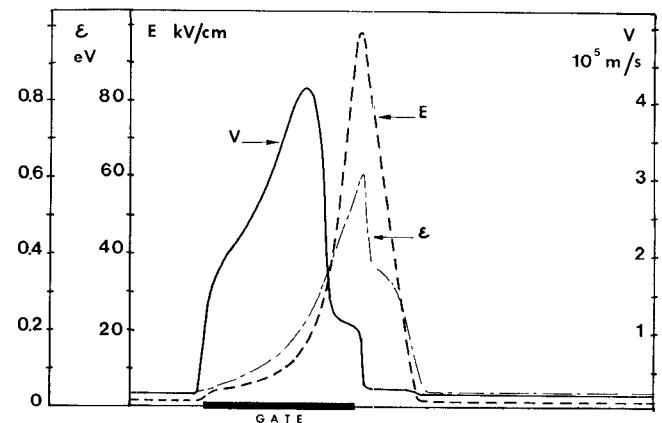


Fig. 15. Electric field, electron velocity, and energy as they evolve along the source-drain axis under the gate, calculated using a one-dimensional model [65] for a typical HEMT structure at ambient temperature: $L_g = 0.5 \mu\text{m}$, $N_d = 10^{18} \text{ cm}^{-3}$, $a = 500 \text{ \AA}$, $V_{ds} = 2.5 \text{ V}$.

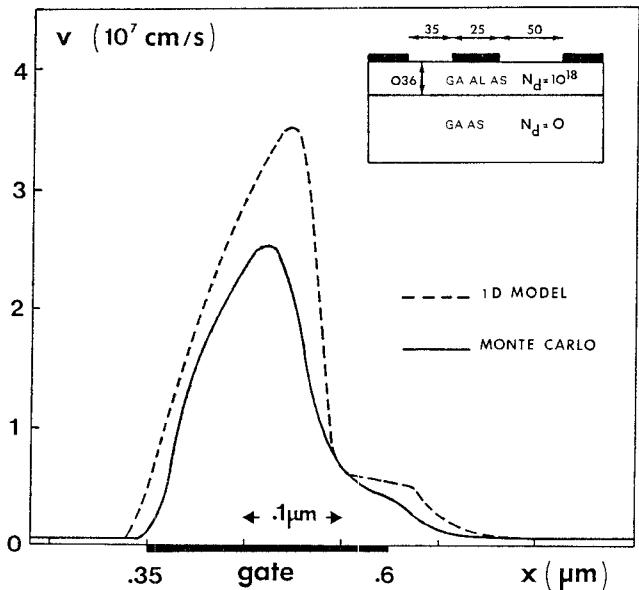


Fig. 16. This figure shows a comparison between the MC solution and a one-dimensional solution of the same HEMT structure shown in the inset under the same bias conditions, the average velocity is $\sim 1.5 \cdot 10^7$ cm/s under the gate.

presented. Therefore, it is not surprising that, when these effects are ignored in a model, much higher "effective" velocities (higher than physical drift velocities) are needed in order to obtain a good fit with experiments. The Trofimenkoff $v(E)$ relation can be considered as essentially incorrect and must be viewed as some "average velocity of the electron channel" and not a local velocity, especially on the submicron scale, where the geometry of the electric field is somewhat complicated.

In the same spirit, diffusion contribution is seldom included in the models. Since diffusion is a fact of nature, and the diffusion current term is generally omitted, fitting the model outcome with experimental data means that diffusion is implicitly plugged into the conduction current. Neglect of diffusion contribution is illustrated in Fig. 16, where we present a comparison between a one-dimensional simulation developed in [65] and a MC simulation of the

same structure. The MC model automatically takes diffusion into account; the one-dimensional model does not. The resulting mean velocity under the gate of the HEMT may be somewhat overestimated. Note, however, that the average value of the electron velocity under the gate can be substantially higher (because of non-steady-state behavior) than the physical v_s in the heterojunction (see Section II-A and [35]). In [99], the additional contribution due to diffusion has been included, assuming the Einstein relation in its equilibrium form to hold everywhere in the channel. Anyway, as mentioned earlier in this paper, a study of diffusion in 2DEG is necessary, especially in out-of-equilibrium systems.

