Three–Dimensional Simulation of $Al_xGa_{1-x}As$/GaAs Gradual Heterojunction Bipolar Transistor

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ABSTRACT

In this work we present the results of the simulation of $Al_xGa_{1-x}As$/GaAs gradual heterojunction bipolar transistor using a parallel three–dimensional semiconductor device simulator. This simulator is based on drift–diffusion transport model. In order to solve the systems of linear equations we have tested different methods of domain decomposition, which present great advantages as opposed to the classic methods, as regards to speed and memory requirements. One considerable advantage of the simulator is that it has been implemented using C and Fortran together with the standard MPI message passing library, so obtaining a portable parallel code for the majority of current architectures. We have shown measures of the parallel execution time and different electrical results.

Keywords: simulation, parallel, solvers, finite element and Gradual HBT.

1 INTRODUCTION

Computer–aided numerical simulation has become an indispensable tool in design and optimisation of semiconductor devices. In this work we have development a simulator based on drift–diffusion transport model using Fermi–Dirac statistics. We have applied this simulator to $Al_xGa_{1-x}As$/GaAs gradual heterojunction bipolar transistor (HBT). Unlike conventional silicon bipolar transistors, a wide energy bandgap emitter is used in HBTs to minimize hole injection from the base and maintain high levels of emitter injection efficiency. The doping concentrations in the base and emitter can thus be optimised for low base resistance and capacitance and the base can be made thinner to reduce transit time and improve high frequency performance.

We have used the finite element method (FEM) in our simulator in order to discretize the Poisson equation, and hole and electron continuity equations in stationary state. The properties of the resulting linear systems and their high range make it necessary to find adequate solvers, as classic methods, such as incomplete factorizations, are highly inefficient. We have used a library of parallel sparse iterative solvers, called PSPARSLIB [1] to solve these linear systems in parallel. A great advantage of this library is that it is optimised for several powerful multicomputers. Using this library, we have studied various domain decomposition methods in order to solve these systems [2]. The possibility of being able to execute the simulator in parallel allows a considerable reduction in the time that is necessary in order to obtain the solution of the simulation, which is a great advantage over sequential simulators.

In the next section we present a description of the three–dimensional parallel simulator, focusing on the physical model and numerical solvers, which we have studied to solve the associated linear systems. Then, in the section 3, results of the simulation of a gradual $Al_xGa_{1-x}As$/GaAs HBT are shown. In the final section, the main conclusions of this work are presented.

2 DESCRIPTION OF THE THREE–DIMENSIONAL PARALLEL SIMULATOR

Our simulator is based on drift–diffusion transport model. Using this model Poisson, electron and hole continuity equations have to be solved in the bulk semiconductor region. These equations can be written in a stationary state as [3], [4]:

$$div(\varepsilon\nabla\psi) = -q(p - n + N_{\rm D}^{+} - N_{\rm A}^{-}) \quad (1)$$

$$div(J_{\rm n}) = qR \quad (2)$$

$$div(J_{\rm p}) = -qR \quad (3)$$

where ψ is the electrostatic potential, q is the electron charge, ε is the dielectric constant of the material, n and p are the electron and hole densities, $N_{\rm D}^{+}$ and $N_{\rm A}^{+}$ are the doping effective concentrations, and $J_{\rm n}$ and $J_{\rm p}$ are the electron and hole current densities, respectively. The term R represents the volume recombination term, taking into account Schokley–Read–Hall, Auger and band–to–band recombination mechanisms [5].

The carrier currents are controlled by drift–diffusion mechanisms, and may be expressed by:

$$J_{\rm n} = -q\mu_{\rm n} n \nabla(\phi_{\rm n}) \quad (4)$$

$$J_{\rm p} = -q\mu_{\rm p} p \nabla(\phi_{\rm p}) \quad (5)$$

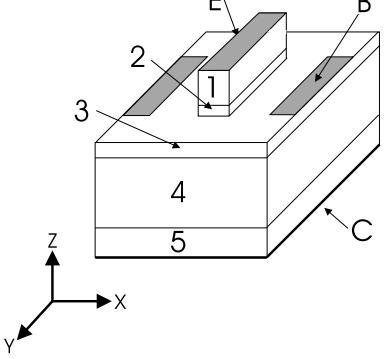

Figure 1: Structure of Transistor

where $\mu_{\rm n}$ and $\mu_{\rm p}$ are the mobilities of electrons and holes, and $\phi_{\rm n}$ and $\phi_{\rm p}$ are the quasi–Fermi potentials of electrons and holes.

