Gummel Iterations for Inverse Dopant Profiling of Semiconductor Devices

M. Burger*
Institut für Industriemathematik, Johannes Kepler Universität, Altenbergerstr. 59, A 4040 Linz, Austria
e-mail: martin.burger@jku.at

INTRODUCTION

Optimal dopant profiling of semiconductor devices is an interesting and challenging task in modern microelectronics (cf. [1], [2]), which is nowadays treated by a combination of mathematical optimization and numerical simulation techniques. Such optimizations of doping profiles involves a high computational effort since a high number of forward simulations have to be carried out in the optimization process. Here we discuss a more efficient approach to the solution of the optimization problem, which is based on a Gummel-type iteration for the optimality system.

MACROSCOPIC DEVICE MODELS

Macroscopic models for semiconductor devices such as the frequently used *drift-diffusion model* (cf. [3]) can be written schematically in the form

$$\lambda^2 \Delta V = Q(\rho) - N, \qquad C(\rho, V) = 0, \quad (1)$$

where V denotes the electric potential, ρ a vector of densities (for electrons and holes), and N the (scaled) doping profile. The first equation is the Poisson equation for the electrical field with scaled Debye length λ and $Q(\rho)$ is the charge generated by the electrons and holes. The equation symbolizes by $C = 0$ is a set of continuity equations, e.g. Nernst-Planck equations for electron and hole densities.

Optimal dopant profiling can be formulated as an optimization problem on top of such a model, namely as a minimization task

$$F(\rho, V, N) \to \min_{(\rho, V, N)} \quad \text{subject to (1).} \quad (2)$$

EFFICIENT OPTIMIZATION

A disadvantage of the optimization model (2) is the strong coupling of the Poisson and continuity equations, which implies a strong coupling of all variables in the first-order optimality system. In order to avoid this problem we use an approach proposed in [4], namely to replace the doping profile by the total charge density $q := Q(\rho) - N$ as the unknown in the optimization. In this way the state equations have a triangular form, the densities do not further appear in the Poisson equation. As a consequence, the optimality system for the minimization of a functional $G(\rho, V, q) = F(\rho, V, N)$ considerably simplifies and one can construct a simple Gummel iteration for this system (based on alternating solution of Poisson and continuity equations), which turns out to be globally convergent and rather efficient.

OPTIMIZATION RESULTS

We illustrate the optimization for the drift-diffusion model, with an objective functional of the form

$$G(\rho, V, q) = (I - I^*)^2 + \epsilon \int (q - q^*)^2 \, dx, \quad (3)$$

where I is the current flowing out over a contact and I^* a reference value to be achieved. The second term in the objective avoids to large deviations from a reference configuration modeled by q^*

Results of the optimization for a PNP-Diode are shown in Figures and 1. Figure shows a comparison of the reference state and the optimal doping profile, and Figure 1 displays the current-voltage curves obtained with these doping profiles.

For a Metal-electron field effect transistor (MESFET), the result of the optimization on an adaptive mesh is shown in Figure 2. Finally, Figure 3 illustrates the convergence history of the optimization method, one observes that the result of the optimization is obtained after few Gummel iterations for the optimality system.

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Conclusion

We have derived an efficient Gummel iteration for optimal inverse dopant profiling, which is easy to implement and globally convergent. With this approach the effort for optimization only doubles the one for simulation.

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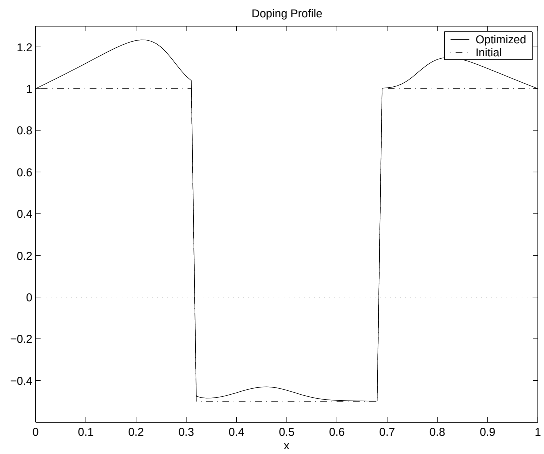

Fig. 1. Optimized Doping Profile of an NPN-Diode.

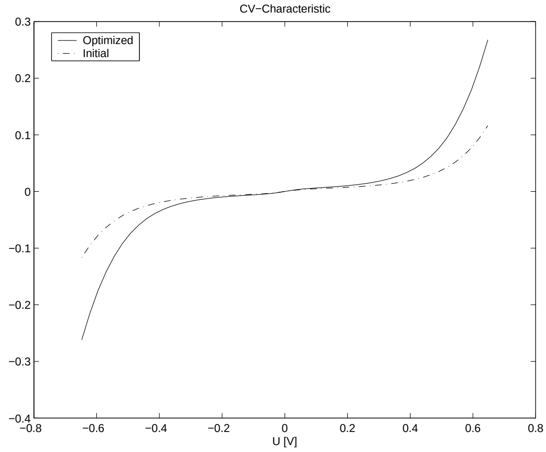

Fig. 2. CV-curve of the NPN-Diode before and after optimization.

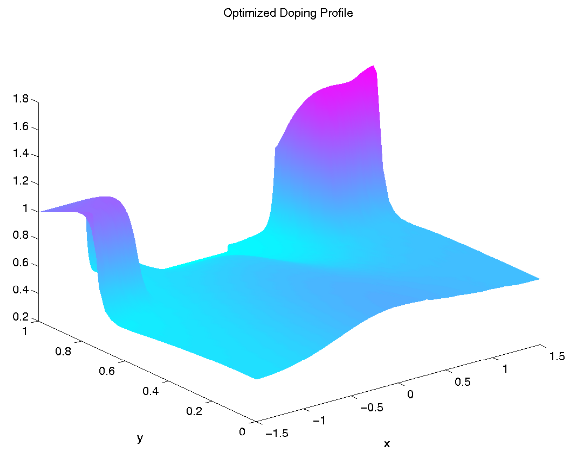

Fig. 3. Optimized Doping Profile of a MESFET.

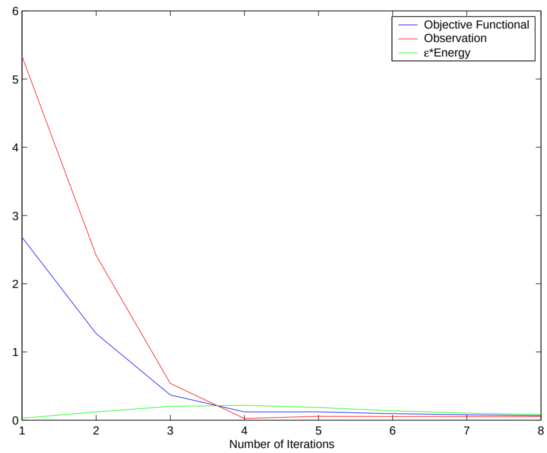

Fig. 4. Convergence History of the Optimization Method