SIMULATION OF MICROWAVE AND MILLIMETER-WAVE SEMICONDUCTOR DEVICES

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Abstract

Classical, semiclassical and quantum mechanical modelling techniques suitable for simulating contemporary microwave and millimeter-wave devices are discussed. Examples of simulation results obtained using the different types of model are given for several microwave devices.

Introduction

The difficulty in representing the operation of microwave devices above 20 GHz, particularly in the non-linear regime, coupled with the desire to optimize performance, has led to increased interest in using physical models to design and improve devices. The type of physical device model used to represent a particular device depends on the nature of the dominant carrier transport mechanisms and in more complex cases the feasibility of solving the model. Many of the commercially available simulation packages utilize bipolar drift-diffusion models, suitable for devices where hot electron effects are less significant. In small-scale devices where the response time of the device approaches the energy (and momentum) relaxation times it is necessary to consider a more detailed treatment than the basic drift-diffusion schemes. The majority of microwave devices intended for operation above 10 GHz require at least an energy-transport model. In very small-scale devices and in many heterostructure devices, a self-consistent quantum-mechanical solution at the interfaces may be required.

Drift-Diffusion Models

The basic drift-diffusion equations, obtained from the time-independent Boltzmann transport equation, consist of the current continuity equations,

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla . J_n - qG \qquad \textit{for electrons} \tag{1}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla . J_p - qG \qquad \textit{for holes} \tag{2}$$

and the current density equations,

$$J_n = qn\mu_n E + qD_n \nabla.n \qquad \textit{for electrons} \tag{3}$$

$$J_p = qp\mu_p E - qD_p \nabla p \qquad \textit{for holes} \tag{4}$$

where n and p are the electron and hole densities, μ_n and μ_p are the electron and hole mobilities and q is the magnitude of the charge on the electron, G is the generation-recombination rate, E is the electric field, D_n and D_p are the electron and hole diffusion coefficients. The diffusion coefficients are usually obtained from the well known Einstein relationships, although it has been demonstrated that the anisotropic nature of compound semiconductor materials leads to diffusion coefficients which depart significantly from the Einstein relations [1]. The drift-diffusion approximation assumes that the average electron temperature throughout the device is fixed at the lattice temperature (T_0, corresponding to the equilibrium energy).

The Poisson equation is solved to obtain the electric field and potential distribution. In the case of homogeneous structures, the Poisson equation simplifies to,

$$\nabla.E = -\nabla^2\psi = \frac{q}{\epsilon_0\epsilon_r}\left(N_D^+ - n + p - N_A^-\right) \tag{5}$$

where ψ is the electrostatic potential, N_D^+ and N_A^- are the ionized donor and acceptor doping densities, ϵ_0 is the permittivity of free space and ϵ_r is the relative permittivity of the semiconductor. In many microwave devices trapping effects are important, modifying both the DC and RF characteristics. In these circumstances it is necessary to include terms in the Poisson and continuity equations which account for trap filling and dynamic charge associated with these trapping centres.

It should be noted that in the case of heterostructure devices, where the material parameters are a function of position and composition (mole fraction x), the Poisson and current density equations are written as,

$$\nabla.E = -\nabla^2\psi = \frac{q}{\epsilon_0\epsilon_r}\left(N_D^+ - n + p - N_A^-\right) - \frac{1}{\epsilon_0\epsilon_r}\nabla\epsilon_0\epsilon_r.\nabla\psi \tag{6}$$

$$J_n = \mu_n n\left(qE - \nabla\chi + \frac{kT}{n}\nabla n - \frac{kT}{N_c}\nabla N_c\right) \tag{7}$$

$$J_p = \mu_p\left(qE - \nabla\chi - \nabla E_g + \frac{kT}{p}\nabla p - \frac{kT}{N_v}\nabla N_v\right) \tag{8}$$

where χ is the electron affinity, N_c and N_v are the conduction and valance band density of states respectively. The electron affinity, density of states and energy band gap E_g are all functions of mole fraction x (see for example [2]).

