J Comput Electron (2006) 5:235–240
DOI 10.1007/s10825-006-8850-1

High order explicit versus quasi-linear implicit finite-difference approximation for semiconductor device time-domain macroscopic modelling on parallel computer

Ali El Moussati · C. Dalle

Abstract Bipolar semiconductor device 2D FDTD modelling suited to parallel computing is investigated in this paper. The performance of a second order explicit approximation, namely the Nessyahu-Tadmor scheme (NT2) associated with the decomposition domain method, are compared to a classical quasi-linear implicit one based on the Alternating Direction Implicit method (ADI). The comparison is performed both from the numerical stability point of view by means of drift-diffusion and energy-momentum simulations and from the computation efficiency point of view. The test structure is a millimetre-wave IMPATT diode the RF as well as internal operation of which is highly non linear. The results demonstrate that high order explicit approximations compete with implicit approximations and allow the development of efficient models well suited to the parallel computation.

Keywords Macroscopic modelling · Finite-difference method · IMPATT diode · Parallel computing

Introduction

Numerical physical modelling is fundamentally limited by computation time. Expected improvements of the monoprocessor PC's or Unix workstation performance mainly depend on the clock frequency increasing but are not sufficient to satisfy the computation requirements such as those of future 3D global modelling. Only the parallel computation is today potentially capable to offer the necessary significant improvements. However, existing codes are generally not designed to fully exploit the potential of such computers. Thus, we are presently working on the development of new FDTD electrical macroscopic semiconductor device models compatible with parallel computing. New code development is a heavy and costly effort because the potential solutions are numerous and cannot be systematically investigated. Indeed, the final choice results from a trade-off between the model formulation, the equation local approximation scheme, the equation global solution algorithm and the available computer operating mode. The purpose of this paper is to compare the computation performance of finite-difference approximations issued form the two main classes of numerical schemes namely the explicit and implicit ones for the two-dimensional simulation of bipolar semiconductor structures.

A. El. Moussati · C. Dalle (✉)
Institut d'électronique, de microélectronique et de nanotechnologie, CNRS, Cité scientifique, Avenue Poincaré, BP. 60069, 59652 Villeneuve d'Ascq cédex, France,
e-mail: christophe.dalle@univ-lille1.fr

I. Time domain electrical macroscopic modelling

Time domain electrical modelling fundamentally relies on the Maxwell's equations solution following the quasi-electrostatic assumption which implies that the electric field only derives from the electrostatic potential V:

$$\text{rot}\, E = 0 => E = -\text{grad}\, V$$

Consequently, the Maxwell's equations are reduced to the Poisson and total current equations:

$$\text{div}\, D = \rho => \blacktriangledown V = -\rho/\varepsilon$$

$$J_{\text{total}} = J_{\text{conduction}} + \varepsilon \delta E/\delta t$$

Thus, from the circuit element modelling point of view, the electrical model allows to determine the instantaneous

