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AN EXTENDABLE MULTI-PURPOSE SIMULATION AND OPTIMIZATION FRAMEWORK FOR THERMAL PROBLEMS IN TCAD APPLICATIONS

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ABSTRACT

We present the capabilities of our optimization framework in conjunction with typical applications for thermal problems. Our software package supports a wide range of simulators and optimization strategies to improve electronic devices in terms of speed, reliability, efficiency, and to reduce thermal degradation due to mechanical influences. Moreover, we show several optimization examples, where we succeeded to extract electro-thermal material and process parameters. These new material parameters can be applied to more complex device structures and to obtain a better insight into the physics of semiconductor devices.

1. INTRODUCTION

State-of-the-art semiconductor process technology nodes require materials working near their limits to meet the proposed performance from the ITRS (International Technology Roadmap for Semiconductor) [1]. In addition to the commonly known properties of the involved materials, parasitic effects have to be considered as well, since even small fluctuations of process parameters cause variations of device geometries. During operation, grain effects or reliability failures may occur, which change the device characteristics dramatically. Therefore, new models and methods have to be developed in order to describe the observed behavior with sufficient accuracy in TCAD (technology computer-aided design) software. Today's semiconductor devices and interconnect structures have already reached a level of complexity, where the behavior of the included materials cannot be rigorously described by simple and basic equations because of limited knowledge of material parameters and material interactions. Different fundamental approaches have been proposed, e.g. ab-initio simulations, but their applicability to structures of industrial interest is still limited. Therefore, parameterized models are required as a sufficient description of the observed device characteristics within reasonable time for computation.

In the following we introduce our simulation and optimization framework, where we present its different operation modes: *calibration*, *parameter extraction*, and *optimization*. Furthermore, we demonstrate these optimization techniques for efficiency maximization of a thermoelectrical generator and model calibration of a thermochemical reaction for material deposition.

2. SIESTA

Highly sophisticated simulation and optimization environment frameworks [2, 3] support a wide range of simulators, optimizers, and optimization strategies. Contrary to commercially available software [2, 4], our framework SIESTA (*Simulation Environment for Semiconductor Technology Analysis*) [5] provides an open architecture for numerous types of simulators and optimizers to be individually chosen for a particular problem. In order to achieve fast and accurate optimization results, this simulation environment offers modular and flexible interfaces by which external tools can be easily integrated [5] and even combined with each other.

Fig. 1 depicts an abstracted data flow for a SIESTA optimization. The presented optimization procedure consists of a loop which terminates when the result has reached the required accuracy determined, for instance, by the first derivative of the objective score function. An-

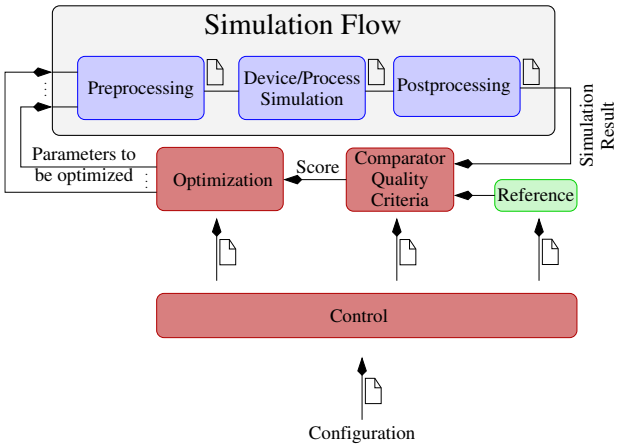

Figure 1: Overview of the data flow during an optimization with SIESTA.

other possible termination criterion is that the optimizer has found a local optimum which cannot be further improved with a gradient based optimizer [6]. For genetic or evolutionary approaches [3], the loop also terminates, if the maximum number of evaluated genomes has been reached.

During start-up, SIESTA generates an initial parameter set based on the user's initial guess within user-defined constraints for each simulation branch. After applying post processing tools, the simulation result is parsed in order to extract a representative quantity for comparing it with reference data. A score value is determined which indicates the quality how well these two data sets match. The optimizers use the computed score value to generate the parameter set to improve the score value that will be evaluated after each simulation run based on the currently generated parameter set. A typical example for reference data are measurements where also additional requirements can be specified to meet specific physical constraints under certain conditions.