Unipolar devices, such as MESFETs, are often modelled using a reduced set of the transport equations, considering only the electron continuity and current density equations (eg [3,4]). This is often adequate for normal operating conditions, but cannot be used to consider breakdown or devices with lightly doped p-type buffer layers below the active layer. Bipolar devices naturally require a full solution of both electron and hole transport equations, together with a suitable treatment of generation and recombination. Other microwave devices which operate with high levels of impact ionization, such as IMPATT devices, also require detailed generation-recombination models.

Non-Stationary Transport

The high electric fields present in the small structures used in microwave devices causes substantial electron heating, and the carriers attain very high energies relative to the equilibrium levels. In these circumstances the carriers experience non-stationary transport conditions and their velocity may transiently exceed the equilibrium value. There are two general approaches to modelling small-scale devices. These are Monte Carlo simulation techniques and simulations based on hydrodynamic equations derived from the Boltzmann transport equation. A useful assessment of the relative merits of the various hydrodynamic approximations is given in [5].

The full set of hydrodynamic equations which describe non-stationary transport for electrons are,

particle (current) conservation,

$$\frac{\partial n}{\partial t} + \nabla(n\boldsymbol{v}) = 0 \tag{9}$$

momentum conservation,

$$\frac{\partial \boldsymbol{v}}{\partial t} = -\frac{q\boldsymbol{E}}{m*(w)} - \frac{2}{3m*(w)n}\nabla(nw) - \boldsymbol{v}\nabla\boldsymbol{v} + \frac{1}{3n}\nabla(m*(w)v^2) - \frac{\boldsymbol{v}}{\tau_m(w)} \tag{10}$$

energy conservation

$$\frac{\partial w}{\partial t} = -q\boldsymbol{v}\boldsymbol{E} - \boldsymbol{v}\nabla w - \frac{2}{3n}\nabla\left[n\boldsymbol{v}\left(w - \frac{m*(w)}{2}v^2\right)\right] - \frac{w - w_0}{\tau_w(w)} \tag{11}$$

where the average electron energy w is given by,

$$w = \frac{1}{2}m*(w)v^2 + \frac{3}{2}kT_e \tag{12}$$

and $m^*(w)$, $\tau_w(w)$ and $\tau_m(w)$ are the average effective mass and the effective energy and momentum relaxation times, T_e is the electron temperature. The parameters $m^*(w)$, $\tau_w(w)$, $\tau_m(w)$, and the equilibrium velocity v_{ss} are all determined from their relationship with the steady-state electric field E_{ss} obtained from Monte Carlo simulations [2,5].

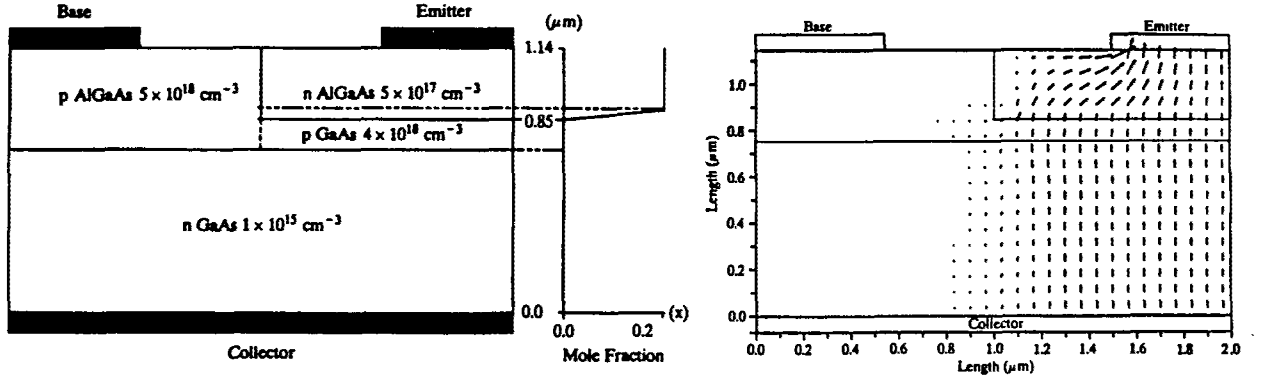

Figure 1. Heterojunction bipolar transistor simulation results, showing current flow in a graded base structure, using a drift-diffusion model with finite-difference discretization.

