Methodology For Predictive Calibration Of TCAD Simulators

Gilles Le Carval, Pascal Scheiblin*, Dominique Poncet, and Pierrette Rivallin
LETI (CEA - Technologies Avancées) DMEL-CENG, BP85X 38054 Grenoble Cedex 9, France
* CISI Région Rhône-Alpes; 6, rue de l'Arcelle, Z.I. des Plans, 38600 Fontaine, France

Abstract— This paper presents an original methodology for calibrating Technology Computer-Aided Design (TCAD) simulators. This approach associates physical analysis of models, statistical analysis of data, and systematic use of Design of Experiments. This new concept, inspired by the Taguchi's methodology, allows to minimise the difference between simulations and measurements while being the less sensitive to the fluctuations of the manufacturing process. The methodology fits well with economic constraints by only using the existing data, and by reusing previous calibration works.

I. INTRODUCTION

In this paper we propose an original strategy to obtain a set of calibrated model parameters for predictive simulations. This methodology associates Design of Experiments (DOE) with Response Surface Method (RSM) but also advanced concepts of statistical analysis: D-optimal filtering and Taguchi's method [1,2]. It has the following characteristics: insensitivity to process conditions, optimal use of existing experimental results, rigorous statistical analysis of the data, and clever selection of the model parameters. Moreover, its capability to continuously incorporate further data confers an increasing robustness on the methodology. The strategy may be adjusted to any type of model and is illustrated with the examples of a numerical oxidation model and a mobility model for electrons.

II. THE METHODOLOGY

One of the greatest desires of device engineers is to dispose of physically based simulators with meaningful predictive capabilities. One way to improve prediction is to implement new models containing more accurate physics in simulators, and to adjust their parameters. Unfortunately, time, money and relevant experimental data are rarely available to achieve this task before processing the new device generations. This leads to a real need for a pragmatic method for calibrating commercially available simulators.

DOE combined with TCAD are now classically used for process optimisation [3,4]; attempts have also been done to use them for calibrating [5] model parameters. These approaches suffer from an inherent weakness: they don't take into account the global behaviour of the experimental domain but only "test points", so the resulting calibrated parameter set is only valid for the experimental conditions that were used for calibration.

The first key point of the method we propose overcomes this difficulty: it makes the calibration independent of the experimental conditions in the domain of interest. For this purpose we use the Taguchi method which allows to optimise a process, while making it robust with regard to experimental variability. The originality of our approach is to define Taguchi's control factors as the model parameters of the simulator, and the noise factors as the process parameters. A consequence of this approach is that the fluctuations due to equipments in real fabs, which are not negligible, will not affect the calibration.

The second key idea of our methodology is to obtain a calibration from the optimal use of existing data, without running any complementary experiment: to reach this objective, we use D-optimal filtering, which ensures the best coverage of a given experimental domain.

For each type of physical model of simulators, the flow consists of three principal steps as outlined in Fig. 1.

Initially, model and process parameters follow parallel treatments. First, they are chosen and sorted according to the physical analysis of the model and the relevance of existing data.

Secondly, a DOE is constructed on the model parameters of the simulator. Concerning experiments, as stated above, a D-optimal filtering permits to choose the necessary set of

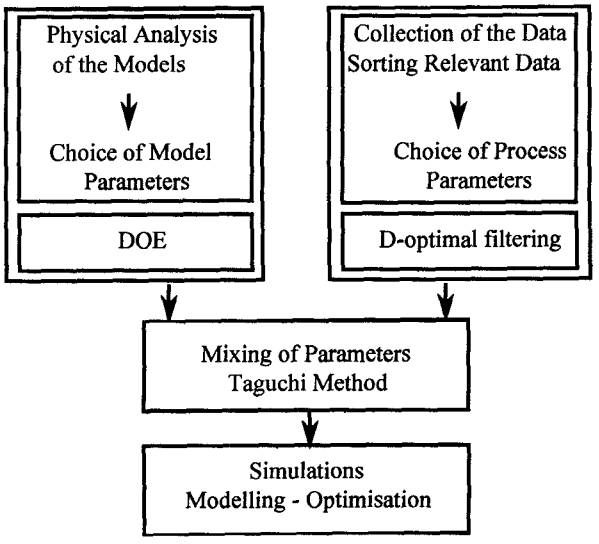

Fig. 1 : Outline of the methodology

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process parameters, among the previously sorted experiments. Then, following the requirements of the Taguchi method, responses and control factors are defined. The responses must be chosen to be the most sensitive to the studied model, and exclusively dependant on it.

