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Two Dimensional Numerical Simulator for Modeling NDC Region in SNDC Devices

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Abstract. This paper deals about making a numerical simulator for observing the self-organization phenomenon like current filament formation in the negative differential conductivity (NDC) region of operation in a device using MATLAB environment. Emphasis is laid on choosing the appropriate boundary conditions in simulator to observe the NDC part of the device Current-Voltage ($I - V$) characteristics along with the appropriate isothermal physical models are included for mobility and the recombination-generation. The simulator used in this paper is designed to observe NDC region in S-shaped NDC (SNDC) devices like BJT and similar conditions can be used to observe the field domains in the N-shaped NDC (NNDC) devices with appropriate changes. Dirichlet and Neumann boundary conditions are applied to BJT and $I - V$ characteristics of the developed device simulator are compared with the commercial available TCAD device simulator (*i.e.*, *Sentaurus*).

1. Introduction

Detailed numerical simulation and modeling have become extremely important over the last four decades to optimize the performance and design of nano-scale semiconductor devices. It has been seen that huge number of trials are required in the experiments to optimize semiconductor device performance however it can be decimated using computer simulation for faster development cycle [1]. Numerical modeling of semiconductor devices are based on basic semiconductor equations which has been first proposed by Gummel et. al in 1964 and many papers have been published in this domain [2]. In general, the numerical simulation of the device includes a basic semiconductor physical models which describes carrier transport models in material such as: drift-diffusion, hydrodynamic etc[3]. Moreover, we solve Poisson's and continuity equations for both electron and hole, to more computationally challenging physical models such as the energy balance, which exemplifies some higher moment simplification of Boltzmann transport approximation (BTE). However, the choice of appropriate physical models are dependent on level of detail is required. In particular, semiconductor device structures whose electronic properties changes on a deep nanometer scale gives an number of examples of nonlinear transport models[4, 5]. In these devices nonlinear transport mechanisms are complex because electrical or optical properties are governed by different nonlinear dynamic processes. The electronic transport properties of a semiconductor material show up most by $I - V$ characteristic form under time-independent voltage bias conditions[4]. It has been determined in a complex manner by microscopic properties of material, which specifies the current density (J) with function of local electric field (E) and by electrodes. Under low voltage or current conditions, the relation between J and E do not always exist, however it is strongly dependent in high voltage or current conditions. Moreover,



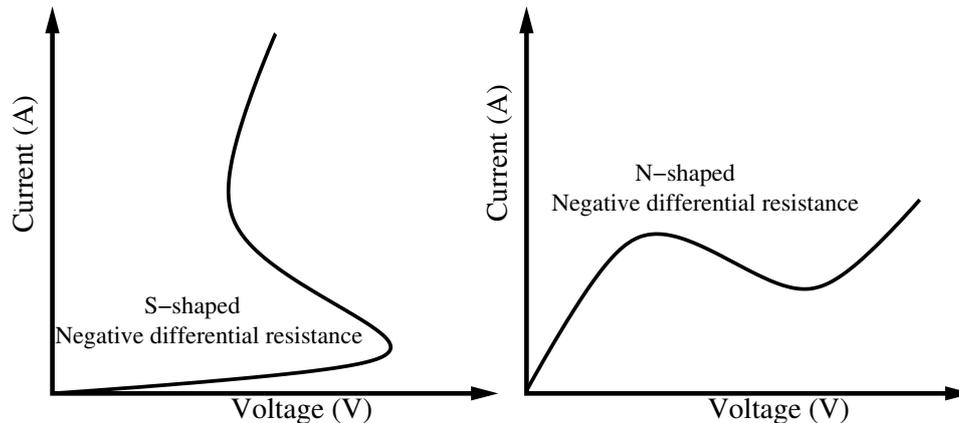


Figure 1. Typical negative differential conductivity (NDC) regions are observed in $I - V$ characteristics of the device structure under high current or voltage conditions[6].

an unstable situation has been observed when current density increases or decreases corresponds to negative differential conductivity region[6].

