AN IMPLICIT COUPLING SCHEME FOR THE USE OF LONG TIME STEPS IN STABLE SELF-CONSISTENT PARTICLE SIMULATION OF SEMICONDUCTOR DEVICES WITH HIGH DOPING LEVELS

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The shrinking dimensions of semiconductor devices and the raising costs of experimental optimization increase the requirement for efficient and accurate CAD modeling over several design levels (process-device-circuit). Stochastical particle simulation is most accurately describing the nonstationary phenomena of the device physics. Although the required CPU time has limited the practical use of such methods till now, the development of a highly efficient full-band MC-code [1] or Cellular Automata (CA) techniques ([2] and [3]) allow characterization of the operation of millimeter-wave devices and optimization of their structures. A major drawback in numerical efficiency arises if the conventionally applied explicit scheme for performing the self-consistent coupling of the time-dependent electric field with the movement of the pseudo-particles is used, and if devices with high doping level are considered [4]. It is known, that instability arises if the time-step ΔT for successive Poisson solutions does not fulfill $\Delta T \cdot \omega_p < 2$, where ω_p means maximum plasma frequency in the device. Moreover, a detailed investigation shows, that ΔT should in general be chosen much shorter than $\Delta T_{max} = 2 \cdot \omega_p^{-1}$ (fig. 1 and [5]). This problem can be solved by using implicit coupling schemes [6].

The aim of the present work is to introduce an efficient iterative implicit coupling scheme which allows to use long time-steps between successive solutions of the Poisson equation even if ω_p is very high, and which easily can incorporate particle-mesh coupling schemes which guarantee weak self-forces and to first order can also incorporate exact integration of the equations of motion across cell-boundaries of the Poisson-grid. The new method can directly improve the computational efficiency of many particle simulators (standard MC, full-band MC, CA-methods) by an order of magnitude if devices with high free carrier densities are under investigation.

The instability of the conventional scheme arises because the total energy of the electrostatic system, consisting of moving and fixed charges, is not conserved within one time-step. The electrostatic field energy increases over many iterations, thus artificially "heating-up" the carrier gas. As far as time-steps are short enough, energy-relaxation due to lattice scattering limits this effect, but microscopical quantities like i.e. particle mean energy become false, which also affects macroscopical quantities, like i.e noise temperature [7].

In the new implicit scheme, the total mean energy of the electrostatic system is conserved to first order in one time-step. To achieve this the Poisson equation is rewritten in discretized form by additionally considering the change of the density vector during the movement of the particles as a function of changing potentials on the knots of the Poisson grid. Iteratively solving the resulting equations enables one to include proper treatment of particles which cross cell boundaries, what in turn leads to high accuracy of the calculated particle motion also in regions of strong electric field gradients (i.e. near heavily doped pn-junctions or at hetero-interfaces).

The stability of the implicit method is illustrated by simulating both heavily doped semiconductor materials and a 0.15 μm recessed-gate MESFET structure. In fig. 1, the stability-phases of the two coupling schemes are compared for self-consistent simulations with different combinations of time-steps, plasma frequency and collisionality (for definition see caption of fig 1). It is found, that the implicit scheme in general allows to use maximum time-steps of 1-2 $\cdot \omega_p^{-1}$ in all cases of simulation which have been investigated. In fig. 2, the calculated microscopical behaviour of carriers in a MESFET is shown, which has been obtained with a two-dimensional MC–code. Using the explicit scheme, the time-steps have to be chosen as small as 1 fs, in order to suppress the onset of errors arising from artificial heating up of the carrier gas in the high-doped contact regions. Applying the implicit scheme makes the use of 10 fs time-steps possible whithout showing any artificial heating effects. Although solving Poisson's equation in the implicit case is more demanding now, the overall increase of the numerical efficiency of the MC–simulator is a factor of 7 in this example because of the longer time-steps which can be used.

A detailed description of the numerical implementation of the implicit method and further results concerning stability conditions, accuracy, and the increase of efficiency when using Monte–Carlo–

and Cellular-Automata codes for simulation of devices consisting of different materials (GaAs, Silicon, SiGe) will be given at the conference.

