Practical Inverse Modeling with SIESTA

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Abstract

We present a simulation system which meets the requirements for a practical application of inverse modeling in a professional environment. A simulation tool interface for the integration of arbitrary simulation tools at the user level is introduced and methodology for the formation of simulation networks is described. A Levenberg-Marquardt optimizer automates the inverse modeling procedure. Strategies for the efficient execution of simulation tools are discussed. An example demonstrates the extraction of doping profile information on the basis of electrical measurements.

1. Introduction

TCAD simulation tools are widely used throughout the semiconductor industry. However, their efficient application requires a sound calibration of the involved models. Their parameters need to be tuned in order to achieve an acceptable accuracy of the simulation results. The complexity of the involved models inhibits a manual calibration and, therefore, an optimizer must be employed to automate the procedure. The simulation environment SIESTA [1] can be utilized to solve generic inverse modeling problems. Fig. 1 illustrates how its optimizer is searching for sets of model parameters which deliver an optimal fit between simulation results and measurements: A simulation model is evaluated with a given set of parameters and its results are compared to measurements; the optimizer receives the difference between simulation and measurement, and uses it to compute improved sets of parameters.

2. Tool Integration

An open simulation tool interface enables the cooperation between SIESTA and arbitrary simulation tools. This interface imposes no restrictions on simulation tools and, in particular, it does not require their modification. Fig. 2 illustrates how SIESTA controls simulators. Dedicated parts of the input deck (e.g. *vt-dose, vt-energy*) are marked by pairs of "<(" and ")>" which are controllable by the simulation environment. Arbitrary results of simulation tools are registered with SIESTA and are

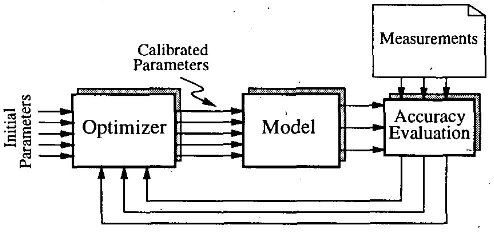


Figure 1: The automated inverse modeling system.

```
defop VTIMPLANT() {
  comment(text : "VT Implant")
  implant(species : bf2,
          dose : <(vt-dose)> /cm2,
          energy : <(vt-energy)> keV,
          side : front,
          type : &Th_Adjust_Impl)
}
```

Figure 2: An input deck template.

accessible for subsequent simulation tools. Users are able to form sequences of simulation tools and link these tools in order to create so called *models* which serve as an encapsulation of that sequence. Additionally, SIESTA offers the capability to create simulation networks of individual models (which themselves encapsulate simulation tools). Fig. 4 illustrates how this feature is utilized in order to include several measurements into the inverse modeling procedure. Each part of this network evaluates the accuracy of the simulation model with respect to specific measurements, and returns a vector of float values quantifying the accuracy. Finally, these vectors are concatenated into a vector which represents an overall measure of accuracy for all measurements under consideration. This vector will be fed back to a Levenberg-Marquardt optimizer. Thus, we are able to enhance the confidence of the inverse modeling procedure by including as many measurements as possible.

3. Parallel Computation

Inverse modeling represents a considerable computational effort. Optimizers typically evaluate the Jacobian of the simulation model with respect to the parameters to be optimized. This means that the modeling network described above has to be evaluated at least once per parameter, and thus numerous evaluations are necessary. SIESTA performs parallel and distributed computation on a heterogeneous cluster of workstations in order to keep simulation time within an acceptable time scale [2]. A dynamic load balancing mechanism optimizes the utilization of the available computer hardware and a tool management mechanism handles simulation tools and their licenses.

4. Application

An example demonstrates the extraction of the channel profile of a CMOS fabrication technology (Fig. 6). Electrical measurements (transfer and output characteristics) of MOS devices with gate lengths of 0.18μm, 0.25μm, and 0.5μm are used to determine the vertical doping profiles of the devices. Fig. 3 depicts the simulation network which evaluates a device with a given gate length and an analytical doping profile defined by several parameters. A model named *gendevice* generates an NMOS device according to the input settings. In the following two models named *mmnt-idvg* and *mmnt-idvd* evaluate the transfer and the output characteristics, respectively, of that device using the device simulator MINIMOS-NT [3]. The models named *compare-idvg* and *compare-idvd* compare the results of device simulation to measurements, and deliver a vector of floating point numbers which describe a measure of *match* for each operating point under consideration. Finally, these match vectors for transfer and

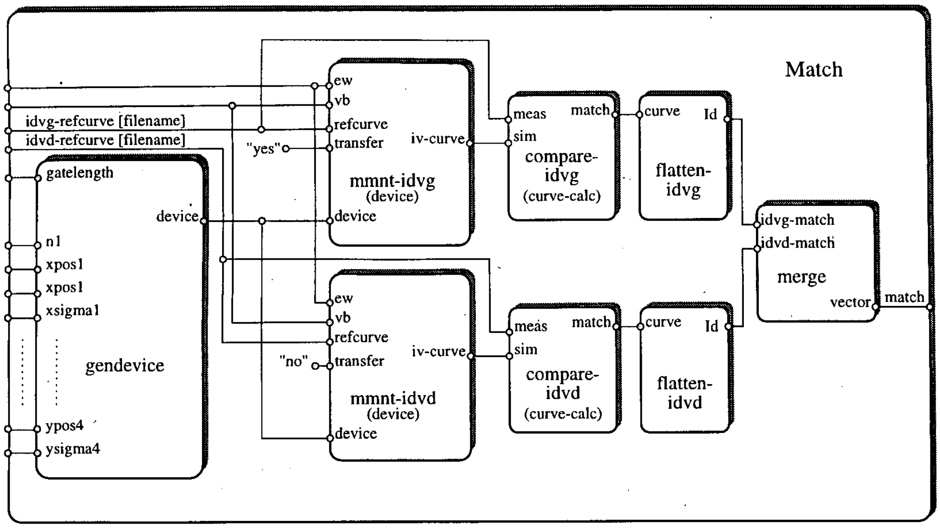


Figure 3: A simulation network for the evaluation of a given device structure defined by the input settings.

output curves are concatenated and delivered as the result of the whole model. An evaluation network as depicted in Fig. 4 is designed on the basis of the model depicted in Fig. 3 in order to evaluate devices with different gate dimensions simultaneously.

