Performance of GaAs Device Simulations at Microwave Frequencies

G P Doades, M J Howes, D V Morgan

Solid State Materials, Devices and Applications Group
Department of Electrical and Electronic Engineering
University of Leeds Leeds LS2 9JT UK

SUMMARY

A two-dimensional numerical simulation of a planar Transferred Electron Device (T.E.D) is used as a specific example of the performance of device simulations when operation at microwave frequencies is required. Particular attention is given to the formulation of the conservation equations and the inclusion of energy relaxation effects of GaAs. The Poisson equation and the energy and momentum conservation equations used are realised in finite difference form for use in a computer model. With the inclusion of mobility and electron temperature data, the model is used in a time domain simulation. The steady-state device behaviour is shown to be adequately modelled using simpler equations, ignoring energy relaxation effects. At microwave frequencies the device admittance is calculated and the results with and without energy relaxation are compared. In the case of the T.E.D. the differences at microwave frequencies are seen to be significant and at 20 GHz and above are dramatic.

INTRODUCTION

The increasing importance and potential of monolithic integrated circuits in the microwave field has led to an increasing demand for the fundamental understanding of monolithic microwave elements on semiconductor material. The semiconductor material normally used at microwave frequencies is Gallium Arsenide (GaAs) because of its higher mobility than silicon and the negative differential mobility region, essential for the operation of Transferred Electron Devices (T.E.D.). An enormous effort has been applied in recent years to the development of GaAs technology and the investigation of the electrical properties and electron transport phenomena of the material. The mechanical properties and crystal purity have progressed to a stage where many useful devices and even whole circuits can be readily fabricated and used. The

understanding of the electrical behaviour, however, has not produced any simple rules by which device behaviour can be accurately predicted. The electron transport phenomena of the material is quite well understood, since it stems from a general analysis of quantum theory. The equations produced to predict electrical behaviour are very complicated and very difficult to use to predict the behaviour of any particular device. The equations must be simplified or approximated in some way to produce a usable model of a semiconductor device.

When considering a model for device analysis it must be borne in mind the types of device that will be simulated and, just as importantly, the conditions under which the actual or proposed device will operate. In producing computer simulations one can either over simplify or overcomplicate the model used. The inherent planar nature of monolithic elements gives rise to large physical non-linearities and complicated two dimensional distributions within the device structure. This makes it very difficult to formulate generally applicable analytic expressions and makes the traditional, simple circuit type approximations inaccurate. The inaccuracy of the analytical models is aggravated at high frequencies, high signal levels and small device dimensions where the electrical behaviour of GaAs becomes very complicated.

At the other extreme, the electrical behaviour of GaAs can be very thoroughly described by solving the Boltzmann equation. This equation can describe a collection of particles travelling through a crystal lattice by some externally applied force, and being retarded and scattered by the various mechanisms which operate in a crystal structure. Obviously this will very accurately simulate device behaviour if all the scattering mechanisms of the material can be programmed into the model. In GaAs, which has two main possible states for an electron in the conduction band, there are very many scattering parameters to be described by the Boltzmann equation. This leads to an equation or set of equations which are very difficult to solve. Many attempts at a solution to this problem have been attempted, either by direct or iterative solutions [1], [2] or by Monte-Carlo methods [3]. Monte-Carlo methods have proven to be very useful for accurately modelling the behaviour of GaAs. In practice, however, these methods take huge computer resources just to simulate small amounts of material. To simulate a complete device by this method is very cumbersome and very slow. To simulate devices at microwave frequencies, runs of over 100 pS will be required, this makes the Monte-Carlo method very impractical for modelling complete devices under practical operating conditions.