Two different $I - V$ characteristics of negative differential conductivity (NDC) regions have been described by S-shaped or N-shaped $J(E)$ characteristic, which have been denoted by SNDC and NNDC respectively, as shown in Figure 1. The NDC nature of the $I - V$ characteristics have been analyzed analytically and the conditions under which SNDC and NNDC curves are formed have been discussed by Scholl et al.[6]. The physics behind the formation of current filamentation in SNDC devices and Field domains in NNDC devices have also been explained[6]. There has been research work done on how to make a device simulator by solving the semiconductor equations and about the NDC operating region of the device individually but very little emphasis has been laid over the conditions to be satisfied by a simulator to observe the NDC region of the $I - V$ characteristics of a device. This paper targets at making a simulator to observe the NDC nature of the SNDC like BJT by applying appropriate boundary conditions. In this paper a generalized method is proposed to apply the appropriate boundary conditions to observe the NDC region of the $I - V$ characteristics and the same is proved by plotting the SNDC $I - V$ characteristics of a BJT. Both Neumann and Dirichlet boundary conditions are applied to the BJT and a comparison is made on choosing different boundary conditions.

The paper is organized as follows: Section II briefs flow of the proposed simulator. Furthermore, two-dimensional discretization scheme is formulated in terms of basic semiconductor equations then the boundary conditions for observing the NDC curves is discussed. Finally, the results are presented and discussed for different boundary conditions.

2. Proposed Flow of Device Simulator

The basic flow of the simulator and device structure used for simulation purpose are shown in Figure 2. The structure for which the simulator is built and boundary conditions tested is a two dimensional (2D) NPN BJT, as shown in Figure 2(b). The structure has three contacts base, emitter and collector out of which emitter and collector contacts are heavily doped n^+ regions with $N_D = 10^{20} cm^{-3}$ and base contact is heavily doped p^+ region with $N_A = 10^{19} cm^{-3}$. The collector-base junction is formed by relatively less doped collector and base regions with $N_{Dn} = 10^{16} cm^{-3}$ and $N_{Ap} = 10^{17} cm^{-3}$ respectively. The contact regions need to be heavily doped to have better contacts and lightly doped region near the junction helps in withstanding the practical levels of operating voltage not limited by tunneling effect. The proposed flow of device simulator is described below:

- (i) Using the boundary conditions as input and the matrix representation of discretized