Apart from purely transport problems, a number of other parameters are involved in one-dimensional models. The principal one is the charge control law by the gate. Delagebeaudeuf *et al.* [108] established the expression

$$qn_s = \frac{\epsilon}{d} (V_g - [\phi_B - \Delta E_c - V_0]) \quad (4)$$

where the term in brackets is the threshold voltage below which the 2DEG disappears and V_0 is the voltage which is necessary to deplete the doped GaAlAs layer of width d . Equation (4) is accurate as long as the position of the Fermi level can be ignored. When the device is in operation, the channel voltage under the gate is $V_c(x)$ and (4) becomes

$$qn_s(x) = \frac{\epsilon}{d} (V_g - V_c(x) - [\phi_B - \Delta E_c - V_0]) \quad (5)$$

where $V_c(x)$ is self-consistently calculated via Poisson's equation. Lee *et al.* [105] presented a similar derivation in which the Fermi level variation across the layers, as a function of n_s , is no longer neglected but rather is considered to change linearly with n_s in the range of interest. This puts an additional $\Delta d \sim 80 \text{ \AA}$ to d in (5) and an additional ΔE_{F0} to the previous threshold voltage ($\Delta E_{F0} \sim 0$ at 300 K and $\sim 25 \text{ meV}$ at 77 K). The main advantage with (4) and (5) is that they deliver a closed linear formula for $n_s(x)$ in which quantum mechanical effects are at least partially accounted for. The Δd has recently been reinterpreted by Khondker *et al.* [109] in terms of average distance of the 2DEG layer from the heterointerface, which is still estimated to be in the order of 80 \AA . Then (4) and (5) are still true. A serious drawback of (5) is that, when included in the model, it leads to a gate capacitance contribution which is a constant with respect to V_g . This is in contradiction with experimental observation. It has been shown by Vinter [110], based on quantum mechanical arguments, that this capacitance has a strong dependence on V_g .

The experimental observations of $C_{gs}(V_g)$ clearly show that additional effects due to the presence of free electrons in the GaAlAs layer and of donor levels mainly control the total charge under the gate. Moreover, in logic applications, the gate is forward biased half of the time, and the flow of current through the gate then almost fully controls the electron density beneath the gate. On the other hand,

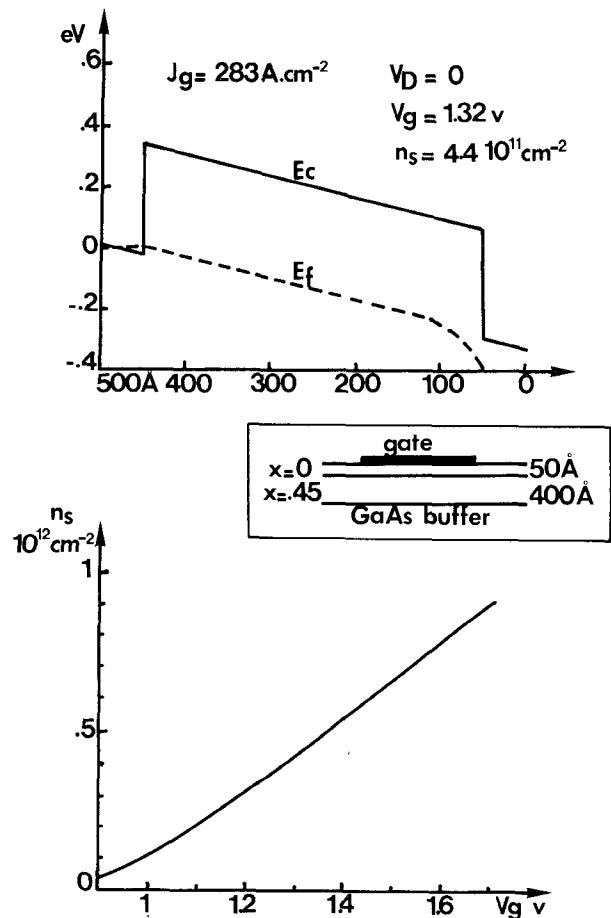


Fig. 17. The structure simulated (all the layers are undoped) is shown in the inset. At the top, the conduction band and the pseudo Fermi level are shown (see text). At the bottom the carrier density in the well (left-hand side of the AlGaAs layer) is shown as a function of gate voltage.

in low-noise applications of HEMT, the subthreshold portion of the charge control law is important. In both cases linear approximations must be relaxed and replaced by more exact functions.