To provide a usable model, some form of compromise between the two extremes is required. The model must be efficient enough to give results in a reasonable amount of time without recourse to huge computers, but accurate enough to give

quantitative analysis of modern GaAs microwave devices. The Boltzmann equation is normally simplified down to a set of phenomenological equations to describe the electron motion on a macroscopic basis. This then usually leads to the formulation and solution of time-dependent conservation equations as a set of partial differential equations. To obtain some degree of reality mobility, diffusion and electron energy data specific to GaAs are normally included. This data is obtained from previous measurements of the material or Monte-Carlo simulations or both. The resultant equations can then be solved much more efficiently than the more complex Monte-Carlo, Boltzman equation methods. The only question which remains is how far to simplify the physics and how valid the approximations are.

The mathematical basis for a complete device model.

CARRIER TRANSPORT

The set of phenomenological equations which govern the motion of electrons in GaAs is determined from the Boltzmann equation. The approximation produced is widely known as the "diffusion approximation". In producing this approximation the following assumptions are often made [4].

a) A non-degenerate semiconductor
b) A single electron-gas model
c) Velocity is an instantaneous function of field alone.

Approximations a) and b) appear to be quite valid for most devices and operating conditions in the microwave regime and allow the device physics and resultant equations to be considerably simplified. Approximation c) is a result of ignoring the time an electron takes to acquire the full energy given to it by an applied electric field. This seems to be an adequate approximation when the field changes only slowly compared to this time. At sufficiently high frequencies, however, this approximation may not be valid.

As a result of these approximations, the equations of carrier transport are:

current continuity

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla.\bar{J}_n \qquad (1)$$

where $\bar{J}_n$ is the electron current and is given by

$$\bar{J}_n = qn\bar{v} \qquad (2)$$

q is the magnitude of the electronic charge, n is the carrier density and and $\bar{v}$ is the average net velocity of the electrons. The velocity $\bar{v}$ arises from the conservation of momentum and is

expressed as

$$\bar{v} = \mu(E)\bar{E} + \frac{D(E)}{n}\nabla n \tag{3}$$

The value used for the diffusion coefficient is normally taken to be the Einstein relationship,

$$D(E) = \frac{kT\mu(E)}{q} \tag{4}$$

where T is the crystal lattice temperature and μ is the electron mobility. The diffusion coefficient may also be taken from measured or Monte-Carlo produced data. The data is often turned into a polynomial curve-fit to be used in a computer model.

The driving electric field $\bar{E}$ is derived from solving the Poisson equation,

$$\nabla^2\phi = \frac{q}{\varepsilon_o\varepsilon_r}(N_D - n) \tag{5}$$

using the relationship,

$$E = -\nabla\phi \tag{6}$$

The set of equations (1) to (6) form the basis of many semiconductor device models [5], [6], [7]. These models are then assuming the instantaneous response of the electrons to an electric field, and produce reasonably good models where the field is varying slowly enough in time and space. In circumstances where the field is changing rapidly in time, or over a short distance, some consideration of the electrons energy is required.

The energy conservation equation takes the following form

$$\frac{\partial(n\varepsilon)}{\partial t} + \nabla.(\bar{v}n\varepsilon) = qn\bar{v}.E - \frac{n(\varepsilon-\varepsilon_o)}{\tau_e} \tag{7}$$

ε is the average energy of the electron gas, τ_e is the energy relaxation time.

In the original derivation of the equations it is assumed that the electrons obey a Maxwellian distribution function. This allows the interpretation of the average electron energy as an electron gas having a 'temperature' T_e. The temperature is obtained from the relation,

$$\varepsilon = \frac{3}{2}kT_e \tag{8}$$

if energy relaxation is included then equation (3) can be altered to become,

$$\bar{v} = \mu(\varepsilon)\bar{E} + \frac{1}{n}\nabla\big(D(\varepsilon)n\big) \tag{9}$$

this now expresses the fact that the net electron velocity is a function of the electron energy not of the electric field alone. Furthermore, the velocity cannot now change instantaneously in response to an electric field, the electrons must 'heat up' in time according to equation (7).