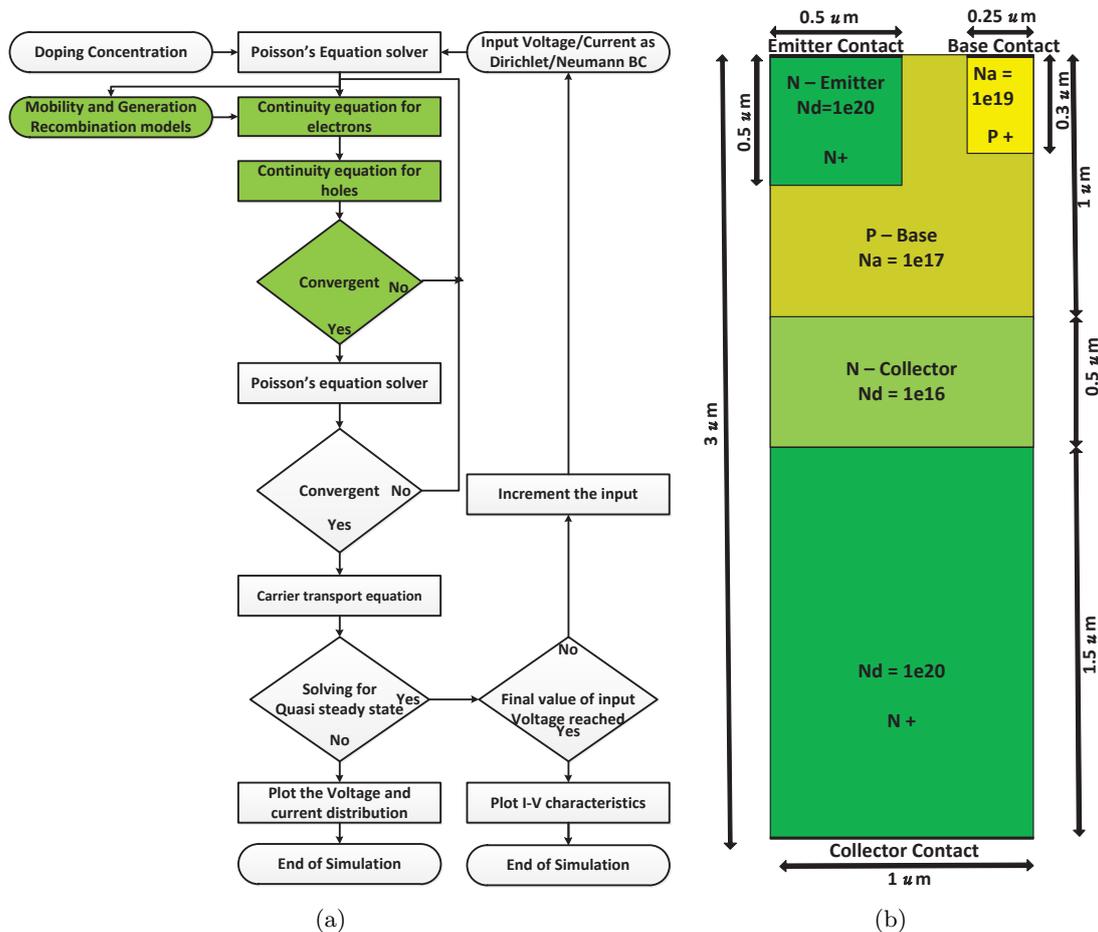


Figure 2. (a) Proposed flow of the device simulator, (b) Device under test for simulation purpose is layered BJT device structure where doping of all the regions are given.

Poisson's equation, determines the potential at every discretized node in the device structure.

- (ii) From the potential obtained in Step 1, we calculate the Electric field at every point using central difference FDM method.
- (iii) It can be seen that, as the mobility and net recombination rate are included into the continuity equations results non linear partial differential equation which cannot be solved directly by matrix method. Therefore, to solve these equations, we use Gummels iteration method [2], while solving the electron continuity equation consider hole concentration (p) as constant (equal to initial doping concentration for the first time) and calculate electron concentration (n).
- (iv) While solving the hole continuity equation consider electron concentration as a constant and equal to that obtained in step 3 and calculate the hole concentration. Now update the hole concentration, mobility and recombination rate in step 3 and repeat these two steps till convergence is reached. At this point the electron and hole concentrations are obtained will be satisfying both the continuity equations.
- (v) Substitute the electron and hole concentration obtained after convergence in step 4 into the Poissons equation and solve step 2 to step 5 until convergence is achieved. At this point the potential and carrier concentrations obtained will satisfy the Poisson's and continuity equations. Now we calculate the current density using the Drift-Diffusion equations.

- (vi) Finally we plot the I-V characteristics by increasing the input and repeat step 1 to step 5 until the final value of input is reached.

2.1. Basic Semiconductor Equations

To analyze the distribution of current density and potential inside any arbitrary semiconductor device under various operating conditions it needs to be modeled mathematically using the following equations:

- (i) Poisson's equation
- (ii) Continuity equations for electrons and holes
- (iii) Carrier transport equation for electrons and holes
- (iv) Mobility and Recombination-Generation rate

2.2. Discretization of Basic semiconductor equations

We need to discretized the basic semiconductor equations to solve them numerically. Though there are many ways of discretization of the Partial differential equations like finite element method (FEM), finite volume method (FVM) and finite difference method (FDM). However, we choose to discretized using five point Finite Difference Method owing to its simplicity and good accuracy. FDM Discretized basic semiconductor equations are:

- Poisson's equation:

$$\frac{n_d}{m_d}\psi(x+1, y) + \frac{n_d}{m_d}\psi(x-1, y) - 2\left(\frac{n_d}{m_d} + \frac{m_d}{n_d}\right) + \frac{m_d}{n_d}\psi(x, y+1) + \frac{m_d}{n_d}\psi(x, y-1) = m_d \cdot n_d \frac{q}{\epsilon}(n-p-C) \quad (1)$$

