# 3D Numerical Modeling of Continuity Equations for Abrupt HBTs at the Heterojunction Interface

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## Summary

In this work we have developed a numerical modeling of the continuity equations for 3D numerical simulation of abrupt heterojunction bipolar transistors (HBT). For this class of transistors it is necessary to take into account that on both sides of the interface between the different regions of HBT devices exist materials with different properties. It implies the standard discretization methods, as FEM or finite differences, can not applied directly. We have applied our modeling combined with the finite element method (FEM), making a specific formulation for the nodes located on the interface of the regions with different characteristics. This way, the effects due to thermionic emission and the tunnel effect may be simulated when these equations are solved in an abrupt HBT.


## Introduction

Heterojunction bipolar transistors (HBTs) are nowadays an active area of research due to interest in their high–speed electronic circuit applications [1]. The main characteristic of bipolar transistors with an abrupt heterojunction is a discontinuity in the energy bands at the emitter–base interface [2]. Development of numerical models for HBTs is essential for a better understanding of their physical behavior and to design optimization, and it is currently an important research area. The first programs enabled one-dimensional simulations to be carried out. Nevertheless, with the reduction of the physical dimensions of the devices to be simulated, the need for carrying out 3D simulations in order to be able to study the diverse factors that affect the devices in a more precise manner has become evident.

Conventional simulators of homojunction and gradual heterojunction bipolar transistors are based on drift–diffusion carrier transport. This model is not valid for abrupt HBTs, since the current through the energy spike formed at the emitter–base interface is controlled by thermionic emission and tunneling transmission [3][4]. Furthermore, HBTs have a very highly doped base region in order to improve their high–frequency performance, and it is therefore necessary to include the Fermi–Dirac statistics [5]. In this paper we propose a new formulation for the electron and hole continuity equations at the heterojunction interface to study these devices combined with finite element method. Commercial programms, like Silvaco, Apsys, etc. do not use this aproximation. Using this model heterojunction bipolar transistors may be simulated using several dimensions, included the thermionic emission and the tunnel effect.

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**Modeling and Simulation of Abrupt HBTs**

For studying electrical behavior of an heterojunction bipolar transistor, the basic equations to be solved are Poisson and electron and hole continuity equations, in a stationary state. In a previous work we have developed a model for Poisson equation [6]. The model described here is a further generalization of that work to study continuity equations.

In all the regions of the device, except at the emitter–base interface, the carrier currents are controlled by drift–diffusion mechanisms, and may be expressed by:

$$J_n = -q\mu_n n\nabla(\phi_n), \qquad J_p = -q\mu_p p\nabla(\phi_p) \tag{1}$$

where $q$ is the electronic charge, $n$ and $p$ are the electron and hole densities, $\mu_n$ and $\mu_p$ are the mobilities of electrons and holes, and $\phi_n$ and $\phi_p$ the quasi–Fermi potentials.

The charge transport through an abrupt discontinuity is based on Grinberg's model [4], which includes tunneling transmission through the spike and thermionic emission over it. The electron current density through the spike in the conduction band is expressed as:

$$J_n = -q\nu_{neff}\left(\frac{N_{cB}}{N_{cE}}n(z_j^+) - n(z_j^-)e^{-\frac{\Delta E_c}{kT}}\right) \tag{2}$$

where $\Delta E_c$ is the discontinuity in level $E_c$ in the heterojunction interface, $N_{cB}$ and $N_{cE}$ are the effective density of states in the conduction band in both regions, $z_j^-$ and $z_j^+$ are the two sides of the emitter–base interface and $v_{neff}$ is the effective electron velocity through the interface, which is expressed as:

$$\nu_{neff} = \sqrt{\frac{kT}{2\pi m_B^*}}(1 + p_t) \tag{3}$$

where $p_t$ is the tunneling factor through the spike and $m_B^*$ is the effective electron mass in the region of base. Expressions similar to 2 and 3 apply for the holes current in the valence band through the interface.