Expanding equation (9) the following may be derived

$$\overline{v} = \mu(\varepsilon)\overline{E} + \left[\frac{k\mu(\varepsilon)}{q} \nabla(T_e) + \frac{kT_e\mu(\varepsilon)}{qn} \nabla(n)\right] \tag{10}$$

comparing this with equation (3), it can be seen that the two forms are very similar except that there is an extra term in the diffusion part of equation (10). This expresses the fact that it is the most energetic (hottest) electrons that will diffuse out of a collection. This may be very important where there is a high degree of local electron heating, at a Schottky junction or the edges of planar contacts for example.

Finally the total current density can be calculated by,

$$\overline{J} = \overline{J}_n + \varepsilon_o \varepsilon_r \frac{d\overline{E}}{dt} \tag{11}$$

and the current flowing through the device may be obtained (in the two dimensional case) by calculating the current through a plane p, which cuts a cross section through the device.

$$I = \int_p \overline{J}\, ds \tag{12}$$

MATERIAL PARAMETERS

In the preceding equations, several parameters in the equations are required before they may be solved. These are the data which refer to the material which will be used for the devices. The characteristics required are the relationships between mobility, field, electron energy or temperature and the energy relaxation time.

The relation between effective electron temperature and applied electric field has been determined theoretically [8] and is presented here as a detailed curve-fitted function and shown in figure 1. The most widely available and most accurately known relation for GaAs is the velocity/field relation. Since the electron energy is a function of applied electric field, the electron drift velocity may be expressed in terms of a field-dependent mobility,

$$v = \mu(E)\overline{E} \tag{13}$$

This leads to the familiar velocity/field relation which is again expressed as a curve fit to measured or simulated data [9].

$$v(E,T,N_D) = \frac{300\mu_o E}{T} \quad \frac{1 + \dfrac{8.5\times10_4 E_3}{\mu_o E_o^4(1-5.3\times10^{-4}T)}}{1 + \left(\dfrac{E}{E_o}\right)^4} \quad m.s^{-1}$$

where $E_o = 4 \times 10^5$ v.m^{-1} and μ_o is given by,

$$\mu_o = \frac{0.8}{1 + \sqrt{(N_D/10^{23})}} \quad m^2v^{-1}s^{-1} \qquad (15)$$

Combining the energy/field parameter and the data for the velocity field as a function of lattice temperature and doping density, a mobility/energy (mobility/electron temperature) relationship may be established. the mobility/temperature relationship is shown graphically in figure 2.

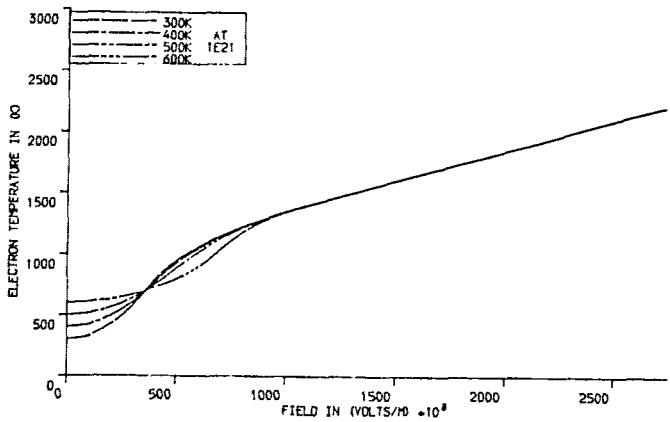


Figure 1
Electron Temperature/field as a function of
Lattice Temperature for GaAs.

The only other unknown here is the energy relaxation parameter τ_e. This can be derived from the steady state energy conservation equation,

$$q\bar{v}.\bar{E} = \frac{3}{2} k \frac{(T_e - T_o)}{\tau_e} \qquad (16)$$

and takes on the form as shown in figure 3.

BOUNDARY CONDITIONS

Most modern devices are made or are preferred in a planar form suitable for monolithic circuit design. This necessitates that any device simulation used in their investigation should be at least two dimensional. The basic two dimensional structure takes the form shown in figure 4.

