Accurate deterministic numerical simulation of p-n junctions

A. Godoy, P. González[1], J.A. Carrillo[2], F. Gámiz
Dep. de Electrónica, Univ. de Granada, Granada 18071, Spain.
[1]Dep. de Matemática Aplicada, Univ. de Granada, Granada 18071, Spain.
[2]ICREA-Departament de Matemàtiques, Univ. Autónoma de Barcelona, Barcelona, Spain.
email: agodoy@ugr.es ; prodelas@ugr.es

It is well known that in order to explain the behavior of devices like p-n junctions or bipolar junction transistors (BJTs), it is necessary to consider the carrier flow both in the conduction band and in the valence band. To do this, different approximations are commonly used to get a numerical solution of the corresponding Boltzmann-Poisson's system of equations. However, not too much work has focused on a deterministic solution of the Boltzmann equation even when this technique has been proved to yield better results than drift–diffusion or hydrodynamic calculations and also a reduced computational cost compared with Monte Carlo simulations. In this paper some variants of a deterministic simulation of bipolar carrier devices are considered using a FD-WENO scheme (finite differences weighted essentially non oscillatory).

Our goal will be the reduction of the computation time while keeping the same precision in our results. To do this we have divided a p-n junction in three different regions. In the neutral regions we solve the transport equation only for the majority carrier and try to approximate the magnitudes related with the other one by an equilibrium assumption. In the space charge region we solve the Boltzmann equation for electrons and holes. The Poisson equation is solved in the entire length of the device. Thus, we get the following system of equations:

$$\partial_t f_{e,h} + \frac{1}{\hbar}\nabla_k \varepsilon_{e,h}(k)\cdot\nabla_x f_{e,h} \mp \frac{e}{\hbar} E\cdot\nabla_k f_{e,h} = Q(f_{e,h}) + R_{e,h}(f_e, f_h)$$

$$\Delta V \equiv \nabla^2 V = \frac{e}{\varepsilon}(\rho_e - \rho_h - N_e + N_h) \qquad t \in \mathbb{R}_0^+,\ x \in [0,L] \subset \mathbb{R}$$

and depending on the region we are working with, two or three equations has to be solved.

The initial conditions for each of the equations consist in local maxwellian distributions, where $f_{e,h} \equiv f_{e,h}(t, \boldsymbol{x}, \boldsymbol{k})$, $t \in \mathbb{R}_0^+$, $\boldsymbol{x} \in [0,L] \subset \mathbb{R}, \boldsymbol{k} \in \mathbb{R}^3$ represent the probabilistic density functions of finding an electron (f_e) or a hole (f_h) with a wave vector $\boldsymbol{k}$, in a position $\boldsymbol{x}$ at a time t. $Q(f_{e,h})$ and $R_{e,h}(f_e, f_h)$ represent, respectively, the collision's operators and the generation-recombination terms present in this type of devices.

We will mainly focus our interest in mechanisms of scattering by means of acoustic phonons in the elastic approximation and optical non-polar phonons with a single frequency ω, along with quite simple terms of direct or indirect generation-recombination. In order to improve the FD-WENO code, both smoothly varying non-uniform grid and some sort of multigrid technique inspired in a multidomain method with interpolation at subdomain interfaces are currently under development, and it will be the subject of future works.

We have confirmed how the numerical results obtained not only correspond quite well with the qualitative behavior expected for these type of devices, but also some exhaustive comparisons with the well-known drift-diffusion simulator PISCES become in great agreement.

A full journal publication of this work will be published in the Journal of Computational Electronics.