2.1. Optimization Methods

SIESTA supports different optimization modes which can be categorized into gradient-based [7, 8] techniques, genetic approaches [9, 10], and heuristic approaches [11]. All these techniques have their own benefits and drawbacks and the user can decide which one to use for a particular problem. To provide the appropriate capabilities for problems related to thermal coupled systems, e.g. a calibration for a chemical vapor deposition (CVD) process model or an optimization to improve the efficiency of an electro-thermal generator, a simulated annealing optimization strategy has been chosen to provide a good combination of a fast local parameter search and the global search character due to its heuristic parts in the optimization algorithm [11].

All in SIESTA available optimization techniques fit well for highly nonlinear optimization problems. For the examples shown in Section 3, some of the input parameters depend implicitly on other input parameters, and, e.g., therefore also constraints may change which can be seen for a special radiosity model [12] that describes a temperature-driven chemical reaction for material deposition. To represent the physics, constraints are used to force the optimizer to use reasonable parameter sets. Due to implicit cross-dependencies between input parameters and boundary conditions, the constraints may also change with a new optimization state. A big challenge are optimizations with restrictions for the simulation, e.g., if the temperature reaches a certain value, where simulation is no longer able to predict the device behavior appropriately [13] due to inadequate physical models, appropriate constraints have to be applied to ensure that the internal states of the simulation models as well as the its output parameter remain valid.

Most of the optimization algorithms used in SIESTA support such restrictions only rudimentary. Therefore, only a limited number of optimizers can be used for these specific tasks. Thus, the user has to carefully design the specifications of a problem, otherwise the optimization can become instable and an interaction with the user is necessary, or the optimization process might not converge at all.

SIESTA itself consists of several functional blocks which are shown in Fig. 2. The experiment and the configuration can be setup either with a graphical user interface (GUI) or using text-based templates. Text-based configuration offers many more possibilities for tool combinations and is more flexible than the GUI where only a limited number of problem classes based on predefined templates can be handled. Once the experiment has been setup, the experiment definition is submitted to the SEILIB (SIESTA *environment interaction library*) which handles the interaction between the optimization software tools and the actual execution on different hosts in a heterogeneous network. Moreover, SEILIB provides a sophisticated host management which enables to use advanced load balancing on a heterogeneous network.

After the scheduled simulations have successfully been finished, the simulation results are submitted to the job database with the experiment definition. The quality of the simulation result is determined by using a user-defined score function to notify the optimizer to submit an updated parameter set for the next optimization loop according to the received quality criterion. The optimization results of SIESTA can be tracked via visualization tools as well as by simple text files for data manipulation and logging purposes.

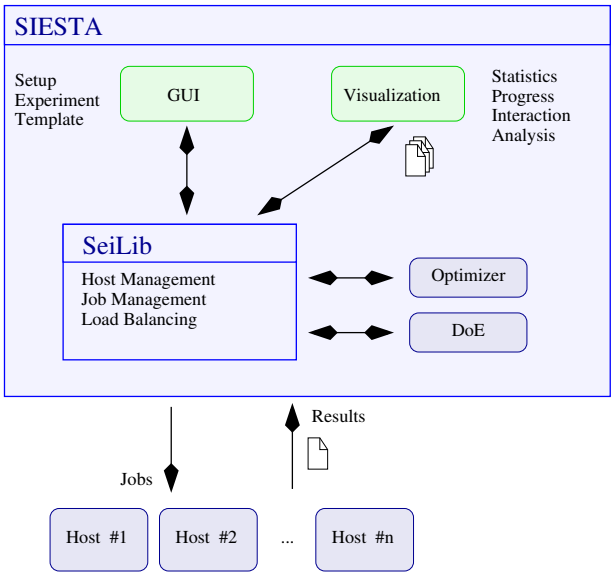

Figure 2: Overview of the internal structure of SIESTA showing various configurable modules.