The characteristics of most semiconductor devices are strongly temperature dependent, yet the majority of simulations assume that the device is at a constant lattice temperature, usually room temperature (300K). A rigorous thermal model requires the solution of the heat flow equation. An example of results obtained for a sub-micron gate length GaAs MESFET simulation incorporating a detailed non-stationary model and thermal modelling is shown in Figure 1. A finite-element discretization was used in this simulation

A further simplification of the full set of hydrodynamic equations leads to the energy-transport model. Here momentum and energy conservation equations reduce to the following forms,

$$v = \frac{\tau_m(w)}{m*(w)}\left(-qE - \frac{2}{3}\nabla w - \frac{2w}{3n}\nabla n \right) \tag{13}$$

$$\frac{\partial w}{\partial t} = -qvE - v\nabla w - \frac{2}{3n}\nabla(nwv) - \frac{w - w_0}{\tau_w(w)} \tag{14}$$

Quantum Mechanical Models

Many contemporary microwave devices, such as HEMTs and RTDs, utilise structures which exhibit quantization of energy levels. In these devices it is sometimes necessary to obtain a quantum mechanical solution for the electron density and potential distribution, requiring a self-consistent solution of the Poisson and Schrödinger equations [6]. This is usually attempted in one-dimension, solving,

$$\frac{\partial}{\partial x}\left(\epsilon_r \frac{\partial V}{\partial x}\right) + \frac{q}{\epsilon_0}\left(N_D^+ - n + p - N_a^-\right) = 0 \qquad \textit{Poisson's Equation} \tag{15}$$

$$-\frac{h^2}{8\pi^2}\frac{\partial}{\partial x}\left(\frac{1}{m*}\frac{\partial \psi_n}{\partial x}\right) + (V_{tot} - E_n)\psi_n = 0 \qquad \textit{Schrödinger's Equation} \tag{16}$$