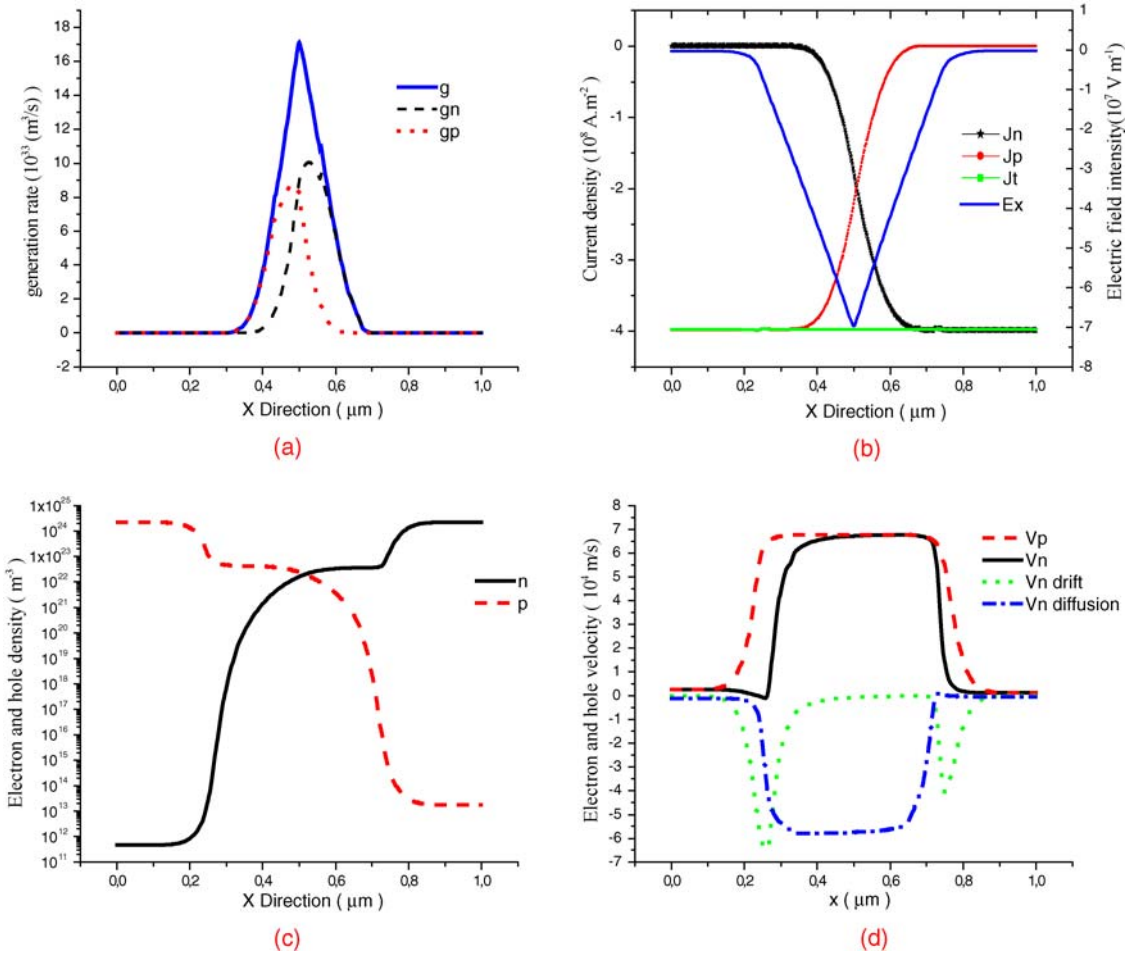

Fig. 1 Spatial evolutions of the electron and hole density (c), current density and electric field (b), velocity (d) and generation rate (a) resulting from the explicit NT2 drift-diffusion modelling. The DC bias voltage is 19.5 V and the DC current is 393 mA

relation $I(t)/V(t)$ between the flowing current and potential across the device terminals. A transport model describing the free carrier kinetics is required to determine the conduction current. The macroscopic approach fundamentally relies on the Boltzmann transport equation the integration of which allows to derive more or less complete conservative equation sets depending on the considered assumptions [1]. The simplest one is the well-known drift-diffusion model following a stationary approach of the carrier transport. Let us just recall that it consists of the continuity and conduction current equations for the electrons and holes written here for a 1D case:

$$\delta n/\delta t = 1/q \,\mathrm{div}\, J_n + g - u; \delta p/\delta t = -1/q \,\mathrm{div}\, J_p + g - u$$

$$J_n = -q\mu_n nE - \mu_n \delta n/\delta x; J_p = +q\mu_p pE - \mu p\, \delta p/\delta x$$

$$J_{\mathrm{conduction}} = J_n + J_p$$

The more accurate but complex one is the non-stationary energy-momentum model which accounts for the momentum and energy carrier relaxation phenomena. It is based on the solution of the continuity, total energy and momentum equations:

$$\begin{aligned}
\delta n/\delta t &= 1/q \,\mathrm{div}\, J_n + g - u;\\
\delta p/\delta t &= -1/q \,\mathrm{div}\, J_p + g - u\\
\delta n\varepsilon_n/\delta t &= J_n E - \mathrm{div}(nv_n(\varepsilon_n + kT_n))\\
&\quad -(n\varepsilon_n - n\varepsilon_{n0})/\tau_{\varepsilon n};\\
\delta p\varepsilon_p/\delta t &= J_p E - \mathrm{div}(pv_p(\varepsilon_p + kT_p))\\
&\quad -(p\varepsilon_p - p\varepsilon_{p0})/\tau_{\varepsilon p}\\
\delta nm_n^* v_n/\delta t &= -qnE - \mathrm{div}(nm_n^* v_n v_n) - \delta nkT_n/\delta x\\
&\quad -nm_n^* v_n/\tau_{mn}\\
\delta pm_p^* v_p/\delta t &= qpE - \mathrm{div}(pm_p^* v_p v_p) - \delta pkT_p/\delta x\\
&\quad -pm_p^* v_p/\tau_{mp}\\
J_n &= -qnv_n; J_p = +qpv_p; J_{\mathrm{conduction}} = J_n + J_p
\end{aligned}$$