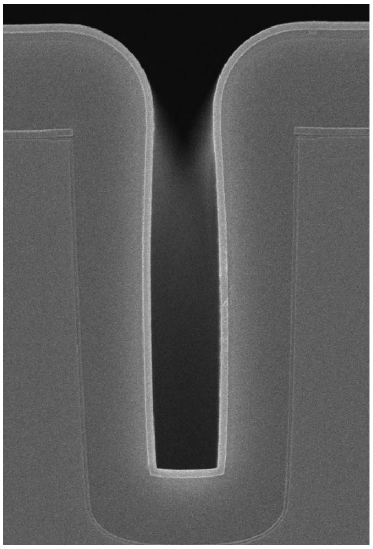

Figure 3: TEM picture of a trench structure for identification of sticking coefficients of a LPCVD TEOS deposition model.

Currently available optimization modes for SIESTA [5] are *optimization*, *calibration*, *parameter extraction*, and *design of experiment* (DOE). Each of the optimization-related modes can be configured for minimization or maximization. The DOE [14] mode computes the score function for a whole parameter space with a certain user-definable algorithm to cover all regions of interest. The output of a DOE can be fed to a database for design engineers to improve their productivity by reducing waiting periods for simulation inquiries. In all these optimization modes, the score function which indicates the quality of the simulation result will be minimized or maximized, depending on the optimization goal. With this abstract modeling of the optimization procedure, the behavior can be tuned for particularly complex needs.

The default operation mode is *optimization*, which targets a specified scalar-valued quantity, for instance the power output of a simulated device, a leakage current of a transistor, or side effects like parasitic capacitances, or the on-resistances of transistors. Furthermore, power consumption, maximum temperature of a device, and the maximum value of the electric field can be optimized with an appropriate setup. In addition, combinations of different device parameters like the gain of amplifier devices, different sorts of yield, efficiencies, or the ratio of capacitance per area for memory cells can be optimized.

The *calibration* mode is commonly used for inverse modeling [2, 5]. In this mode SIESTA optimizes parameters in order to fit specific requirements consisting of output characteristics or constraint equations. The simulation results shown in Section 3.1, depict the outcome of the calibration of a given model, where the quality criterion is the difference between the simulation result and the reference measurement.

The operation of *calibration* and *parameter extraction* is quite similar. Calibration requires a good initial guess, whereby the initial parameter vector for the parameter extraction is not well known. Therefore, parameter extraction often requires a global optimization techniques due to the possibly large uncertainty of the given initial values.

2.2. Simulation Tool Flow

Since SIESTA offers a text-based open application interface [15], it is very easy to add additional simulation software tools to a particular simulation tool flow. SIESTA provides several interfaces to commercial as well as to tailor-made simulation tools.

3. APPLICATIONS

3.1. TEOS Deposition

Material deposition processes can be accurately described by thermo-chemical reaction mechanisms [16, 17]. However, the quantitative predictability of such fairly complex models is still limited for processes of industrial interest [18] in terms of time and in terms of accuracy due to fluctuations in the process conditions. Thus, simple calibrated process models applying sticking coefficients are a good alternative for process investigations [19]. Especially for problems with high temperature variations, this approach reduces the computational effort drastically by orders of magnitude. Our attempt

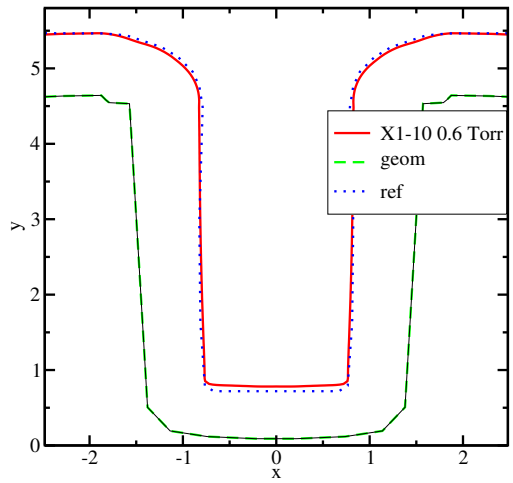

Figure 4: Comparison of simulation and measurements for LPCVD TEOS deposition for a trench with a low aspect ratio at 0.6 Torr.