But, in a forward biased gate regime, the assumption of a flat Fermi level across the entire structure is no longer true, since a substantial gate current can go across the AlGaAs layer. This regime has been studied by Ponce *et al.* [111]. When gate current is taken into account, one observes a steep increase of n_s (when the gate forward bias V_g is increased) above the n_{s0} value, corresponding to the maximum electron concentration which can be normally obtained in the 2DEG channel. This phenomenon, which results from the variation of the Fermi level across the AlGaAs layer, must be taken into account in the study of SISFET structures, for instance, of power HEMT or in logic applications. Therefore, it appears that in many cases control laws like (4) and (5) must be properly modified. A model taking these facts in account has been developed in [62]. Fig. 17 illustrates a MIS-like FET in which the charge control law actually depends on the variation of the pseudo Fermi level in the AlGaAs layer when a gate current is flowing. This current is taken into account by considering that the pseudo Fermi level which varies across the

AlGaAs barrier is related to the electron density via Fermi-Dirac statistics such that current continuity is obtained across the AlGaAs layer and the boundary conditions $E_c - E_F = -e\phi_B$ is met at the metallic contact. ϕ_B is taken to be 1 V.

To sum up this part we can say that i) one-dimensional models are necessary because they allow fast, cost-free simulations of rather complex structures; ii) the merit of a model is deeply linked to the amount of physics which can be included in it; and iii) a realistic model which includes a significant amount of physics, and as such can only be treated computationally, will ultimately allow a better knowledge of the key parameters which must be employed in pure analytical models. Finally, the comparison with experiments must not be restricted to the static $I(V_d)$ curves, but rather must also be performed with high-frequency parameters [112].

IV. MODELING OF NEW HETEROJUNCTION STRUCTURES

At the beginning of this paper several new heterojunction structures were mentioned:

- SISFET [4]
- inverted MODFET [5]
- MODFET with superlattice [6]
- multichannel structures [3]
- InAlAs/GaInAs MODFET's [7]
- pseudomorphic AlGaAs/GaInAs [8].

Some other improvements of usual AlGaAs/GaAs structures have also been realized, for instance:

- the introduction of a Si atomic-planar doped AlAs/GaAs/AlAs quantum well structure instead of n^+ AlGaAs layer [113];
- multilayer structures including graded $Al_xGa_{1-x}As$, as proposed by Cirillo [114].

The problems encountered when modeling these devices may vary considerably from one structure to the other. Simulation methods that are used for usual MODFET's could be extended in some way to the study of inverted structures. The situation is different for SISFET modeling, which requires a very accurate determination of the subband energy levels with respect to the Fermi level in the potential well if an accurate prediction of carrier concentration in the 2DEG and drain current must be obtained. For this purpose, the most accurate method would be a self-consistent solution of the Schrödinger equation. Hopefully, analytical formulations remaining accurate enough can be obtained and exploited rather easily. In SISFET's and related structures, an accurate calculation of gate current is needed; for this purpose, we have to account for the various phenomena (tunneling effect, hopping process) which control this current.

Multilayer structures, with graded x layers for instance, do not require taking into account quantum effects in a deeper way than is usual with MODFET's, but they need accurate solutions of Poisson's equation taking into account

the existence of several doping levels in the AlGaAs layers (see Section II).

On the other hand, device modeling including superlattices or planar doped or multichannel structures requires an exact solution of the Schrödinger equation in the direction perpendicular to the gate, in order to give an accurate value of the free carrier concentration in the different regions. This is important for superlattice structures, where specific properties of a superlattice must be taken into account, for instance, the relative positions of Fermi level, conduction bands, and donor levels in GaAs layers.

In all these structures, the 2DEG exists in the GaAs layer and consequently electron dynamics may be quite similar to what occurs in normal MODFET's. In some inverted or multichannel structures, the mobility may be somewhat lower than in normal MODFET's; then the interactions with impurities diffusing from the AlGaAs layers to the GaAs layers must be considered.

On the other hand, when modeling GaInAs MODFET's knowledge of electron dynamics in the 2DEG formed in this kind of material and also in bulk InAlAs or InP is required. Although electron dynamics in bulk GaInAs, InP, and InAlAs are now well known, the situation is quite different for the 2DEG formed in GaInAs. In the earliest simulations [115] of AlInAs/GaInAs devices, the authors postulated that the electron dynamics is quite similar to that of the bulk material, as is done in many models of AlGaAs/GaAs devices.

