

Hydrodynamic and Energy-Balance Models Based Numerical Solvers for Semiconductor Structures

Mario Kupresak¹, Philippe Peter¹, Jasmin Smajic¹, *Senior Member, IEEE*, and Juerg Leuthold¹, *Fellow, IEEE*

¹Institute of Electromagnetic Fields (IEF), ETH Zurich, Zurich 8092, Switzerland, mario.kupresak@ief.ee.ethz.ch

Semiconductor topologies are fundamental building blocks of many conventional devices used in daily life, and accurate modeling and simulation tools of those topologies are thus of great relevance. To account for the nonclassical effects in the charge transport, the hydrodynamic model (HDM) and the energy-balance model (EBM) have been employed. In this work, we develop a numerical solver that incorporates HDM, using the discontinuous Galerkin finite element method. Besides the HDM solver, we make use of a commercial EBM implementation. The analysis has been performed for a n^+nn^+ junction, under the excitation of a voltage source. The obtained results have been compared with the ones of the classical drift-diffusion model. It is shown that the studied models may result in quite different predictions of the response of the investigated structure. We are currently developing an EBM solver, that will be validated with the above commercial tool. A detailed comparison of the HDM and EBM solvers will be performed.

Index Terms—Charge transport models, finite element analysis, numerical simulation, semiconductor devices.

I. INTRODUCTION

SEMICONDUCTOR DEVICES are of paramount importance to the modern research and technology. To understand and confirm the behavior of these devices, accurate descriptions of the semiconductor physics and the associated simulations are required. To this end, several charge transport models have been proposed in the literature [1]. A classical approach, namely the drift-diffusion model (DDM) [1], [2], has been employed, to investigate the properties of different structures, e.g., pn- and n^+nn^+ -junctions [3], [4]. Essentially, this model studies the drift and diffusion currents that flow in the structures, while adopting the concepts of the mobility and diffusivity of charge carriers.

However, considering the recent miniaturization trend, where the characteristic dimensions of the semiconductor topologies are comparable to the carriers' mean free paths, the nonclassical effects, such as the carrier inertia, ballistic effects, hot electrons, etc. [4], [5], govern the structure's response. As a consequence, the same topologies may no longer be fully described by DDM, and more advanced approaches are required. To capture the above effects, the following models: 1) the hydrodynamic model (HDM) [1], [4]–[6] and 2) the energy-balance model (EBM) [1], [5], have been widely used. Beyond DDM, these models are based on the carriers' mass, momentum and energy density. We note that in [5], a preliminary comparative study of HDM and EBM has been reported, within the framework of the finite difference method.

The current work performs a computational study, incorporating the aforementioned models. More precisely, a numerical solver for HDM has been realized, using the finite element method (FEM). On top of the HDM solver, a commercial EBM implementation in SILVACO Atlas has been considered [7]. Note that Atlas does not include the full HDM, investigated in this work. Additionally, our previously established DDM solver has been used as a reference [8]. The study has been conducted for a semiconductor n^+nn^+ junction, commonly encountered in the literature [4], [5], [8].

The in-house developed HDM solver will be complemented by an EBM one, that is currently in implementation. The results

of the EBM solver will be validated with the ones of Atlas, mentioned before. A detailed comparison, concerning the performances of our HDM and EBM solvers and the impact of the studied models on the analyzed structure, will be performed. To the best of our knowledge, the targeted computational study has not been previously done. The associated results will be presented at the conference and in the subsequent full paper.