II. Numerical approach

Explicit and implicit methods are the two main classes of finite difference approximations. In the explicit schemes, the local variables are directly determined from previously known quantities. Thus, these schemes are naturally appropriate for parallel calculations. However, explicit schemes are reputed to be intrinsically unstable and requiring short time increments. By contrast, implicit schemes present better intrinsic stability properties but they lead to non linear matrix systems the solution of which is often based on recurrent calculations and consequently is not directly suited to the parallel computing. These two possibilities have been considered in the present study and compared and tested firstly in term of numerical stability by means of the development of two dimensional (2D) drift-diffusion and energy-momentum models and secondly in term of computer efficiency by means of their implementation on a parallel IBM/SP3 computer comprising 4 nodes each including 16 processors (but the computer practical use was limited to one node namely 16 processors with a shared memory).

The first modelling is based on the implicit approximation and is issued from our existing code previously optimized for sequential computing on a monoprocessor workstation. The implicit approximation is based on a linear approach [2] in order to avoid iterative matrix system solution method resulting from the fully non linear formulation [3]. Thus, the transport equation finite-difference approximation is based on an implicit scheme using the first and second upwind method for the spatial derivatives [4] associated to the alternating direction implicit method (ADI) for the time derivation [5]. This leads to the solution of $A \cdot X = B$ equations where A remains a simple tridiagonal matrix, performed by means of the parallel engineering and scientific subroutine IBM library (PESSL). The Poisson's equation solution leads to a five band matrix.

The second modelling is based on the explicit approximation. In a first step, we have experimented first order approximations like the Lax-Friedrich, Lax-Wendroff and Godunov schemes but they have appeared unstable especially for energy-momentum simulations. Thus, we have used higher order approximations such as the second (NT2) and third order (NT3) Nessyahu-Tadmor schemes [6]. They are predictor-corrector type schemes using non oscillatory approximations allowing to improve the stability [7] but to the detriment of a higher number of intermediate calculations. The decomposition domain method has been used to optimally solve the equation systems. It allows to split up a simulated structure in domain each associated to an elementary processor. A difficulty relies in the management of the domain boundaries [8]. This method is associated to the message passing interface parallel programming model (MPI) [9].

III. Simulations

The test-problem was a PN junction device. Indeed, the simulation of such a bipolar semiconductor structure is more constraining from a numerical point of view than the often considered unipolar Gunn diode in which the diffusion effect are less pronounced [10]. The structure along the X axis is a 0.15/0.32/0.25/0.15 μm long 2.2 10^{24}/2. 10^{23}/2. 10^{23}/2.2 10^{24} m^{-3} doped P^+PNN^+ 100 GHz silicon IMPATT diode. The device thickness along the Y axis is 2 μm. The associated mesh consists of $500 * 20$ nodes. The time increment is 5. 10^{-15} s. The simulations have been performed under DC avalanche operating mode at 500 K. Indeed, such a steady-state one-dimensional carrier transport operating mode is useful to test the algorithm capability to account for time and spatial null derivatives. Large signal simulations have been also performed but are not more significant in the present study.