Finally, using the simulation results and subsequent optimisation, the analytical modelling of responses versus the model parameters of the simulator supplies the set of calibrated parameters, the less sensitive to the experimental conditions.

III. Calibrating Numerical Oxidation

A. Application of the Methodology

The growth of SiO_2 is modelled following the Deal and Grove relationship, modified to account for the fast initial growth regime. The oxide thickness (*Tox*) obeys the law:

$$\frac{dTox}{dt} = \frac{B}{A + 2\,Tox} + Rth, \qquad (1)$$

where *B/A* and *B* are respectively the linear and parabolic constants, and *Rth* the growth rate of the initial thickness.

In the case of oxidation, the number of experiments available at our site is quite high, and the complexity of the furnace recipes is a real difficulty: each recipe contains many oxidising steps, with different time, temperature and gas flows characteristics. The calibration of the model over the whole range of these experimental conditions would lead to about fifty model parameters and a tenth of process parameters to consider. This is obviously not tractable, so we decided to classify the recipes: we focus in this paper on the calibration of dry oxidation of low doped silicon below 950°C, in presence of Chlorine.

In the chosen experimental range *B/A*, and *Rth* express as:

$$\frac{B}{A} = \boldsymbol{l0} \exp\left(\frac{-\boldsymbol{le}}{kT}\right) (P_{O2})^{\boldsymbol{p}}\, \boldsymbol{L_{HCl}(T)}, \qquad (2)$$

$$Rth = \boldsymbol{t0} \exp\left(\frac{-Tox}{\boldsymbol{tl}}\right) \exp\left(\frac{-\boldsymbol{te}}{kT}\right) \qquad (3)$$

As the parabolic regime will not be reached for the thickness range in this work, the parabolic constant *B* is kept to its default value. In (2) and (3) *T* is the temperature, and P_{O2} the partial oxygen pressure. The model parameters are indicated in bold fonts.

The selected oxidation recipes consist in two oxidising steps with some additional inert anneals. The experimental parameters are the durations of the two oxidising steps, the HCl partial pressure and a bloc variable indicating the step in which HCl is introduced. We assumed a linear model on these 4 process parameters, the D-optimal sorting chose the 6 most relevant experiments among the set of candidates.

For the 8 model parameters, an algorithmic DOE allows to build a quadratic model with 79 trials. The range of parameters is given in Table 1.

TABLE 1
PARAMETERS RANGES DETERMINED FROM DEFAULT VALUES [6].

Model parameter	Minimum value	Maximum value
l0 (μm/min)	60216	63305
le (eV)	1.95	2.05
t0 (μm/min)	6.24e+6	6.9e+6
te (eV)	2.32	2.42
tl (μm)	0.006	0.0078
p	0.5	1
LHCl(900)	1.67	1.83
LHCl(950)	1.54	1.7

Finally we mixed these 2 designs to define the inner and outer arrays of the Taguchi design. The 474 resulting numerical simulations were performed and automatically managed by a commercially available software package [6].

Here the responses are the differences between simulated and measured oxide thickness. The objective of the Taguchi method is to maximise the signal to noise ratio *Z*:

$$Z\_Tox = -10 \log\left(\frac{1}{n} \sum \left(\frac{Tox_{\,exp} - Tox_{\,simul}}{Tox_{\,exp}}\right)^2\right) \qquad (4)$$

where *n* is the number of experiments of the outer array.

B. Results

The following regression model was found for *Z* (centred parameters):

$$Z = 1.9 + 8.4\,\boldsymbol{le} - 2.9\,\boldsymbol{te} - 0.39\,\boldsymbol{L_{HCl}(950)} - 138\,\boldsymbol{le.te} + 2954\,\boldsymbol{le.tl} + 17\,\boldsymbol{le.L_{HCl}(950)} - 5.5e\text{-}7\,\boldsymbol{p.t0} - 1370\,\boldsymbol{te.tl} + 6\,\boldsymbol{L_{HCl}(950).L_{HCl}(900)} - 212\,\boldsymbol{le}^2 - 1.44\,\boldsymbol{p}^2$$

This model was maximised to obtain the optimal point. The improvement of the simulation due to calibration is evaluated by the mean square difference between simulated and measured thickness over the whole set of experiments. We obtained a set of calibrated model parameters leading to a simulation accuracy of 3%, now insensitive to process

fluctuations. These parameters are summarised in Table 2.