II. MATHEMATICAL DESCRIPTION

The implemented unipolar HDM solver is based on the following equations, given in the 1-D form [4]:

$$\frac{\partial n}{\partial t} + \frac{\partial(vn)}{\partial x} = 0 \quad (1)$$

$$\frac{\partial p}{\partial t} + \frac{\partial(vp)}{\partial x} + k_B \frac{\partial(nT)}{\partial x} = -qnE - \frac{p}{\tau_p} \quad (2)$$

$$\begin{aligned} \frac{\partial \omega}{\partial t} + \frac{\partial(v\omega)}{\partial x} + k_B \frac{\partial(vnT)}{\partial x} \\ = -qnvE + \nabla \cdot (\kappa \nabla T) - \frac{\omega - \frac{3}{2}k_B n T_L}{\tau_\omega} \end{aligned} \quad (3)$$

$$p = mnv \quad (4)$$

$$\omega = \frac{3}{2}k_B n T + \frac{1}{2}mnv^2. \quad (5)$$

In (1)–(5), n is the electron concentration, p is the momentum, ω is the energy density, v is the electron velocity, T and T_L are the electron and lattice temperatures, respectively, E is the electric field, τ_p and τ_ω are the momentum and energy density relaxation rates, respectively; k_B is the Boltzmann constant, q is the electron charge, m is the effective electron mass, κ is the heat conduction coefficient; x and t are the space and time variables, respectively. The governing equations of EBM may be obtained by removing the convective term $\frac{\partial(vp)}{\partial x}$ in (2) and the kinetic part of ω in (5) [5].

To implement (1)–(5), we have employed a well-known numerical technique for solving highly nonlinear hyperbolic systems, namely the discontinuous Galerkin FEM, and the two-stage Runge-Kutta method for the space and time

discretizations, respectively [9]. Particularly, the electric field distribution has been computed from the Poisson equation, using the continuous Galerkin FEM [10]. Additionally, to ensure stable solutions, slope limiters have been utilized. In the simulations, 150 line elements and the time step of 0.5 fs have been specified. Besides the HDM solver, we have also employed an EBM solver of Atlas. For detailed discussion of the simulations performed, we refer the readers to the associated user manual [7]. The results of the above solvers have been compared with the ones of DDM.

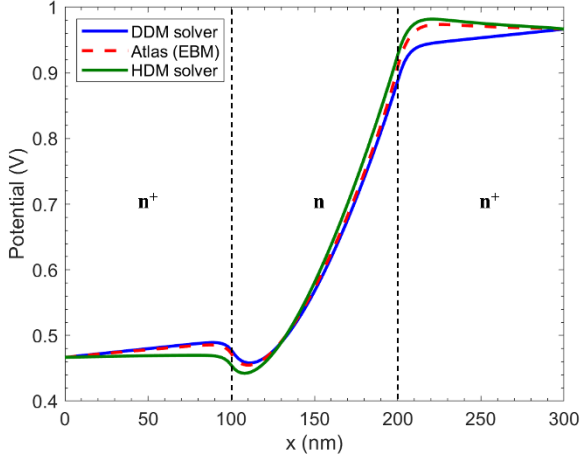


Fig. 1. Potential distributions of the studied models for a n^+nn^+ junction, excited by a bias of 0.5 V.

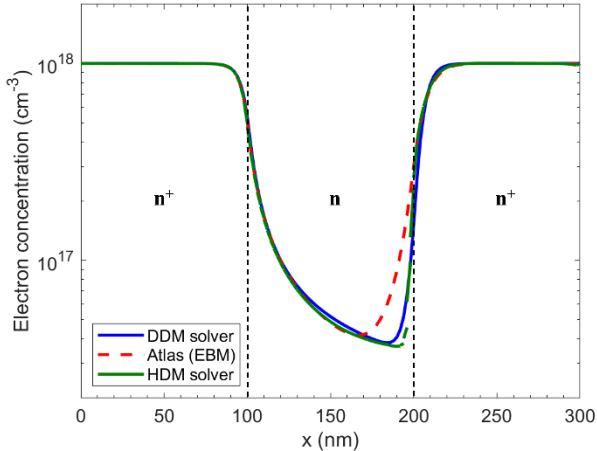


Fig. 2. Electron concentration distributions of the studied models for a n^+nn^+ junction, excited by a bias of 0.5 V.