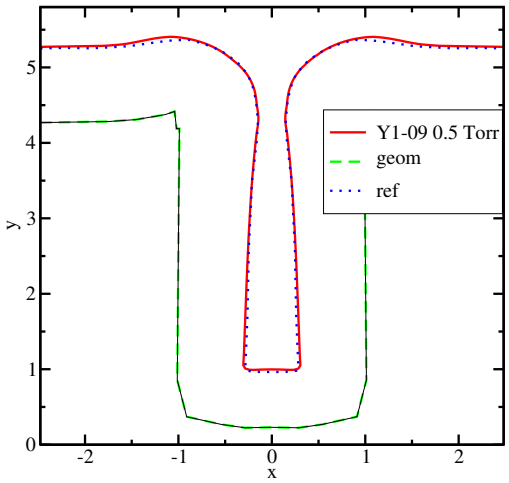

Figure 5: Comparison of simulation and measurements for LPCVD TEOS deposition for a trench with a high aspect ratio at 0.5 Torr.

is to investigate whether it is possible to determine a valid parameter set for LPCVD (low pressure chemical vapor deposition) of TEOS at different temperatures and ambient pressures. The simulator ELSA (enhanced level-set applications) [12, 20] has been calibrated by measurements from literature [21] for typical trenches filled with silicon oxide from TEOS deposition as depicted in Fig. 3.

As input parameters for the calibration process we provided the sticking coefficients for a LPCVD TEOS deposition model proposed in [20] to describe the pyrolytic thermo-chemical reaction for deposition.

The calibration result for the first trench presented in Fig. 4 excellently agrees for the highly nonlinear equation system, and also other trenches for different temperatures and ambient pressures (cf. Fig. 5) show good agreement with measurements.

In addition, the identified parameter set is valid for a whole series of available test trenches, where the aspect ratio is in the range of 1.1 to 3.5. Typically, according to the depletion of the reactant at the bottom of the trench, the deposition model with sticking coefficients produces a larger error, if applied to trenches with larger aspect ratios.

3.2. Thermo-Electric Generator

Thermo-electric power generators made of SiGe alloys which exploit thermal gradients [22] are interesting for future waste heat recovery applications because of their potentially high reliability.

Several device structures based on the SEEBECK effect have been proposed to the conversion of heat to electrical power. As of yet, however, none of these approaches is suitable for industrial application or economical use.

We investigated and optimized a novel device structure for electro-thermal energy conversion with the goal to gain optimum power outputs as well as efficiencies for given thermal environments. A principle sketch of the device is depicted in Fig. 6.

This presented thermo-electric generator consists of a large scale pn-junction with different thermal boundary conditions at each side of the junction. The heated side implies a zone where free electron-hole pairs are thermally generated and separated by the built-in potential of the pn-junction [23]. Electrical contacts are mounted at the cold side of the structure where an actively cooled heat sink forces the temperature at the cold side to room temperature.

Due to the strong temperature gradient along the pn-junction, the free carriers experience a driving force towards the cooled side. As a limiting factor, the thermal conductivity of the involved materials causes also a high heat flux from the heated to the cooled side. This in principle parasitic heat flux has to be minimized in order to obtain good efficiencies. Therefore, our goal is to obtain high power output through the introduction of graded material compositions Si_xGe_{1-x} as well as proper device geometries in order to achieve an appropriate temperature distribution for maximized carrier generation, optimum electrical transport conditions, and minimized heat flux.

For our investigations we used the three-dimensional device simulator MINIMOS-NT [24] and SIESTA in the advanced two-loop *optimization* mode, where we extract the necessary load resistance for power match in the

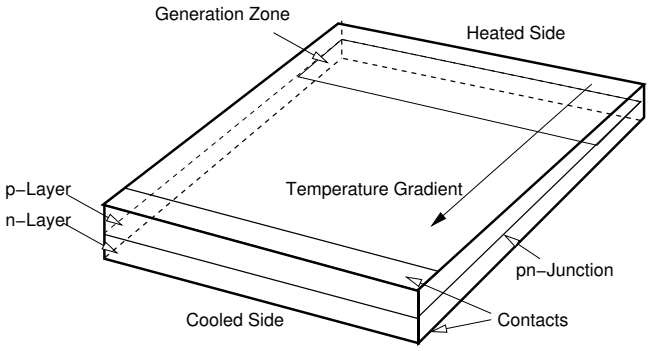

Figure 6: Thermo-electrical power generator structure using a temperature gradient to exploit the SEEBECK effect.