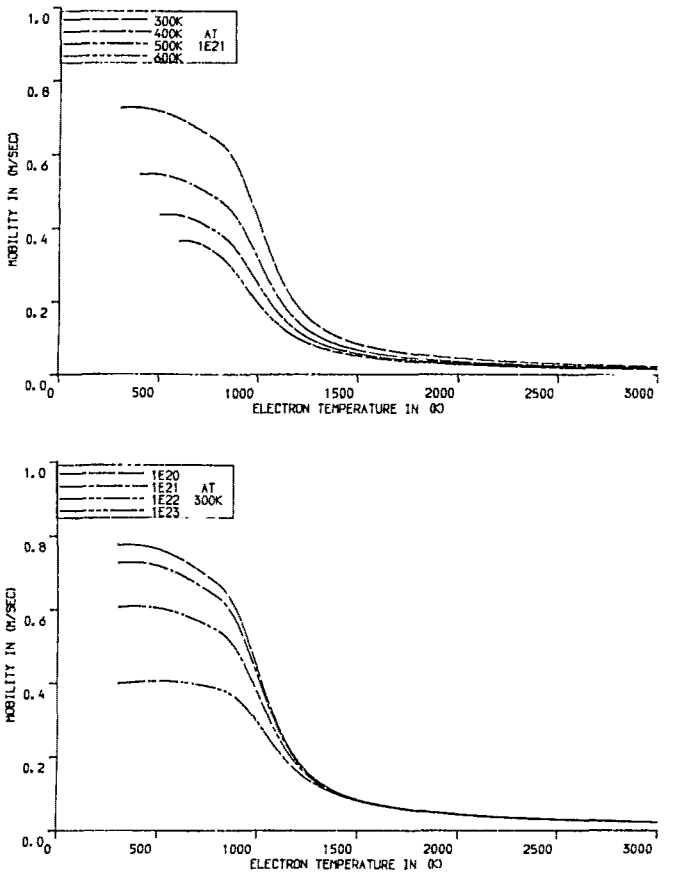


Figure 2
Mobility/energy characteristics for GaAs

This structure as it stands may be a planar T.E.D., or resistor or, with the addition of a third electrode, become an F.E.T. structure. As can be seen, this type of structure is essentially rectangular, and well suited for finite difference analysis using cartesian co-ordinates.

Most of the boundaries are assumed to be 'free'. The boundary conditions needed to solve the set of differential equations are therefore differential boundary conditions at these free surfaces so,

$$\frac{d\psi}{dx} , \frac{dn}{dx} = 0 \qquad @ \text{ boundaries parallel the y axis} \qquad (17)$$

$$\frac{d\psi}{dy} , \frac{dn}{dy} = 0 \qquad @ \text{ boundaries parallel the x axis} \qquad (18)$$

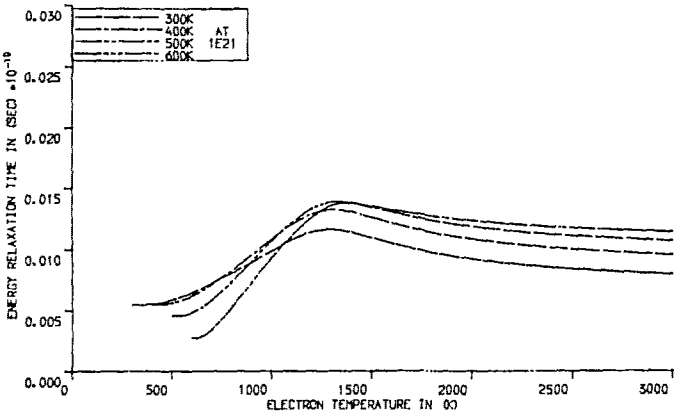


Figure 3
Energy relaxation function of GaAs.