- Continuity equation for electrons:

$$n(x+1, y) \left[\frac{n_d}{m_d} - \frac{n_d}{2v_t} E_x \right] + n(x-1, y) \left[\frac{n_d}{m_d} + \frac{n_d}{2v_t} E_x \right] + n(x, y+1) \left[\frac{m_d}{n_d} - \frac{m_d}{2v_t} E_y \right] + n(x, y-1) \left[\frac{m_d}{n_d} + \frac{m_d}{2v_t} E_y \right] - n(x, y) \left[2\left(\frac{m_d}{n_d} + \frac{n_d}{m_d}\right) + temp \right] = m_d n_d \left(\frac{R(\psi, n, p)}{D_n} + \frac{1}{D_n} \frac{\partial n}{\partial t} \right) \quad (2)$$

- Continuity equation for holes:

$$p(x+1, y) \left[\frac{n_d}{m_d} + \frac{n_d}{2v_t} E_x \right] + p(x-1, y) \left[\frac{n_d}{m_d} - \frac{n_d}{2v_t} E_x \right] + p(x, y+1) \left[\frac{m_d}{n_d} + \frac{m_d}{2v_t} E_y \right] + p(x, y-1) \left[\frac{m_d}{n_d} - \frac{m_d}{2v_t} E_y \right] - p(x, y) \left[2\left(\frac{m_d}{n_d} + \frac{n_d}{m_d}\right) - temp \right] = m_d n_d \left(\frac{R(\psi, n, p)}{D_p} + \frac{1}{D_p} \frac{\partial p}{\partial t} \right) \quad (3)$$

Where

$$E_x = \frac{\partial \psi}{\partial x}; dE_x = \frac{\partial^2 \psi}{\partial x^2}; \text{ and } E_y = \frac{\partial \psi}{\partial y}; dE_y = \frac{\partial^2 \psi}{\partial y^2};$$

m_d/n_d = horizontal/vertical differential length and E_x , dE_x , E_y and dE_y in the continuity equation can be calculated using the central difference and five point discretization method.

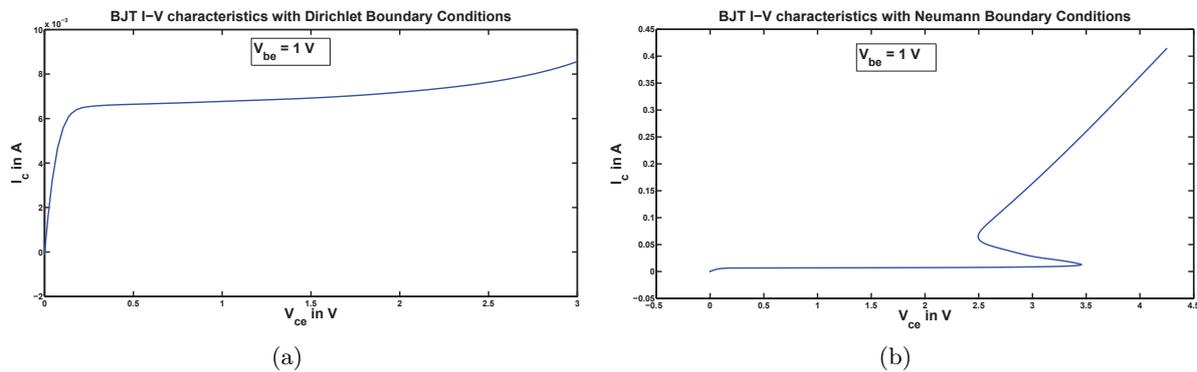


Figure 3. Proposed device simulator results when different boundary conditions are considered. (a) Dirichlet boundary conditions and voltage input are considered, (b) Neumann boundary conditions and current input are chosen.

2.3. Boundary Conditions For Observing NDC Region

Boundaries of a semiconductor device can be classified into two types such as: Physical Boundaries and Artificial Boundaries. Physical boundaries include the boundaries which physically exist like contacts and interface to the insulating material while artificial boundaries are the ones which is introduced for the purpose of simulation or calculations so that it can separate one device from the neighboring devices. Boundary conditions are mathematical conditions which are specified at the boundaries to solve the partial differential equations. In general the boundary conditions are decided by the type of contacts which is dependent on the type of the input given to the device. Broadly boundary conditions are divided as:

- Dirichlet boundary: Dirichlet boundary condition states the value of the solution parameter so that solution of the partial differential equation needs to take at the boundaries of the domain. We solve the Poissons equation with potential as the parameter and stating Dirichlet boundary condition at the boundaries which means we are fixing the value of the potential at the boundaries which is equivalent to connecting the device to a voltage source. To plot the I-V characteristics of a device with Dirichlet boundary conditions is physically equivalent to connecting the device to a variable voltage source and checking the current flowing through the device.
- Neumann boundary: Neumann boundary condition states the derivative of the of the solution parameter on the boundary of the domain that must be satisfied by the solution of the partial differential equation. Physically Neumann boundary condition is applied when you have to connect the device to a current source. When a current source is to be connected to the device it can be done in simulation terms by applying Neumann boundary conditions.