Assuming a single parabolic conduction band, the electron and hole density can be expressed as [6]:

$$n = n_{\rm ien} \exp\left(\frac{q\psi - q\phi_{\rm n}}{kT}\right) \tag{6}$$

$$p = n_{\rm iep} \exp\left(\frac{q\phi_{\rm p} - q\psi}{kT}\right) \tag{7}$$

where $n_{\rm ien}$ and $n_{\rm iep}$ are the intrinsic carrier concentrations. The formulation for carrier concentrations is simple and compact. Parameters $n_{\rm ien}$ and $n_{\rm iep}$ may include different phenomena that affect the concentrations at high doping levels: influence of Fermi–Dirac statistics, changes in the energy levels and variations in the effective densities of states.

These equations are scaled using the scaling presented in [7]. Next, the finite element method [8], [9] should be applied in order to discretise the scaled equations, thus obtaining a system of nonlinear equations, with range N, where N is the number of nodes of the

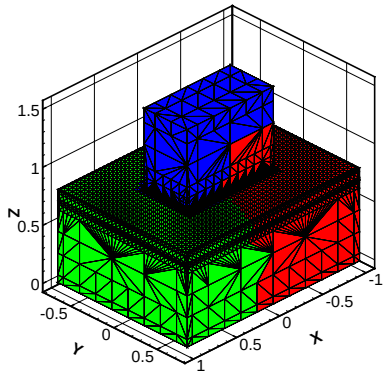

Figure 2: Mesh and partition of the transistor

discretisation [10]. However, the discretisation of J_p and J_n require particular care. It is necessary to use special schemes such as the Scharfertter–Gummel one [7].

We have applied QMG package to generate the tetrahedral meshes [11]. That software can generate finite element meshes in two and three dimensions. We use the three dimensional mesh generator which it is based on octree algorithm. We have shown the structure of the transistor we have simulated in figure 1, and the mesh with 26411 nodes and 142358 elements we have obtained in figure 2. We have used a mesh grading control function to place small tetrahedral near of interface between different region where the values of the simulation change very quick. If a mesh refinement is necessary, it is possible to use a routine which subdivides every tetrahedron into eight smaller tetrahedra.

2.1 Numerical Solvers

The part relating to the resolution of linear systems is the one that uses the most computational time, above all in the three-dimensional case in which the dimensions of the associated linear systems are very high. Amongst the different types of iterative methods that exist we have implemented domain decomposition methods in our simulator.

In order to be able to apply these techniques it is necessary to partition the mesh into subdomains. We have selected Metis program to partition the mesh because it provides high quality partitions, it is extremely fast, and it provides low fill orderings. In the first place, we use it to divide the mesh in p parts to execute our simulator and to solve the associated linear systems on a parallel computer. The main problem is to partition the vertices of a graph in p roughly parts, such that the number of edges connecting vertices in different parts is minimized. The algorithms in Metis are based on multilevel graph partitioning [12]. We have indicated a mesh of the transistor in 3 subdomains in figure 2 using different colours. Also, we have used a Metis function in our simulator to compute fill reducing orderings which is based on the multilevel nested dissection algorithm.

Then, we have used the library of parallel sparse iterative solvers, called PSPARSLIB to solve these linear systems in parallel. The preconditioners provided with the library encompass a number of "standard" options for preconditioning distributed sparse matrices, such as overlapping block Jacobi (overlapping additive Schwarz), multicolor block SOR (overlapping multicolor multiplicative Schwarz), Schur complement techniques, distributed ILU(0), approximate inverse preconditioners, etc. A great advantage of this library is that it is optimised for several powerful multicomputers, and it has been tested on the CM5, CRAY–T3D, CRAY T3E, Convex Exemplar, IBM SP2, IBM and SGI workstation clusters. We have tested some of these solvers, and in

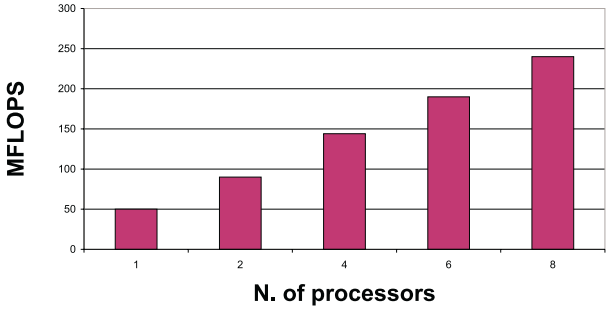

Figure 3: Parallel performance for the gradual heterojunction transistor

general the best results were obtained using Schur combined with ILU preconditioner [2].

3 RESULTS

We have applied the simulator to a device with a gradual heterojunction of $Al_xGa_{1-x}As/GaAs$ [13]. It has five zones: the sub–collector (SC), the collector (C), the base (B), the gradded–emitter (GE) and the emitter (E) as it is showing in figure 1. The aluminium mole fraction changes from 0.3 to 0.0 in 1000 Å, where it reaches the emitter–base junction. The doping profile and the dimensions of each zone are shown in table 1 and table 2.