More difficult problems appear in pseudomorphic n^+ AlGaAs/undoped GaInAs/undoped AlGaAs MODFET modeling. There, the materials are not lattice-matched and a mechanical constraint may exist in the vicinity of the heterojunction. If the GaInAs layer is very thin (~ 100 Å) the mechanical characteristics and then the electrical properties of the GaInAs layer may be quite different from those of the bulk GaInAs material. Work is necessary in order to understand the main parameters controlling electron dynamics in a 2DEG formed in this way.

V. CONCLUSIONS

A large number of MODFET models of various kinds are presently available. However much effort is needed in order to introduce some physical effects which occur in the more recent devices of usual structure or which are of particular importance under low-temperature conditions. Among these, we have discussed electron dynamics in a 2DEG, the influence of the exact positions of donor levels and their evolution with Al mole fraction, and finally, the frequency behavior of the source access zone. A detailed study of presently available models shows the specific advantages of accurate particle models (Monte Carlo, for instance) allowing these effects to be included. Moreover, it is clear that some work must also be done in order to specify the domain of validity of the most simple models, the analytical one-dimensional models, which are very interesting for the CAD of digital and microwave integrated circuits. Finally it appears that most of the avail-

able MODFET models cannot be used for predicting the behavior and performance of improved new structures. For instance, a quantum mechanical treatment must often be properly introduced. Additional work is needed in the field of superlattices and constraint lattice properties and must be developed for that purpose in the future.

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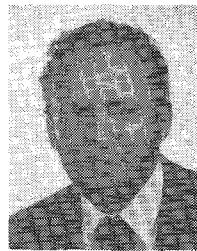
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Georges Salmer was born in Besançon, France, on August 7, 1939. He received the Dipl. Eng. degree from the Institut Supérieur d'Electronique du Nord, Lille, France, and the Doctorat ès Sciences Physiques degree from the University of Lille, Lille, France, in 1961 and 1966, respectively.

He joined the Centre Hyperfréquences et Semiconducteurs, University of Lille I, Villeneuve d'Ascq, France, in 1968. Currently, he is a Professor at the University of Lille and Head of the Centre Hyperfréquences et Semiconducteurs. He is working on microwave solid-state devices, mainly on device modeling and characterization. His early work dealt with IMPATT and BARITT devices, especially high-efficiency Read and high-low GaAs devices. Since 1977, he has worked on low-noise and power submicronic GaAs MESFET's and TEGFET's.



Jacques Zimmermann was born in Blida, Algeria, in 1948. He received the master's degree in electrical engineering in 1972 and the Ph.D. degree in physical sciences in 1980, both from the University of Lille-Flandres-Artois.

Since 1975 he has been a CNRS (Centre National de la Recherche Scientifique) fellow and has worked at the Centre Hyperfréquences et Semiconducteurs, except for an 18-month period with the Department of Electrical Engineering at Colorado State University, Fort-Collins, CO, where he worked as a postdoctoral fellow. He began his early research on essential carrier transport properties in silicon and MOS inversion layers at high electric fields, using Monte Carlo techniques. Then he turned to III-V semiconductor compounds and to carrier dynamics in heterojunctions, work which led to the development of complete device simulation programs based on Monte Carlo techniques at the CHS. In parallel, his experimental work was on millimeter-wave conductivity measurements at high fields and diffusion noise experiments using Dicke radiometers. His work at CSU concerned the development of a theory for high field carrier transport in semiconductors based on a retarded Langevin equation approach, revealing some new non-Markoffian aspects of transport.

Dr. Zimmermann was one of the organizers of the 14th ESSDERC (European Solid State Devices Research Conference) and coedited the conference proceedings as a special issue of *Physica*.



Renaud Fauquembergue was born in Carvin in 1941. He received the Thèse de 3ème cycle degree in electrical engineering in 1968 and the Doctorat ès Sciences degree in physics in 1977, both from the University of Lille Flandres-Artois (France), where he has been working at the Centre Hyperfréquences et Semiconducteurs (CHS) since 1965.

His early research work was devoted to the study of molecular dynamics in the liquid phase using simulation methods and spectroscopic investigations (dipolar and infrared absorption, Raleigh and Raman diffusion). Then his research interests turned to III-V semiconductor compounds and he uses Monte-Carlo techniques to study high field carrier transport properties and carrier dynamics in heterojunctions. His present work deals mainly with two-dimensional Monte-Carlo simulation of submicronic devices such as MESFET's, TEGFET's, MISFET's, and SISFET's.

Dr. Fauquembergue is currently Professor at the University and Head of the Département Génie Electrique et Informatique Industrielle at the Institut Universitaire de Technologie (IUT) of Lille.