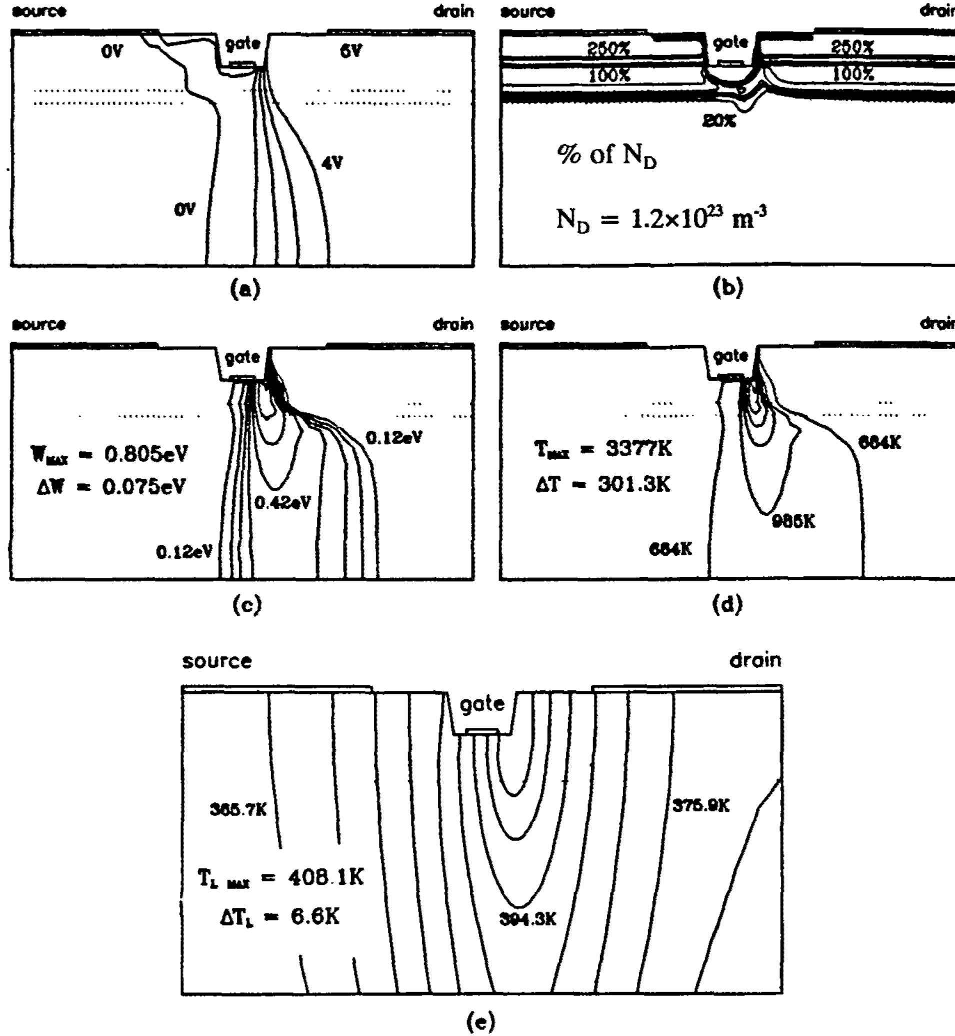

Figure 2. Simulation results for a 0.5 micron gate length GaAs MESFET using a full non-stationary model and including a thermal model based on the heat flow equation. (a) potential (b) electron density (c) electron average energy (d) electron temperature (e) lattice temperature contours.

and the two-dimensional electron gas density associated with quantized energy levels shown in Figure 3 is obtained from,

$$n_{2d} = \frac{4\pi m^* kT}{h^2} \sum_n |\psi_n|^2 \ln\left[1 + \exp\left(\frac{E_F - E_n}{kT}\right)\right] \tag{17}$$

where ψ_n is the wave function corresponding to sub-band n, E_n is the energy at the bottom of sub-band n, and V_{tot} is the sum of the electrostatic potential and exchange correlation potential. Figure 3 shows the conduction band profile, quantized energy levels and electron density for a multi-channel HEMT profile. In many small-scale structures a treatment based on Fermi-Dirac statistics has been found to provide an adequate model. It is found that for simple structures quantum mechanical simulation tends to 'smooth' the conduction band profile compared with results obtained from models based on Fermi-Dirac statistics.

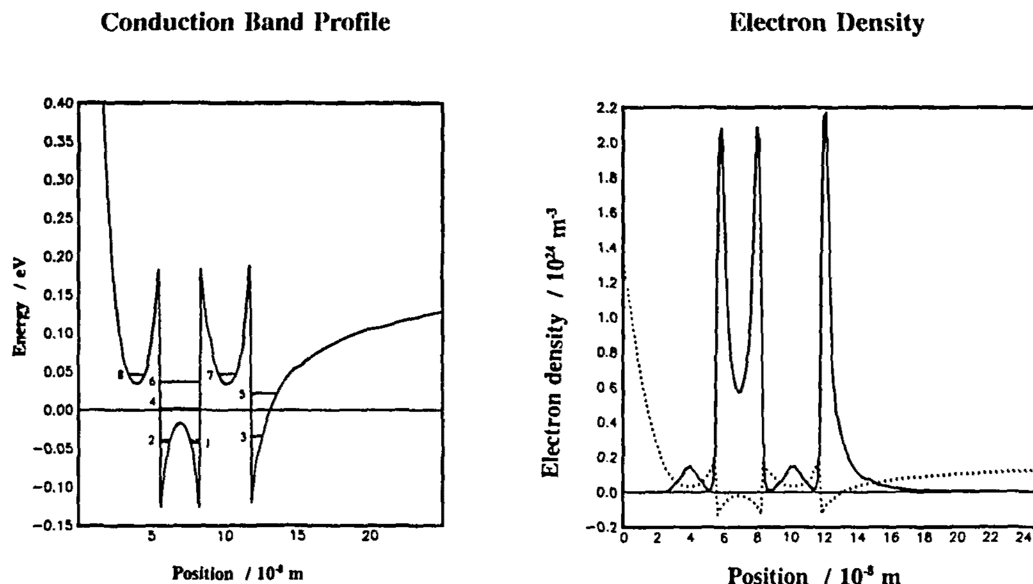

Figure 3. *Conduction band profile showing quantized energy-levels and electron density for a multi-channel HEMT profile obtained from a quantum mechanical model.*

Conclusions

This paper provides a brief summary of physical models available for modelling contemporary microwave and millimeter wave structures.

References

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