TABLE 2
DEFAULT AND CALIBRATED OXIDATION MODEL PARAMETERS.

Model parameter	default value	calibrated value
l0 (μm/min)	61761	60326
le (eV)	2.0	2.04
t0 (μm/min)	6.57e+6	6.24e+6
te (eV)	2.37	2.31
tl (μm)	0.0069	0.007
p	0.75	0.9
LHCl(900)	1.75	1.61
LHCl(950)	1.618	1.8

IV. SECOND APPLICATION: LOW FIELD MOBILITY OF ELECTRONS

The same methodology has been applied for the calibration of the low field mobility of electrons (CVT model) [6], on a 0.25 μm technology. In this case, 8 parameters of the model have been calibrated, and 27 experimental splits of channel and/or source-drain architectures have been used. The chosen responses are 3 SPICE model parameters (M0, R_T, Ilin) for the linear current (5), (6):

$$Id = \left(M0 \frac{Vg - V_T}{1 + Tg(Vg - V_T)} \right) (Vd - R_T Id) \quad (5)$$

$$\text{with } M0 = \frac{\mu_0 Cox W}{L} \quad (6)$$

They are related to the microscopic phenomena included in the CVT mobility model [6]. These parameters are given with their ranges in Table 3.

TABLE 3
PARAMETER RANGES FOR THE MOBILITY MODEL

Model parameter	Miminum value	Maximum value
B (cm/s)	4.75e+7	9.5e+7
C	1.74e+5	5.22e+5
τ	0	0.375
μ0 (cm^2/(Vs))	26.1	156.6
Cr (cm^{-3})	4.84e+16	2.904e+17
α	0	1.36
β	2	4
δ	5.82e+14	1.164e+15

Table 4 gives the calibrated parameters and Table 5 shows the improvement of the signal to noise ratios for each response evaluated with the increase of the ratio Z.

TABLE 4
DEFAULT AND CALIBRATED MOBILITY MODEL PARAMETERS

Model parameter	Default	Optimum
B (cm/s)	4.75e+7	7.125e+7
C	1.74e+5	3.48e+5
τ	0.125	0.375
μ0 (cm^2/(Vs))	52.2	26.1
Cr (cm^{-3})	9.68e+16	4.84e+16
α	0.68	0.68
β	2	2
δ	5.82e+14	1.164e+15

TABLE 5
IMPROVEMENT OF SIGNAL TO NOISE RATIOS.

	Default	Optimum
Z_M0	13.33	13.40
Z_RT	8.31	10.37
Z_Ilin	15.30	16.37
sum of Z	36.93	40.14

V. CONCLUSION

We have proposed a global strategy for optimising TCAD simulators and reach prediction. This approach overcomes the insufficiencies of the physical models by tuning the parameters of the simulator, but casts off the effect of process fluctuations, thanks to the Taguchi method. Then, the same set of model parameters is expected to be convenient, even when changing to the further device generation. Therefore, our methodology clearly appears wafer-saving. The calibration flow can be carried out using existing experimental data without extra experiments, and updating is easy by incorporating any new results as soon as available: the initial work is then reusable and enriched at each iteration of the procedure. These advantages of the methodology make it suitable to be involved within an industrial manufacturing environment.

REFERENCES

[1] G. E. P. Box, N. R. Drapper, "Empirical model-building and response surface," Wiley N. Y. 1987.

[2] G. Taguchi, Y. I. Wu, "Introduction to off-line quality control systems," Central Japan Quality Control Assoc., 1980.

[3] A.R. Alvarez *et al.*, "Application of statistical design and response surface methods to computer-aided VLSI device design," IEEE trans. on CAD, vol. 7 no. 2, pp 272-288, February 1988.

[4] G. Le Carval D. Poncet, G. Guegan and J. P. Caire, "Advantages of the methodology using DOE and simulation for optimizing advandced technologies,", Proc. of ESSDERC 94, Edinburgh 1994, pp 841-844.

[5] R. Cartuyvels, R. Booth, S. Kubicek, L. Dupas and K. M. De Meyer, "A powerful TCAD system including advanced RSM techniques for various engineering optimization problems," Proc. of SISDEP 93, Vienna 1993, pp 29-32.

[6] SILVACO user's manual, SILVACO International, 1995.