These equations are scaled using the scaling presented in [7]. Next, the finite element method should be applied in order to discretise the scaled equations, thus obtaining a system of nonlinear equations, using Scharfertter–Gummel schemes. This new formulation is based on a previous 1D model developed using finite differences [2][3]. The finite–element approach is more useful than the finite–difference method for obtaining solutions for non rectangular, irregularly shaped device geometries, where its inherent flexibility can lead to a more efficient solution than the one that can be obtained using the finite–difference method [8]. Nevertheless, in the case of abrupt HBTs, this method cannot be applied directly, as the properties of the material of the different regions that form abrupt HBT transistors are different. To avoid this problem, we have introduced a modified mesh, which is

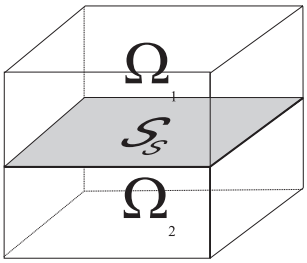


Figure 1: Structure formed by two different materials

characterized by the fact that we have separated the nodes that belong to each region of the HBT. In this way we have two nodes in the same physical position belonging to different regions and each element belonging to a single region.

In order to simplify the analysis, we can consider a 3D volume $\Omega$ formed by 2 regions $\Omega_1$ and $\Omega_2$ with different properties, and a common surface $S_S$, as the one shown in the Figure 1. The scaled and simplified hole continuity equation with boundary conditions we have to solve in the whole domain $\Omega$ is:

$$\nabla J_p(\phi_p(r)) = -R(\phi_p(r)) \qquad r \in \Omega \tag{4}$$

$$p|_{\partial\Omega_D} = p_{eq} \tag{5}$$

$$\left.\frac{\partial p}{\partial \nu}\right|_{\partial\Omega_N} = 0 \tag{6}$$

where $p_{eq}$ is the hole concentration in equilibrium, $\nu$ represents the unit normal vector, and the boundary $\partial\Omega$ splits into "Neumann segments", $\partial\Omega_N$, and "Dirichlet segments" $\partial\Omega_D$ with $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$ and $\partial\Omega_D \cap \partial\Omega_N = \phi$.

As the equations must verify themselves in each region we can restrict the potential function $\phi_p$ to the subdomains $\Omega_1$ and $\Omega_2$, such as is verified that,

$$(\phi_p^1, \phi_p^2) \in H^1_{\Gamma_{D1}}(\Omega_1) \times H^1_{\Gamma_{D2}}(\Omega_2) \tag{7}$$

$$\phi^1_{p|\Gamma_{D1}} - \phi^2_{p|\Gamma_{D2}} = h \tag{8}$$

where $H^1_{\Gamma_{Di}}(\Omega_i)$ is a subset of functions in $H^1_0$(Sobolev class), whose functions are not null on the $\Gamma_{Di}$ boundary, with $\Gamma_{Di} = (\partial\Omega_1 \cap \partial\Omega_2)_{|\Omega_i}$, and $h$ is a specific function.

The mesh that we have used is adapted perfectly to this situation. The equations for each regions are:

$$\nabla J_p(\phi_p^1(r)) = -R(\phi_p^1(r)) \qquad r \in \Omega_1 \tag{9}$$

$$\nabla J_p(\phi_p^2(r)) = -R(\phi_p^2(r)) \qquad r \in \Omega_2 \tag{10}$$

Based on this formulation and considering the physicals characteristics of the hole current densities, we can deduce the conditions that must be verified on the interface points:

$$(J_p|_{\Gamma_{D1}})|_z = J_p^{\text{et}} \tag{11}$$

$$\int_{\Omega_1} J_p \nabla \xi dV + \int_{\Omega_2} J_p \nabla \xi dV - \int_{\Omega} R\xi dV = 0 \tag{12}$$

where in the equation 11 the term $(J_p|_{\Gamma_{D1}})|_z$ indicates the $z$ component of the hole current density in $\Omega_1$ region on the $\Gamma_{D1}$ boundary, and $J_p^{\text{et}}$ is the hole current density due to the thermionic emission. This expression can be written as,

$$J_p^{\text{et}} = q\nu_{\text{peff}} \left( \frac{N_{v2}}{N_{v1}} p(z_j^-) - p(z_j^+) e^{-\frac{\Delta E_v}{KT}} \right) \tag{13}$$