The simulator was developed for distributed–memory multicomputers using the MIMD strategy (*Multiple Instruction–Multiple Data*) under the SPMD paradigm (*Single Program–Multiple Data*). It was implemented using C and Fortran together with the MPI (*Message Passing Interface*) message passing standard library [14]. The main advantage of using this library is that it is presently implemented in many computers, which guarantees the portability of the code. A CRAY T3E distributed memory multicomputer was used to simulate these devices. This computer is a very powerful and flexible parallel scalable system. It comprises up to 2,048 processors connected by a wide bandwidth bidirectional 3–D torus network. Using this computer we have measured the number of MFLOPS (Million of Floating Point Operations Per Second) that are obtained for this gradual heterojunction bipolar transistor. The results obtained are shown in figure 3. It can be seen that the values obtained in this simulation show that the simulator obtained is scalable.

We show the different values that were attained for current density in figure 4. The voltage for this gradual HBT is shown in figure 5 using $V_{BE} = 1.4\ v$. We calculated the parameters of a small signal [15], which are shown in table 3.

Table 1: Doping profile of $Al_xGa_{1-x}As/GaAs$ gradual HBT.

Zone	Region	Doping	$N_{eff}(\mathrm{cm}^{-3})$
1	Emitter	n–$Al_{0.3}Ga_{0.7}As$	$2.0{\cdot}10^{17}$
2	Graded Emitter	n–$Al_xGa_{1-x}As$	$2.0{\cdot}10^{17}$
3	Base	p–GaAs	$5.0{\cdot}10^{18}$
4	Collector	n–GaAs	$5.0{\cdot}10^{16}$
5	Sub–collector	n–GaAs	$2.0{\cdot}10^{17}$

4 CONCLUSIONS AND FUTURE WORK

In this work we have presented the simulation of an $Al_xGa_{1-x}As/GaAs$ gradual heterojunction bipolar transistor (HBT) using a three-dimensional parallel simulator of bipolar devices. This simulator is based on drift–diffusion transport model, and the equations of which are discretized by using the finite elements method (FEM). Fermi–Dirac statistics is considered in our model and a compact formulation is used that makes it easy to take into account other effects such as the non–parabolic nature of the bands or the presence of various subbands in the conduction process.

The program was implemented using C, Fortran and the message passing interface library MPI, due to which we have obtained a portable parallel code in the majority of current architectures, which is a great advantage over sequential simulators. All the data were measured on a CRAY T3E distributed–memory multicomputer. We have applied the simulator to a gradual heterojunction of $Al_xGa_{1-x}As/GaAs$, and we have given the different values that were attained for small signal parameters and current densities.

As future work, we are going to simulate other gradual HBTs, and we are going to implement a new numerical algorithms in our simulator to study abrupt HBT.

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Table 2: Dimensions of $Al_xGa_{1-x}As/GaAs$ gradual HBT.

Region	Δ X(μm)	Δ Y(μm)	Δ Z(μm)
Emitter	1.0	0.5	0.6
Graded Emitter	1.0	0.5	0.1
Base	2.0	1.5	0.1
Collector	2.0	1.5	0.5
Sub–collector	2.0	1.5	0.2

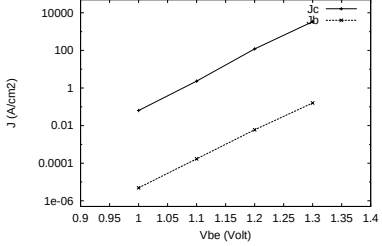

Figure 4: Collector and Base current densities

Table 3: Parameters of small signal for the gradual HBT

	V_{BE} (V)	
	1.4	1.5
g_m *(A/V)*	$6.4 \cdot 10^{-02}$	$2.2 \cdot 10^{-02}$
C_T *(F)*	$7.5 \cdot 10^{-14}$	$4.8 \cdot 10^{-14}$
f_T *(Hz)*	$7.2 \cdot 10^{+10}$	$1.3 \cdot 10^{+11}$
τ_{EC} *(seg.)*	$2.1 \cdot 10^{-12}$	$1.1 \cdot 10^{-12}$

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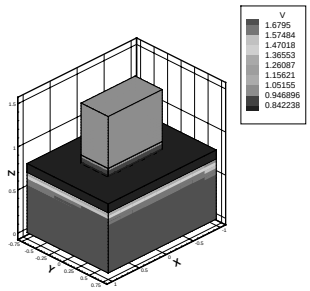

Figure 5: Voltage

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