Fig. 6 shows the measured transfer curves, the simulated results corresponding to the initial channel doping, and the transfer curves obtained from the channel profile which resulted from inverse modeling. As can be seen from Fig. 6 the system is able to identify a doping profile which delivers an excellent fit. The example can easily be extended in order to include additional measurements (e.g. different potentials at the bulk contact etc.). Despite the enormous effort which is related to these device

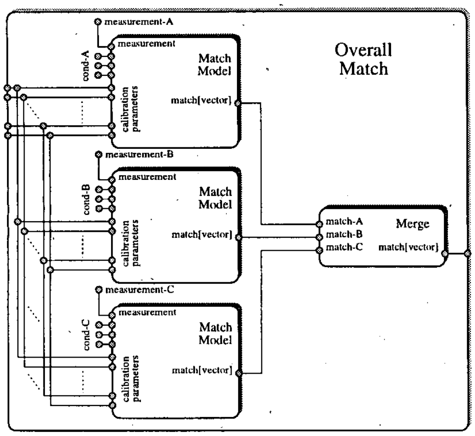
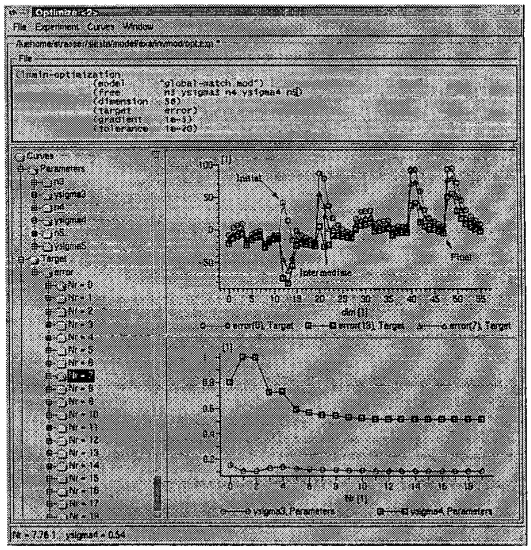


Figure 4: Overall accuracy evaluation.



```
(main-optimization
              (model      "global-match.mod")
              (free       n3 ysigma3 n4 ysigma4 n5)
              (dimension  56)
              (target     error)
              (gradient   1e-3)
              (tolerance  1e-20)
```

Figure 5: A graphical user interface.

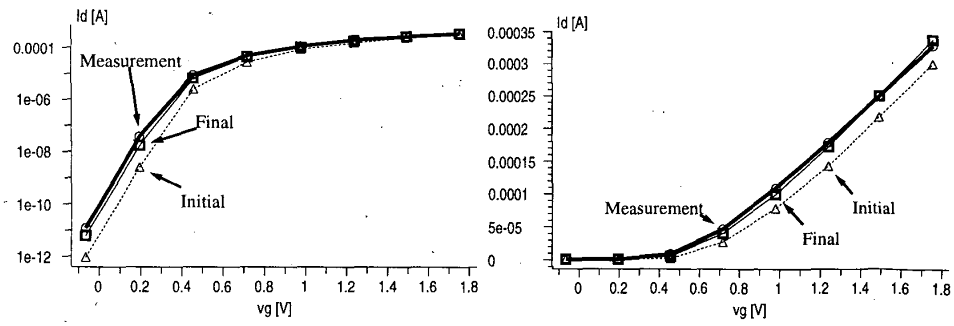


Figure 6: The drain current for $V_d = 1.5\text{V}$ of the $0.5\mu\text{m}$ device as measured, for the initial doping profile, and for the final doping profile.

simulations during the optimization procedure, the experiment takes no more than a couple of hours on a cluster of twenty workstations. A graphical user interface assists users during the inverse modeling experiment (Fig. 5). The history of the model's parameters and its accuracy can be browsed graphically.

5. Conclusion

The presented system has successfully been applied to calibration problems, parameter identification/extraction, and to the extraction of doping profiles on the basis of electrical measurements. In practice the open tool interface has proven to be extremely valuable since arbitrary simulation tools can either be calibrated or they can be utilized to extract doping profiles. State of the art TCAD tools (PROMIS, DIOS, TSUPREM, MINIMOS, DESSIS, and MEDICI) have been used in conjunction with SIESTA. The performance as well as the robustness of the system encourage SIESTA's usage for routine tasks in an industrial environment. Due to parallel computation the overall computation time is no longer a severe constraint for TCAD experiments of this kind.

References

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[3] T. Binder, K. Dragosits, T. Grasser, R. Klima, M. Knaipp, H. Kosina, R. Mlekus, V. Palankovski, M. Rottinger, G. Schrom, S. Selberherr, and M. Stockinger, *MINIMOS-NT User's Guide.* Institut für Mikroelektronik, 1.0 ed., 1998.

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