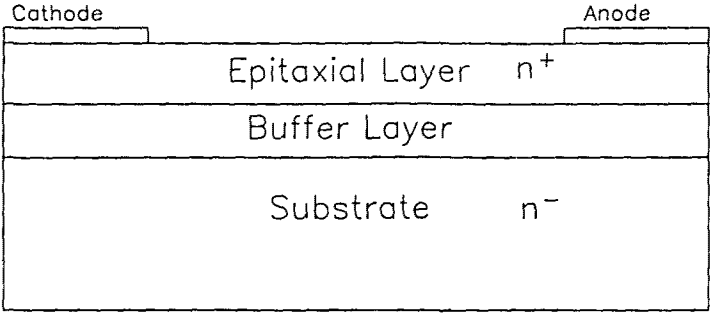


Figure 4
Basic two-dimensional structure

In addition to these there are the fixed electrode boundary conditions in which

$n > N_D$ and $\psi = \psi_c$ the potential applied to the contact.

NUMERICAL ANALYSIS

The preceding set of equations form a linked set of highly non-linear first and second order differential equations. The only practical way to produce a quntitative solution is by numerical means. For certain equations, integration or other 'direct' techniques can be used. The Poisson equation for example is often solved by Fourier transform techniques [10]. The remaining equations, however, are usually discretized in some way by splitting the region of solution into a mesh of

nodes on which the equations are defined. The two main techniques for this are finite elements and finite differences. Again the need for efficiency of the model as a whole must be realised. It is of little value to simplify the physical equations and not choose the most efficient solution method for the particular application. The finite element method is undoubtedly the most flexible, but partly because of its flexibility, if is the least efficient of the two. The finite difference method is both mathematically easy to understand and computationally efficient and easy to program. For the essentially rectangular structures used in this model, the finite difference method has proved to be best method to use.

The finite difference equations for approximating differential equations may be derived using standard techniques such as Taylor series expansion or variational methods [11]. Throughout the model, whenever possible, central difference approximations are used to reduce errors. In two dimensions the use of central difference equations leads to the 'five point formula' and hence a penta-diagonal coefficient matrix to be solved. This type of sparse matrix is particularly well-suited to an iterative solution using Gauss-Seidel or S.O.R. techniques. As well as using significantly less memory, the iterative methods are much faster than most direct methods in practice. For a time domain simulation, the initial solution for each equation is the value of the equation of the last time step. In this way it was found that on average 2-4 iterations were required for each equation at each time step. Only the time-zero value required a significant number of iterations. In contrast, for the same conditions, a Gaussian elimination method takes the equivalent time of about 20 iterations. This is much faster for the time-zero value but much slower for the rest of the simulation!

The current continuity equation is expressed in a central difference form using the half point values surrounding the point of solution, thus,

$$\frac{dn}{dt} = \frac{J_{l+\frac{1}{2}} - J_{l-\frac{1}{2}}}{\Delta X} + \frac{J_{j+\frac{1}{2}} - J_{j-\frac{1}{2}}}{\Delta Y} \qquad (19)$$

In contrast to many other simulations, the values of J at the half points are actually calculated using $\mu_{\frac{1}{2}}$, $E_{\frac{1}{2}}$, $N_{\frac{1}{2}}$, etc. This has been seen to reduce errors arising from the second order terms ($\nabla^2 n$) and produces a more accurate and stable solution.

The continuity equations may be solved in one of two ways, either explicitly or implicitly. The time derivative term is given by,

$$\frac{dn}{dt} = \frac{n^{k+1} - n^k}{\Delta t} \qquad (20)$$

where the k superscripts denote the time step value. The continuity equations may therefore be defined by taking this forward difference in time on the left hand side and a central difference in space on the left hand side. This has the advantage that the equations are simple and the new value of n is given explicitly at each step by the old values of n and the values of J just calculated. One disadvantage is that there is a mixed order of accuracy between the forward difference in time and the central difference in space. The main disadvantage however is that there is a limit to the space and time step that can be used when a stability analysis is done on this type of equation [11]. In an effort to overcome these limitations a partially implicit Crank-Nicholson type equation is used.

