Accurate Three-Dimensional Simulation of Electron Mobility Including Electron-Electron and Electron-Dopant Interactions

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The continuous scaling of MOSFET devices into the nanoscale regime requires refined models for electron transport. Coulomb interactions must be considered because of two reasons. First the Coulomb force is a long range force implying that both the short and the long range interactions must be included in a particle ensemble. Second the hot-carrier and short-channel effects will have a significant impact on device performance due to the small number of carriers and impurities in the active region of nanoscale devices.

Although ensemble MC simulators usually do not include the full Coulomb interactions due to the necessary computational time and resources, two techniques have been used in the past for properly including the short and the long range electron-electron and electron-ion interactions in particle based simulations: P^3M (particle-particle particle-mesh) methods [1], adapted to the boundary conditions necessary for semiconductor devices, and the corrected Coulomb approach [2]. However both approaches suffer from drawbacks when used in the context of transport simulations in semiconductors as explained in the paper.

We propose to use a FMM (fast multi-pole method) [3, 4] instead. The FMM is based on the idea of condensing the information of the potential generated by point sources in several truncated series expansions. After calculating suitable expansions, the long-range part of the potential is obtained by evaluating the truncated series at the point in question and the short-range part is calculated by direct summation. Its computational effort is only $O(n)$ where n is the number of particles.

In this work the two previously used methods, namely the P^3M method and the corrected Coulomb approach, are compared to the FMM and experimental data [5] for the case of a n^+–n–n^+ resistor. The particle based MC simulations were performed in three spatial dimensions for five different doping concentrations (cf. Figure 1 and Figure 2). The corresponding simulation times are shown in Table I. It is found that for higher doping concentrations the FMM result agrees best with experimental data and significantly better than the previous approaches.

Since the FMM approach is independent of the grid used during the MC simulation, it can be included into existing MC device simulation codes in a straightforward way. In summary simulation times were halved and the simulation results agree better with experimental data than previously used methods while accounting rigorously for short-range and long-range electron-electron and electron-ion interactions.

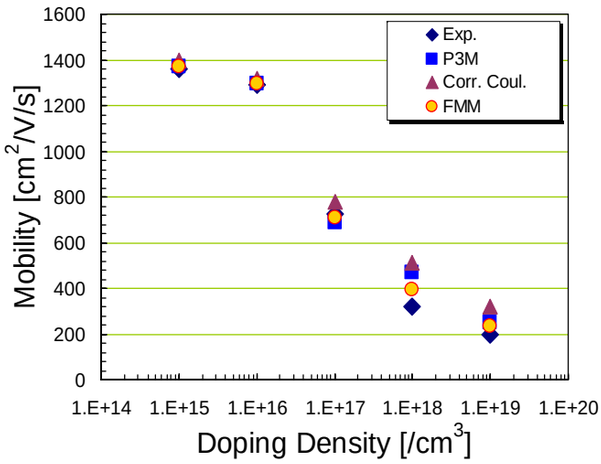

Figure 1: The electron mobility for five doping concentrations (from $10^{15}\,\mathrm{cm}^{-3}$ to $10^{19}\,\mathrm{cm}^{-3}$) as obtained experimentally and by three simulation methods.

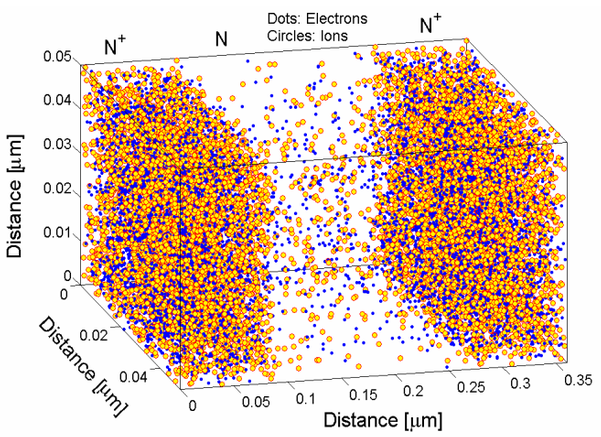

Figure 2: The electron distribution within the resistor ($360\,\mathrm{nm} \cdot 50\,\mathrm{nm} \cdot 50\,\mathrm{nm}$).

Method	Average time per iteration	Total Time (400 iterations)
P^3M	35 s	233 min
FMM	17 s	113 min

Table I: The simulation times on a 600 MHz Pentium III computer. The total number of charges is $\approx 22\,000$, and the MC mesh size is $50 \cdot 20 \cdot 20$.

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