3. Results and Discussion

In the simulation it is observed that, when we apply Dirichlet boundary conditions to an SNDC device like BJT, the resulting $I-V$ characteristics are negative differential resistance as shown in Figure 3(a). But in the most cases when we use Newtons method, it doesn't converge at the first breakdown point from where the curve goes into NDC part. This is due to triggering of impact ionization in the device, which results avalanche-generated electrons and avalanche-generated holes thus current sharply increases across the terminal which results in instability in the device and does not satisfy the outer boundary conditions. However, applying Neumann boundary condition at collector contact of the BJT and Dirichlet boundary conditions at emitter and base contact, shows S-shaped negative differential resistance region as shown in Figure 3(b).

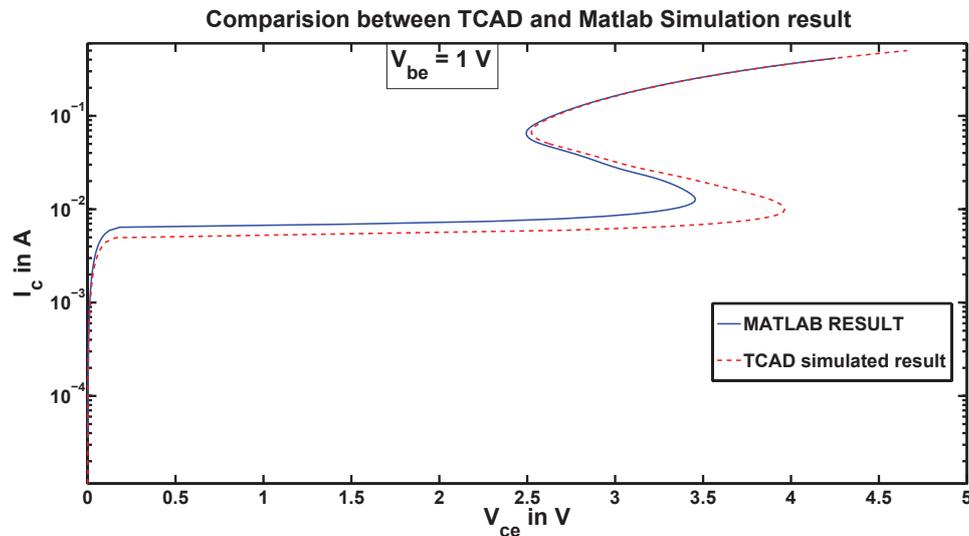


Figure 4. Comparison between commercial device simulator (Sentaurus) results and our proposed device simulator result of BJT $I - V$ characteristics with base voltage = 1 V and Neumann Boundary conditions.

To verify our results with commercial device simulator we have used Sentaurus, which is a set of TCAD tools which simulates and characterize semiconductor devices. The BJT given in Figure 4 is compared simulated results with the same base voltage and boundary conditions but using Sentaurus TCAD and the result obtained is exported and plotted in matlab and compared with the result observed from matlab. The output is showing some variation between the matlab simulated graph and TCAD simulated graph this might be because of reasons like different mobility models being used and the effects like temperature which is not used in the matlab simulator but are taken into consideration in sentaurus TCAD.

4. Conclusion

In summary, we have developed a numerical device simulator to observe negative differential conductivity region in SNDC devices such as BJT. For the simulation purpose, we have used BJT as a device structure and applied different boundary conditions across the collector terminal, It has been observed that Dirichlet boundary conditions shows NNDC behavior while applying Neumann boundary condition results SNDC nature of the device. The proposed flow of the device simulator has been discussed and further results of developed device simulator have been compared with the commercial TCAD device simulator (i.e, Sentaurus).

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