$$\frac{n^{k+1} - n^{k}}{\Delta t} = \tfrac{1}{2}\left[\nabla J \left(n^{k+1}, \mu^{k}, E^{k}\right) + \nabla J \left(n^{k}, \mu^{k}, E^{k}\right) \right] \quad (21)$$

This equation is now implicit in n but totally explicit in μ and E. This allows a much wider choice of time and space steps and an improvement in stability and accuracy. If the equation were also implicit in μ and E then the whole set of equations would have to be iterated at each time step, considerably slowing down the whole simulation, with a marginal improvement in the results. Equation (21) is solved by iterative methods similar to the Poisson equation but using Successive Under Relaxation (S.U.R.) in this case.

The energy continuity equation is expanded into its numerical equivalent equations and is then solved in a method similar to the current continuity equation.

NUMERICAL PARAMETERS

In the numerical equations several parameters must be specified before the solutions may be obtained. The space step is determined by the Debye length for the material, which is in general a function of the doping density. For a TED the doping density is $\sim 10^{22}\ m^{-3}$, giving a space step of $\sim 0.1\mu m$ for a satisfactory accuracy. For reasonable stability of the simulation it was found that a time step of 0.1 pS gave good results. A larger time step may be desirable to reduce the total number of time steps required. In practice, a larger time step leads to the Poisson solver and continuity solvers taking more iterations to achieve the same accuracy, the total cpu time may therefore be greater. The mesh size used by the computer program is determined by the physical size of the device being modelled and the space step. For a 10 μm device with an epi layer thickness of ~ 2μm a mesh size of 100 x 35 was used.

SIMULATION PERFORMANCE

Using the set of numerical equations above, the time domain simulations proceeds according to figure 5.

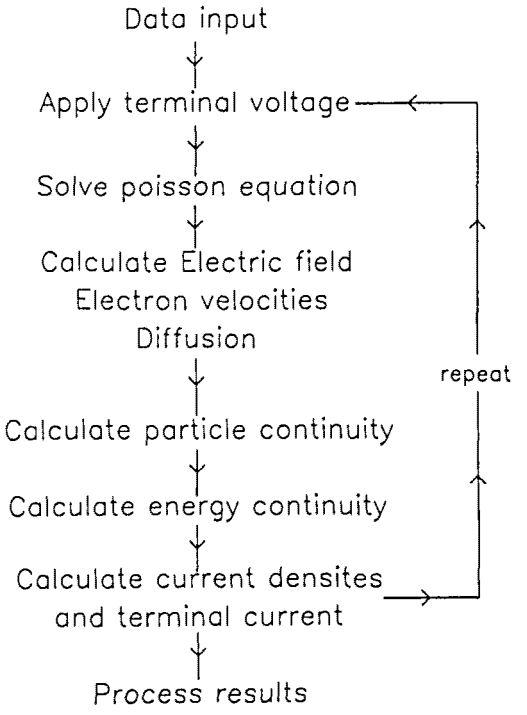


Figure 5
Flow diagram of computer simulation

The simplest solution obtained from the model is for the D.C. (steady-state) case. The simulation is run for just a few picoseconds until initial transients have died out. For some devices such as F.E.T.'s a reasonable amount of information may be derived from the d.c. characteristics. For proper device design, however, the characteristics at the frequency of operation must be used. Since the device behaviour is a non-linear function of frequency and amplitudes of the operating signal, the d.c. characteristics may only be used as a guideline. For

many other devices, the T.E.D. for example, the d.c. characteristics are of little use. To obtain more useful design information, a technique is used which involves finding the equivalent one-port admittance of the device or oscillator at the intended operating point. To obtain this information, the simulation must be run for one or more cycles at the required frequency. At 10 GHz this involves running the program for at least 100 pS and this involves at least 1000 time steps at time step of 0.1 pS. Any simulation which takes a significant amount of cpu time for each time loop is obviously going to take large computer resources for this type of problem. In order to reduce the computer time required the energy conservation equation is often omitted. Indications have been in the past that this equation does not become important until frequencies of 30 GHz or above are involved and since this is the largest equation in the set, considerable computer time will be saved by its omission. Using the set of equations presented in this paper, a computer simulation has been performed on a 10 μm planar transferred electron device. The simulation was run for several cycles at various frequencies.