As an example, Fig. 1 details the spatial evolutions of the internal physical quantities along the Y axis such as the electric field, electron and hole densities, current densities, generation rate and velocities. They have been obtained from the explicit NT2 drift-diffusion model. Thus, the diode appears punched through namely the NP active zone is fully depleted for the considered DC bias point. These curves point out the sharpness of the carrier density where the minority electron and hole penetrate the carrier multiplication high field zone inducing a strong diffusion effect clearly pointed out in the case of the electrons by the velocity diffusion component near the P^+P transition zone. The results obtained by means of the implicit drift-diffusion model for similar operating conditions are perfectly consistent. In connexion with this question, Fig. 2 shows the spatial evolution of the total current along the carrier drifting X direction obtained from the implicit and explicit NT2 drift-diffusion simulations. A

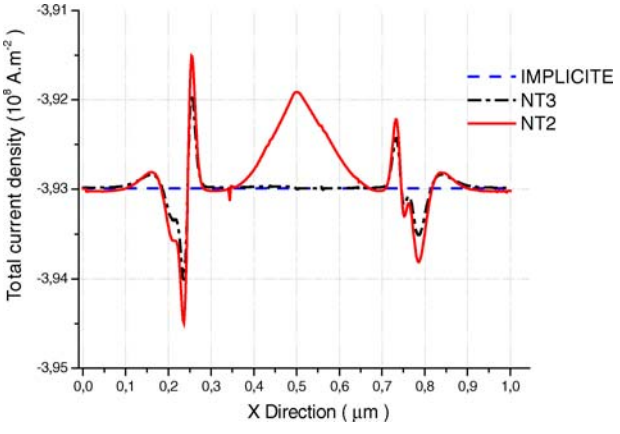

Fig. 2 Total current density spatial evolutions along the X direction resulting from the implicit and NT2 and NT3 explicit drift-diffusion modelling