It is possible to use a similar procedure with the electron current density. The interface nodes must be verified,

$$(J_n|_{\Gamma_{D1}})|_z = J_n^{\text{fet}} \tag{14}$$

$$\int_{\Omega_1} J_n \nabla \xi dV + \int_{\Omega_2} J_n \nabla \xi dV + \int_{\Omega} R\xi dV = 0 \tag{15}$$

where $(J_n|_{\Gamma_{D1}})|_z$ is the $z$ component of electron current density in $\Omega_1$ on the boundary $\Gamma_{D1}$, and $J_n^{\text{fet}}$ is the electron current density due to the thermionic emission and tunnel effect, it can be expressed as,

$$J_n^{\text{fet}} = -q\nu_{\text{neff}} \left( \frac{N_{c2}}{N_{c1}} n(z_j^-) - n(z_j^+) e^{-\frac{\Delta E_c}{KT}} \right) \tag{16}$$

## Parallel Implementation and Numerical Results

Our simulator was developed for distributed–memory multicomputers, using the MIMD strategy (*Multiple Instruction–Multiple Data*) under the SPMD paradigm (*Simple Program–Multiple Data*). Our program was implemented using the MPI message passing standard library [9]. The main advantage of using this library is that it is presently implemented in many computers, and this guarantees the portability of the code.

Poisson and continuity equations are discretized using the FEM with this new specific formulation, as we have explained in the previous section. We have obtained a set of $N$

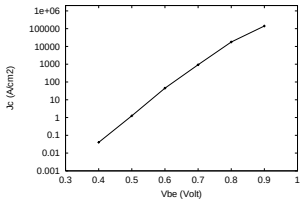


Figure 2: Collector current density for InP/InGaAs HBT

nonlinear equations that is necessary to linearize and solve. With the purpose of linearizing the previous assembly set of equations, we have applied a modified iterative Newton method. The coefficient matrices of these systems have a high rank,high sparse, very badly conditioned and not diagonally dominant due mainly to the equations that we have had to introduce in the interface nodes. To solve these problems we have used domain decomposition techniques. In order to be able to apply these techniques it is necessary to implement a partitioning of the mesh into subdomains for which we have used the METIS program [10]. This program is an unstructured graph partitioning and a sparse matrix ordering system.

We have used a library of parallel sparse iterative solvers to solve these linear systems in parallel [11]. The library consists of four major components, accelerators, preprocessing tools, preconditioning routines, and message–passing tools. The accelerators are based on Krylov subspace methods. These methods often work poorly without preconditioning. The preconditioners provided with the library encompass a number of 'standard' options for preconditioning distributed sparse matrices, such as additive Schwarz, multicolor block SOR (overlapping multicolor multiplicative Schwarz), distributed ILU(0), approximate inverse preconditioners,etc. A great advantage of this library is that it is optimized for several powerful multicomputers. Using MPI library, our program was tested on various platforms such as the CRAY–T3E, a SUN clusters of workstations, the SGI Origin 2000, and Beowulf cluster. With this library we have studied several domain decomposition techniques and solvers. In domain decomposition methods the equations are solved by means of a succession of solutions of local residual equations at each step. Also, we have tested several preconditioners and the best results were obtained with the Additive Schwarz and Schur complement methods. We have applied our simulator to a HBT transistor [12]. We have used a nonstructurated tetrahedral mesh to simulate this device. The obtained collector current density, is shown in Figure 2, and it is close to the experimental results.

## Conclusions

In this work, we have developed a new formulation of electron and hole continuity equations on the heterojunction interface. This model can be combined with finite element method, and, in this way it is possible simulate abrupt HBT using multidimensional models.

In order to solve systems of linear equations, which is the most CPU time–consuming part of the program, we have implemented a parallel simulator and we have tested different

methods of domain decomposition, which present great advantages as opposed to the classic methods as regards speed and memory requirements. We have subsequently selected the best ones to implemented in the simulator. The parallel code was implemented and tested using the message passing interface library MPI on several platforms.

We have applied our model, and we have simulated a InP/InGaAs HBT using three–dimensional numerical simulator. This model combines the drift–diffusion transport model on the bulk on the semiconductor device with the thermionic emission and tunnel effect at the heterojunction interface of abrupt HBT using finite element method.

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