The first point to note is that the velocity-field curve shown in figure 2 changes depending on the frequency at which the field is varied. Figure 6 shows the velocity field curve at various frequencies these curves are actually obtained from a solution of equations (1)-(12) at each frequency.

Built into the simulation was the ability to "switch out" the energy dependent equations. The simulation was then run at 10 GHz both with and without energy relaxation terms. Looking at the carrier distribution in the device both with and without energy relaxation, little difference may be seen (figure 7). The current voltage wave forms are shown in figure 8 and it is only by the Fourier analysis of these waveforms that the difference may be seen clearly. If the admittance is expressed as G + jB then without the energy relaxation terms a figure of -2.4 + j2.7 is obtained and with the energy relaxation terms gives a figure of -1.7 + j3.1. The figures given are in mSiemens. The operating point determined by the two methods is clearly different. The computer time taken by each method is, with the energy relaxation terms each time loop takes 0.08 seconds of c.p.u. on an Amdahl V7 computer and without these terms, each time loop takes 0.06 seconds.

The results shown here are simply an example of the fact that the energy relaxation terms do make a significant difference to device and circuit behaviour, even at 10 GHz. The practical vindication of these conclusions with the use of an F.E.T. simulation and measurements is the subject of a paper by C.Snowden also in these proceedings.