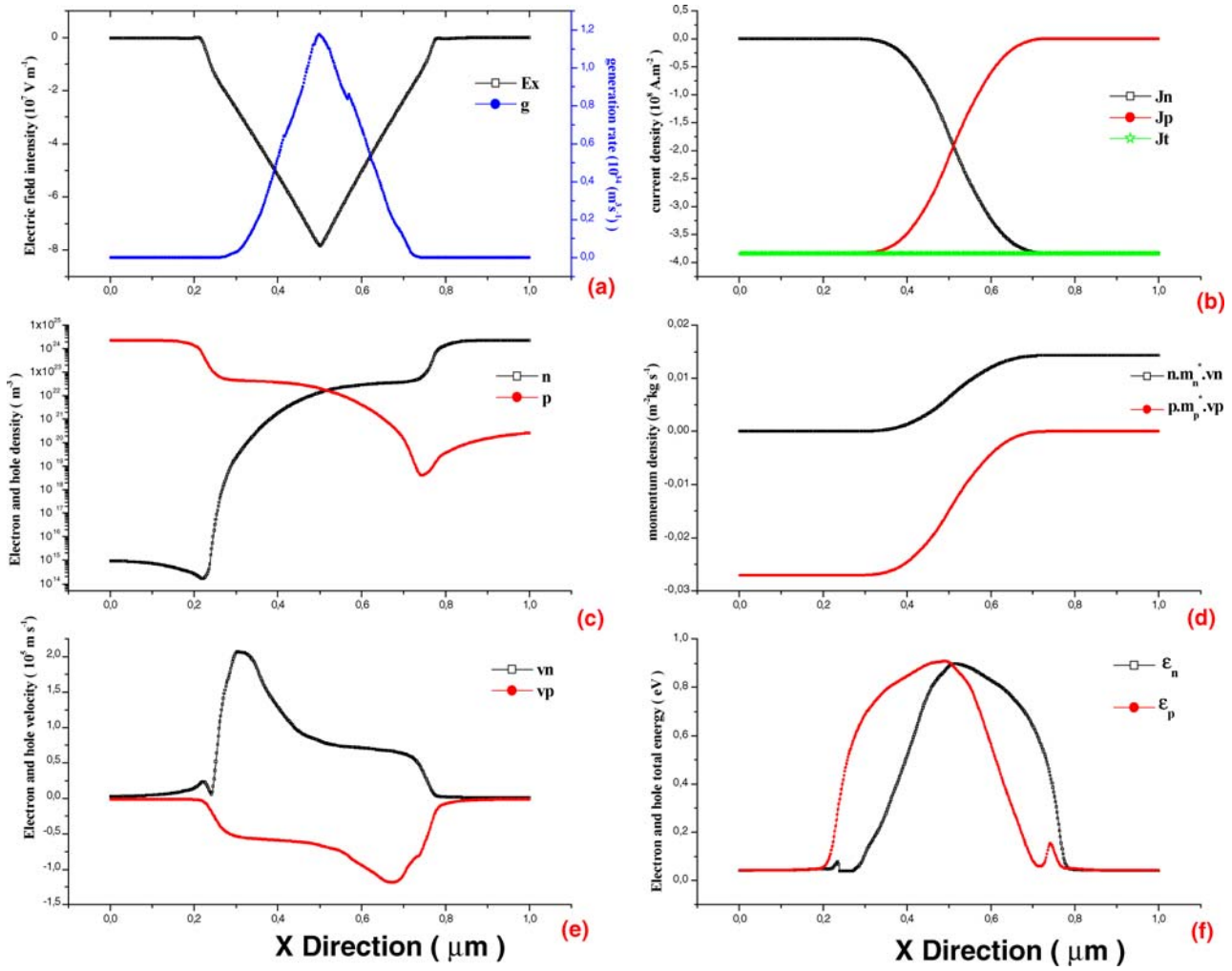

Fig. 3 Spatial evolutions of the electron and hole density (c), current density (b), velocity (e), total energy (f), momentum density (d) and generation rate and electric field (a) resulting from the explicit NT2 energy-momentum modelling. The DC bias voltage is 21.6 V and the DC current is 360 mA

result obtained from a modelling performed by means of the explicit third order Nessyahu-Tadmor scheme (NT3) has been added. These results demonstrate that the explicit finite-difference approximation does not allow to reach a total current density conservation as perfect as that obtained from the implicit approximation but the spatial variations remain weak enough (of the order of 0,4% for the NT2 scheme). They occur where the diffusion effects are the strongest namely at the P^+P and NN^+ interfaces and near the PN junction where the carrier transport is the more convective and the electric field intensity is the highest. Note that the NT3 scheme leads to a better description of the high field transport than the NT2 scheme. However, this improvement is obtained by means of a greater amount of intermediate calculations. Consequently, this method has been later given up because it has appeared slower than the implicit one.

As previously, Fig. 3 details the spatial evolutions of the diode internal physical quantities but now obtained from the explicit NT2 energy-momentum model under similar operating conditions. Thus, the evolutions of the electron and hole total energy and momentum density have been added. The DC current density is similar but the DC bias voltage must be higher. This feature results from the carrier ionization process description in which the ionization rates are considered as function of the carrier energy instead of the electric field intensity as in the drift-diffusion approach [11]. Moreover, by contrast with the drift-diffusion approach, the energy-momentum modelling points out overvelocity effects in the high diffusion zones. However, these spectacular effects do not influence the device RF global operation because they only concern still minority carriers [11]. The comparison of these results with those obtained from the implicit modelling demonstrates a perfect consistency. As previously, the total current density conservation obtained from the explicit modelling is worse than that resulting from the implicit modelling but the spatial variations remain negligible.

The intrinsic performance of the different schemes have been quantitatively compared in term of computer efficiency by means of simulations performed in the same conditions on a one processor IBM workstation. Concerning the drift-diffusion modelling, the computer time, respectively for the explicit NT2 and NT3 schemes, is about 50% and 100% higher than that of the implicit scheme. Concerning the energy-momentum modelling, the computer time required by the NT2 scheme is about 150% higher than that of the implicit scheme. Thus, high order explicit schemes appears slower than implicit ones. Indeed, in comparison with simple one-order explicit, the additional intermediate calculations required by the high order explicit schemes clearly make heavy the computer time. However, the explicit computer programs were not perfectly optimized while the older implicit computer program was well optimized and based, concerning the matrix equation systems, on the extremely efficient IBM/ESSL mathematical library. Moreover, explicit schemes are a priori well suited to the parallel computing.

Thus, the former simulations have been performed using a number of processor varying from one to sixteen. Figure 4 shows the evolution of the acceleration factor as a function of the number of used processors for simulations performed by means of the explicit and implicit drift-diffusion and energy-momentum models in comparison with an ideal linear acceleration factor. Firstly, from a general point of view, the results show that the acceleration factor is well an increasing function of the number of processor but the gradient of the acceleration factor is a decreasing function of the number of processor. This result demonstrates the influence of the increasing importance of the interprocessor communications in the global computation time. The explicit modelling leads to better performance close to be two times higher than the implicit modelling. An improvement of a ten factor is demonstrated with the use of 16 processors for the explicit modelling. It could be expected to be close to sixteen. It is close to six for the implicit modelling.