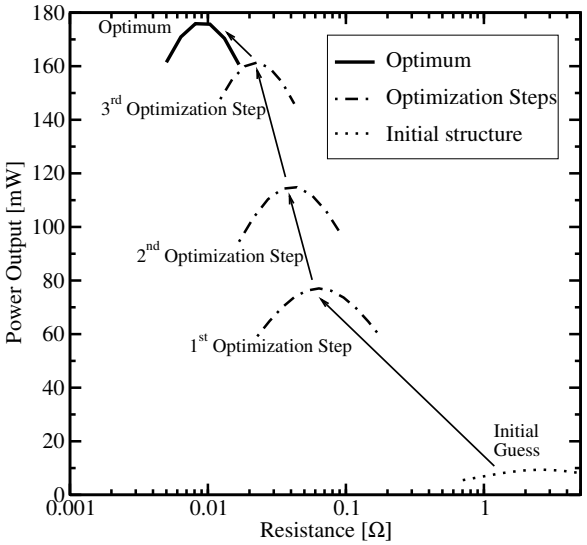

Figure 7: Comparison of different optimization results after different stages of optimization.

first optimization loop to obtain the best result for each single material composition. The thereby obtained intermediate result is provided for the calculation of the corresponding power output and for determining the device's power conversion efficiency. The efficiency has been taken as an objective target for the overall optimization process (second optimization loop).

As a result we achieved the position-dependent concentration of Ge and the predicted power output of the semiconductor device structure. The sensitivity of the power output to several parameters is tracked in order to remain within the manufacturing tolerances. Fig. 7 presents the optimization procedure in four major steps.

As an initial guess, a Si-based device structure has been optimized by introducing a step-like Ge concentration profile as a first enhancement. As a second step and further improvement, the Ge content has been adapted to obtain a good local temperature distribution in order to maximize the total amount of generated carriers as well as the local SEEBECK effect.

Moreover, a layout optimization further improved the efficiency by adapting the electrical transport conditions in a third optimization step. The global optimum for the power output was obtained by introducing certain doping profiles which maximizes the power output.

4. CONCLUSIONS

We have presented SIESTA as a powerful and highly sophisticated optimization tool which can deal with thermal problems to perform optimizations on non-linear electro-thermal semiconductor equations systems in MINIMOS-NT as well as on technology-related processes in ELSA including transient thermo-chemical simulation tasks.

Moreover, these two applications have demonstrated the capability of this optimization tool to deal with a wide range applications due to its open application interface to other commercial and tailor-made tools, which enables to provide appropriate optimizations techniques for highly complex systems like thermally coupled electrical and chemical systems.

5. ACKNOWLEDGMENTS

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6. REFERENCES

[1] Semiconductor Industry Association, "International Technology Roadmap for Semiconductors - 2005 Edition", 2005, `http://public.itrs.net`.

[2] Synopsys, *TCAD Sentaurus Y-2006.06 User Manual*, Synopsys, Mountain View, 2006.

[3] C. Heitzinger and S. Selberherr, "An Extensible TCAD Optimization Framework Combining Gradient Based and Genetic Optimizers", in *Proc. SPIE International Symposium on Microelectronics and Assembly: Design, Modeling, and Simulation in Microelectronics*, Singapore, 2000, pp. 279–289.

[4] ISE Integrated Systems Engineering AG, Zürich, Switzerland, *GENESISe, ISE TCAD Release 10.0*, 2004.

[5] Institute for Microelectronics, *SIESTA – The Simulation Environment for Semiconductor Technology Analysis*, Technische Universität Wien, Austria, 2003.

[6] R. Plasun, *Optimization of VLSI Semiconductor Devices*, Dissertation, Technische Universität Wien, 1999.

[7] P. Spellucci, *Donlp2 Users Guide*, NetLib Project, 1995.