References

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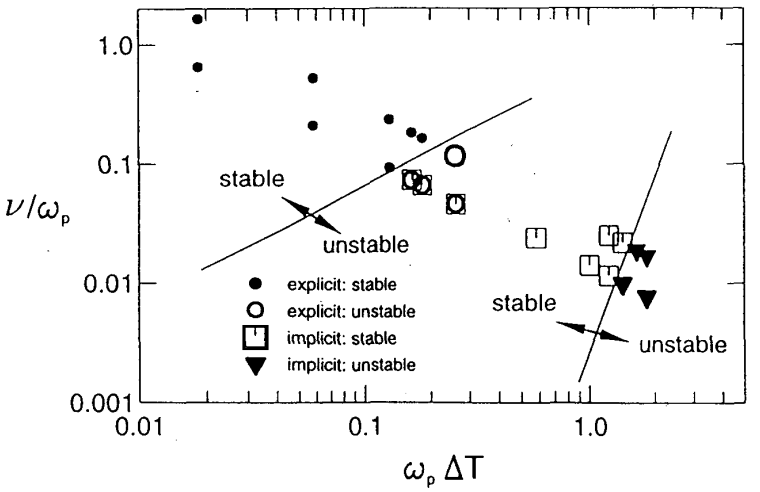

Fig. 1: Recorded conditions of stable or unstable self-consistent calculations using MC- or CA-techniques. Considered materials are GaAs and Silicon. Different time-steps (ΔT), doping levels (determining ω_p) and collisionalities (defined by ν/ω_p where ν is the mean scattering rate) have been adjusted, and some 10.000 iterations in the simulation have been performed to decide wether the simulation is stable or not.

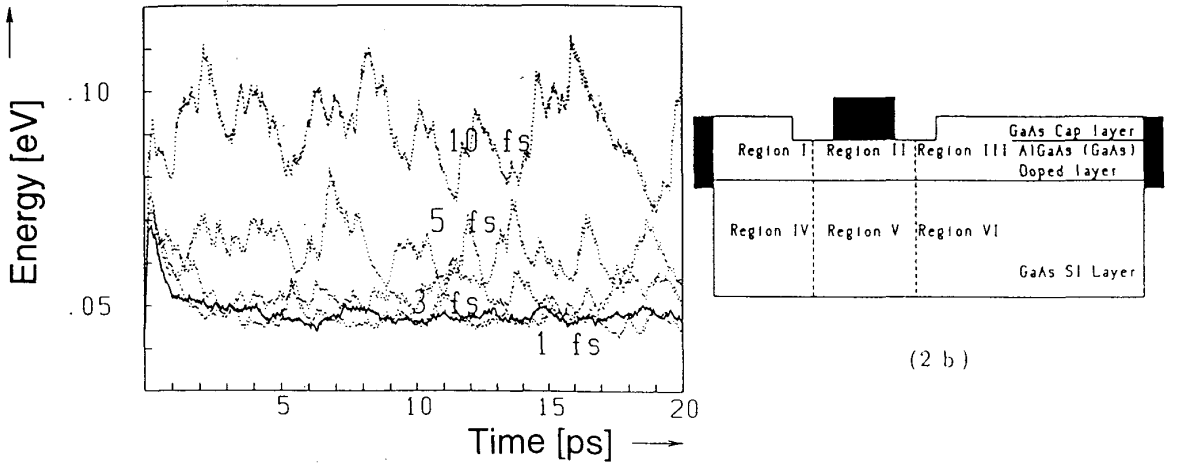

Fig. 2: Calculated total mean energy of electrons in the contact (region 1 of figure 2 b) of a Gallium Arsenide MESFET for a switching-on situation. The doping concentration in the contact region equals $2 \cdot 10^{18}\mathrm{cm}^{-3}$ ($\omega_p = 8.64 \cdot 10^{13}\mathrm{s}^{-1}, \Delta T_{max} = 23$ fs). The dotted lines show the results calculated with the explicit scheme using ΔT= 1, 3, 5 and 10 fs. The full line shows the result for $\Delta T = 10$ fs applying the implicit technique.