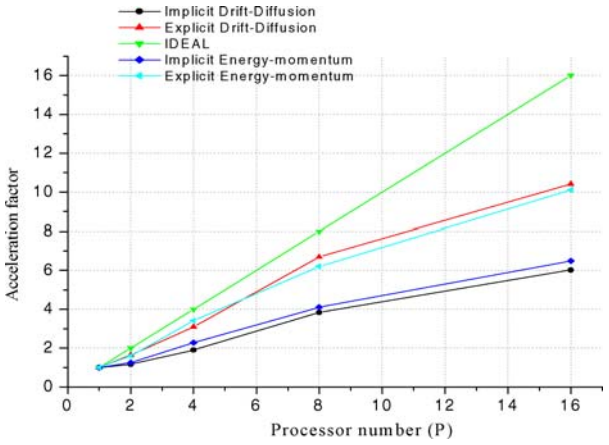

Fig. 4 acceleration factor as a function of the processor number for the implicit and NT2 explicit drift-diffusion and energy-momentum modelling

Conclusion

In conclusion, from a general point of view, our comparative study demonstrates that:

- the explicit NT2 approximation based finite-difference scheme associated with the decomposition domain method can lead to better computation performance than the implicit scheme even when this method is associated with an efficient mathematical library. However, the use of the decomposition domain method and the associated code implementation with MPI is heavy to program.
- the acceleration factor is not proportional to the number of used processors. Indeed, the influence of the inter-processor communications tends to decrease the computing efficiency.
- in comparison with first order explicit approximations, the use of high order explicit finite-difference approximation now allows the development of reliable 2D bipolar semiconductor models (even energy-momentum). Such models allow the use of time increment similar to those used with the implicit modelling. However, a higher number of intermediate calculations make heavy the computer time.

These conclusions are not definitive since all possible numerical schemes could not be all tested but they point out the improvements resulting from the high order explicit schemes. This question could be now studied thoroughly by considering still constraining numerical model-problem such as bipolar heterojunction structures in which occur more important gradients and shocks.

References

1. Blotekjaer, K.: Transport equations for electrons in two-valley semiconductors. IEEE Trans. Electr. Dev. **17**, 38–47 (1970).
2. Reiser, M.: Large scale numerical simulation of microwave gallium arsenide submicronic gate field effect transistor. Comput. Methods Appl. Mech. Engrg. **1**, 17–38 (1972)
3. Selberherr, S., Schütz, A., Pötzl, H.W.: MINIMOS— A two dimensional MOS transistor analyser. IEEE Trans. Electr. Dev. **27**(8), 1540–1550 (1980)
4. Gardner, C.L.: Numerical simulation of a steady-state electron shock wave in a submicrometer semiconductor device. IEEE Trans. Electr. Dev. **38**(2), 392–398 (1991)
5. Xiao, S., Huang, C.: A transient numerical scheme for the simulation of GaAs MESFETs and circuits. Solid-State Electr. **12**, 1519–1524 (1990)
6. Nessyahu, H., Tadmor, E.: Non-oscillatory central differencing for hyperbolic conservation laws. J. Comput. Phys. **87**, 408–463 (1990)
7. Liu, X.-D., Tadmor, E.: Third order nonoscillatory central scheme for hyperbolic conservation laws. Numerishe Mathematik **79**, 397–425 (1998)

8. Toselli, A., Widlund, O.: Domain decomposition methods—Algorithms and theory. Springer series in Comput. Mathemat. **34** (2004).
9. Gropp, W., Lusk, E., Skjelum, A.: Using MPI: Portable Parallel Programming with the Message-Passing-Interface. MIT Press, Cambridge, Massachussetts (1994)
10. Fatemi, E., Jerome, J., Osher, S.: Solution of the hydrodynamic device model using high-order nonoscillatory shock capturing algorithms. IEEE Trans. Comput.-Aid. Design **10**(2), 232–244 (1991)
11. Dalle, C., Rolland, P.A.: Drift-diffusion versus energy model for millimetre-wave IMPATT diodes modelling. J. Numer. Model.: Electr. Networks, Dev. Fields **2**, 61–73 (1989)