III. NUMERICAL RESULTS AND DISCUSSION

The structure-under-study is a 1-D n^+nn^+ junction. Similar to the work reported in [8], the length of the n^+ and n regions is 100 nm, and the corresponding doping concentrations are 10^{18} cm^{-3} and $2 \cdot 10^{15} \text{ cm}^{-3}$, respectively. The metallic electrodes, modeled as perfect Ohmic contacts, are placed at $x = 0$ and $x = 300$ nm, and a bias of 0.5 V is applied to the latter electrode.

Figures 1 and 2 illustrate the potential and electron concentration distributions for the investigated topology. For both studied features, the results generated by the employed models clearly differ. As shown in Fig. 1, the potentials of EBM

and DDM agree closely throughout the left n^+ and n regions. However, around the n - n^+ interface, the two models start deviating from each other, and furthermore, in the right n^+ region, EBM and HDM reveal decreasing potentials, contrary to the increasing one for DDM. One may also notice the discrepancies between EBM and HMD, and DDM, in the corresponding electron concentrations. Notably, EBM predicts considerably larger concentrations in parts of the n region, in comparison to the other two models, as depicted in Fig. 2.

The above observations will be carefully scrutinized in future studies. Moreover, an EBM solver will be developed within the discontinuous Galerkin FEM, similar to the aforementioned HDM solver. The generated results will be verified with the ones of the EBM solver of Atlas, discussed before.

IV. CONCLUSION

This work conducted a computational study of different charge transport models in semiconductors, namely HDM and EBM. An in-house developed HDM solver was reported, within the framework of the discontinuous Galerkin FEM. A commercial EBM implementation within SILVACO Atlas was also considered. The obtained results were compared with the ones of DDM. The study was done for a 1-D n^+nn^+ junction, excited by a voltage source. It was demonstrated that the implemented solvers may generate different solution features of the studied structure. Based on the above HDM solver, an EBM solver will be realized, and the associated results will be tested against the ones of the commercial tool. A thorough analysis of the performances of the HDM and EBM solvers will be performed.

REFERENCES

- [1] T. Grasser, T.-W. Tang, H. Kosina, and S. Selberherr, "A review of hydrodynamic and energy-transport models for semiconductor device simulation," *Proc. IEEE*, vol. 91, pp. 251-274, February 2003.
- [2] H. K. Gummel, "A self-consistent iterative scheme for one-dimensional steady state transistor calculations," *IEEE Transactions on Electron Devices*, vol. 11, no. 10, pp. 455-465, October 1964.
- [3] A. C. Gungor, J. Smajic, F. Moro, and J. Leuthold, "Time-domain coupled full Maxwell- and drift-diffusion-solver for simulating scanning microwave microscopy of semiconductors," in *IEEE PIERS-Spring*, pp. 4071-4077, Italy, June 2019.
- [4] A. C. Gungor, T. Ehrenguber, J. Smajic, and J. Leuthold, "Coupled electromagnetic and hydrodynamic modeling for semiconductors using DGTD," *IEEE Trans. Magn.*, vol. 57, pp. 1-5, June 2021.
- [5] A. Aste and R. Vahldieck, "Time-domain simulation of the full hydrodynamic model," *Int. J. Numer. Model.*, vol. 16, pp. 161-174, February 2003.
- [6] D. Vasileska, S. M. Goodnick, and G. Klimeck, *Computational electronics: semiclassical and quantum device modeling and simulation*, CRC Press, 2010.
- [7] SILVACO, <https://silvaco.com/tcad/>.
- [8] M. Kupresak, J. Smajic, and J. Leuthold, "Modeling and simulations of semiconductor structures at highest frequencies," in *IEEE 21st Biennial Conference on Electromagnetic Field Computation (CEFC)*, pp. 1-2, Republic of Korea, June 2024.
- [9] B. Cockburn and C.-W. Shu, "Runge-Kutta discontinuous Galerkin methods for convection-dominated problems," *J. Sci. Comput.*, vol. 16, pp. 173-261, September 2001.
- [10] J. Smajic, *How to perform electromagnetic finite element analysis*, The International Association for the Engineering Modelling, Analysis & Simulation Community (NAFEMS), NAFEMS Ltd, 2016.