[8] D. W. Marquardt, "An Algorithm for the Estimation of Nonlinear Parameters", *J. Soc. Ind. Appl. Maths.*, vol. 11, pp. 431–441, 1963.

[9] J. Holland, "Adaption in Natural and Artificial Systems", *University of Michigan Press, Ann Arbor, MI*, 1975.

[10] M. Wall, "GAlib A C++ Library of Genetic Algorithm Components", *Massachusetts Institute of Technology*, 2000, `http://lancet.mit.edu/ga`.

[11] L. Ingber, "Genetic Algorithms and Very Fast Simulated Re-Annealing: A Comparision", *Mathematical and Computer Modelling*, vol. 16, pp. 87–100, 1992.

[12] A. Sheikholeslami, C. Heitzinger, H. Puchner, F. Badrieh, and S. Selberherr, "Simulation of Void Formation in Interconnect Lines", in *SPIE's first International Symposium on Microtechnologies for the New Millennium: VLSI Circuits and Systems*, Gran Canaria, Spain, May 2003, pp. 445–452.

[13] S. Holzer, R. Minixhofer, C. Heitzinger, J. Fellner, T. Grasser, and S. Selberherr, "Extraction of Material Parameters Based on Inverse Modeling of Three-Dimensional Interconnect Fusing Structures", *Microelectronics Journal*, vol. 35, no. 10, pp. 805–810, 2004.

[14] T.J. Lorenzen and V.L. Anderson, *Design of Experiments*, Marcel Dekker, New York, 1991.

[15] S. Holzer, A. Sheikoleslami, S. Wagner, C. Heitzinger, T. Grasser, and S. Selberherr, "Optimization and Inverse Modeling for TCAD Applications", in *Symposium on Nano Devices Technology 2004*, Hsinchu, Taiwan, May 2004, pp. 113–116.

[16] G. Schumicki and P. Seegebrecht, *Prozeßtechnologie*, Springer, 1991.

[17] G.B. Raupp, F.A. Shemansky, and T.S. Cale, "Kinetics and Mechanism of Silicon Dioxide Deposition Through Thermal Pyrolysis of Tetraethoxysilane", *J.Vac.Sci.Technol.B*, vol. 10, no. 6, pp. 2422–2430, 1992.

[18] M. E. Coltrin, P. Ho, H. K. Moffat, and R. J. Buss, "Chemical Kinetics in Chemical Vapor Deposition: Growth of Silicon Dioxide from Tetraethoxysilane (TEOS)", *Thin Solid Films*, vol. 365, no. 2, pp. 251–263, 2000.

[19] T. S. Cale, T. P. Merchant, L. J. Borucki, and A. H. Labun, "Topography Simulation for the Virtual Wafer Fab", *Thin Solid Films*, vol. 365, no. 2, pp. 152–175, Apr. 2000.

[20] A. Sheikholeslami, S. Holzer, C. Heitzinger, M. Leicht, O. Häberlen, J. Fugger, T. Grasser, and S. Selberherr, "Inverse Modeling of Oxid Deposition Using Measurements of a TEOS CVD Process", in *PhD Research in Microelectronics and Electronics - PRIME 2005*, Lausanne, 2005, vol. 2, pp. 279–282.

[21] C. Heitzinger, J. Fugger, O. Häberlen, and S. Selberherr, "Simulation and Inverse Modeling of TEOS Deposition Processes Using a Fast Level Set Method", in *Simulation of Semiconductor Processes and Devices*, Kobe, Japan, Sept. 2002, pp. 191–194.

[22] G. Span, M. Wagner, and T. Grasser, "Thermoelectric Power Generation Using Large Area pn-Junctions", in *The 3rd European Conference on Thermoelectrics Proceedings ECT2005*, Nancy, Sept. 2005, pp. 72–75.

[23] G. Span, M. Wagner, and T. Grasser, "Thermoelectric Power Generation Using Large Area Si/SiGe pn-Junctions With Varying Ge-Content", in *2006 International SiGe Technology and Device Meeting Conference Digest*, Princeton, May 2006, pp. 216–217.

[24] Institut for Microelectronics, *MINIMOS-NT 2.1 User's Guide*, Technische Universität Wien, Austria, 2004.