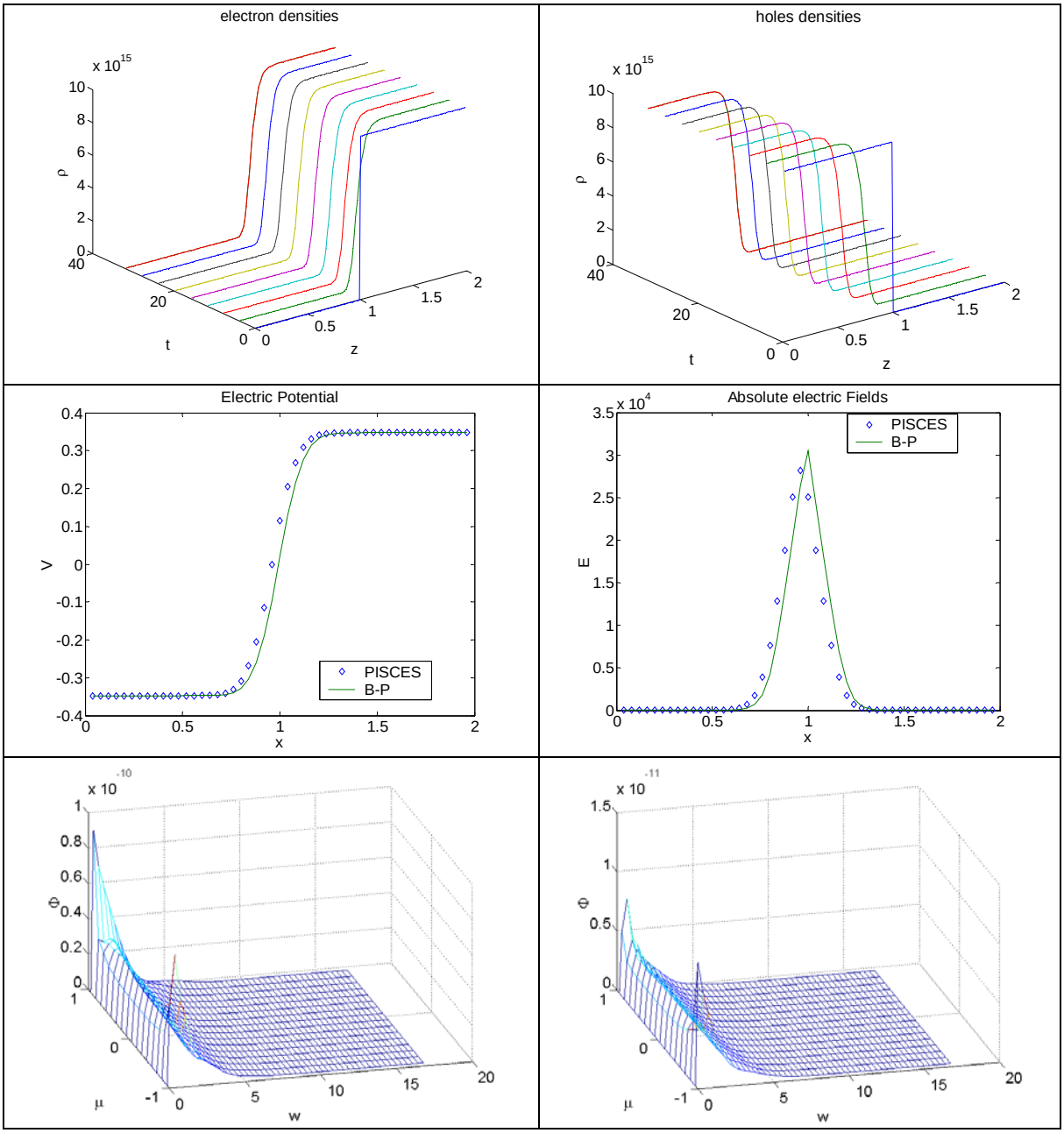

Figure 1: (top-left) Evolution of electron densities; (top-right) Evolution of hole densities; (mid-left) Final electric potential of Boltzmann-Poisson versus PISCES; (mid-right) Final absolute electric field of B-P versus PISCES; (bottom-left and bottom-right, respectively) Probability density functions of electrons and holes near the middle of a p-n junction of 2 μm of total length with uniform doping profiles, $N_D = N_A = 10^{16}$ cm^{-3}, and no applied bias.

A full journal publication of this work will be published in the Journal of Computational Electronics.