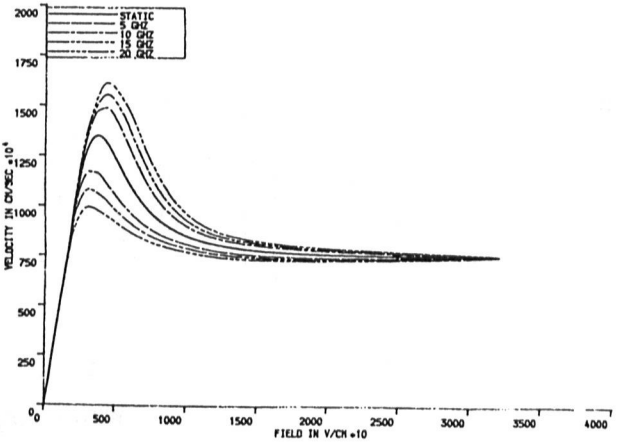


Figure 6
Velocity curves of GaAs at different frequencies

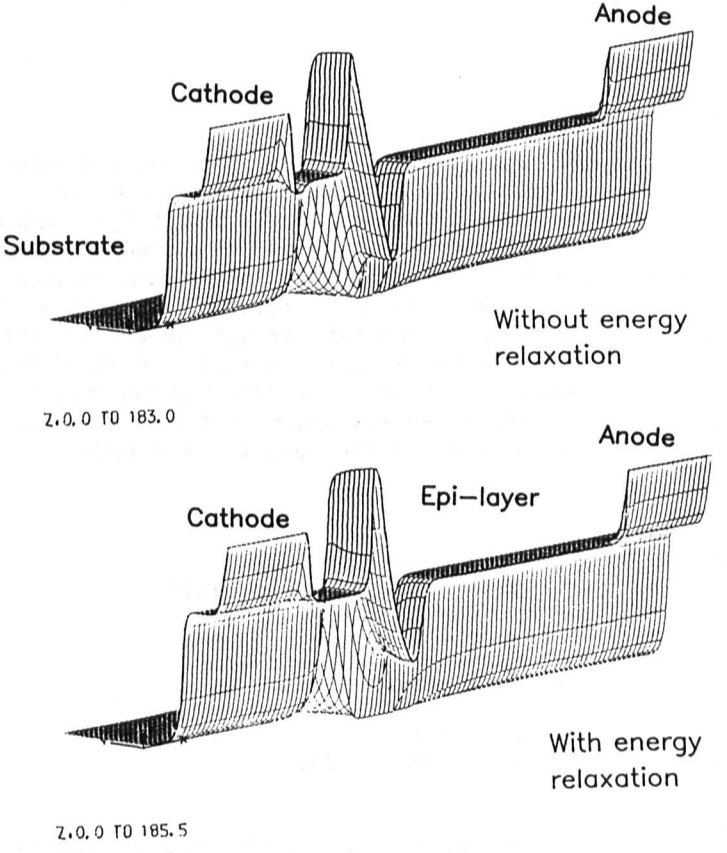
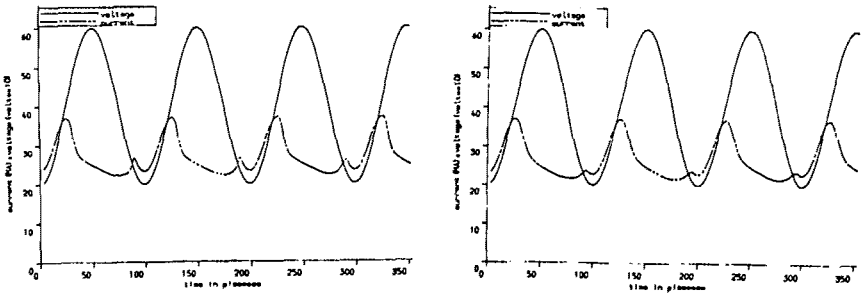


Figure 7
Carrier distributions for a planar T.E.D.



Without energy relaxation

With energy relaxation

Figure 8
Current/voltage waveforms for the T.E.D.

CONCLUSIONS

An efficient computer simulation has been produced to model devices operating at microwave frequencies as well as steady-state. The model is slower than circuit type models but much more accurate and flexible. It is less accurate than more exact Boltzmann equation solutions, but efficient enough to be used to model complete devices and integrated circuits. It has been found necessary to incorporate energy dependent terms in the model since these effects have proved to be significant at microwave frequencies. Even at d.c. the characteristics were modified by the energy dependent terms and the simulation was found to more accurately model the device behaviour.

REFERENCES

1. Lebwohl, P A and Price, P
J, Appl. Phys. Lett., Vol-19, p 530, 1971.

2. Rees, H D,
J Phys. C., Vol 6, p 262, 1973.

3. Jones, D J and Rees, H D,
J.Phys. C., Vol 6, p 1781, 1973.

4. Carrol, J E,
"Hot Electron Microwave Generators", Edward Arnold (Publishers), 1970.

5. Reiser, M,
"Large Scale Numerical Simulation in Semiconductor Device Modelling", Comp. Meth. Appl. Mech. Eng., Vol 1, p 17, 1972.

6. Reiser, M,
"A Two Dimensional Numerical FET Model for DC, AC and Large Signal Analysis", IEEE Trans. Electron Devices, Vol ED-20, No 1, p 35, 1973.

7 Snowden, C M, Doades, G P, Howes, M J and Morgan, D V,
"Two Terminal Characterization of Microwave Monolithic Elements", Proc. 11th European Microwave Conference, Microwave Exhibitions and Publishers Ltd, Kent, England, p 633, 1981

8 Stratton, R,
"The Influence of Interelectronic Collisions on Conduction and Breakdown in Polar Crystals", Proc. Roy. Soc., A246, p 402, 1958.

9. Freeman, K R and Hobson, G S,
"The V_{FT} relation of CW Gunn Effect Devices", IEEE Trans. Electron Devices, Vol ED-19, p 62, 1972.

10 Hockney, R W,
"The Potential Calculations and Some Applications," Meth. in Comp. Phys., Vol 9, pp 133-211, 1970.

11. Gerald, C F,
"Applied Numerical Analysis", Addison-Wesley, London, 1973.