From process simulation to device optimization: how to satisfy the requirements of both research and industry.

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Abstract: while the complexity of microengineering increases, the need for simulation tools becomes mandatory to help process engineers to optimize processes. Numerical simulation is used for various purposes and at various stages of process development, ranging from basic research to industrial processes development and optimization. The requirements of these different kinds of users sometimes appear contradictory. This paper shows how a unique integrated tool can satisfy these different demands. Examples of use of the simulator TITAN, coupled with the optimizer PROFILE, illustrate the possibilities offered by automatic optimization

Introduction

Numerical simulation is now widely used in microengineering process development. The requirements, however, in terms of software quality and generality apparently differ from one usage to another. In an industrial environment, simulation is used for process optimization; the need is expressed for dedicated tools, easy to use, integrating process and device simulation, capable of describing the device geometry under consideration, accurate and valid in the range of applications considered, proposing adapted post-processing and, if possible, able to provide sensitivity analysis and automatic optimization.

On the other hand, simulation is also used during the development and validation of new models. The validation of a model related to a given process step, or to electrical simulation, can often be achieved on simple structures, and does not necessarily require accurate simulation of the complete chain. For these reasons, the time and effort required to implement a new model in a complete simulator is generally considered as disproportionate, especially when the model is only at an early stage of development, so that very often separate programs are developed working under limiting conditions.

Finally, in advanced process development, simulation can also help process engineers to understand parasitic effects or to foresee the behaviour of new devices. This requires a flexible program integrating process and device simulation, containing as much physics as possible, so that unexpected effects can be predicted, possibly providing a choice between different models and access to the model parameter values, but also general enough to accept new geometry descriptions. However, this generality may render such a program difficult to use for a non-experienced user.

One simulator for multiple uses

The considerations above tend to support the idea that for each usage a different tool must be developed: research programs for developing models, dedicated industrial tools for optimizing technologies, more general integrated simulators for "advanced" users. However, the maintenance problems associated with multiple software tools leads to the question of why a general process and device simulator does not meet the requirements of industry. Indeed, the main reasons are that the industrialist does not want to deal with models and numerical considerations, and that the size of the user manual of such a program is discouraging. Consequently, a general tool will satisfy industry's requirements, if a dedicated user guide is proposed, and if choices by default have been made concerning the numerical and physical features. The main problem lies in adapting pre- and post-processing of a general program to a particular cause.

The approach proposed here for making a general program adaptable centres around two key-points: programmable input parser, programmable graphics processor.

First of all, the input language has to be simplified as much as possible, by the distribution of the numerous commands in consistent fields ("process", "device", "process>model" ...). For example, the description of a process chart will be made by using the commands accessible at the level "process"; access to the corresponding models will be made at the sub-level "process>model". For people interested in process

simulation, it should be possible to restrict themselves to the field "process" and ignore the other fields.

At the same time, the language description and default models associated with each physical effect for each material and dopant must be contained in external files, so that the program can be adapted to a given purpose by modifying these files to suppress unnecessary features or change the default models.

The graphics processor must also be programmable, and the description of the different pictures, default colors associated with dopants or currents, etc. be contained in an external file, so that it can be adapted to the needs of a specific use without changing the program itself.

This approach has been followed in the development of the TITAN program [1]. Consistency between the different process steps, the electrical simulation, the input parser and the post-processing is ensured by the use of general data structures [2], for both model description and device representation (geometry, meshing, dopants, electrical potentials...); this data structuring helps increase the evolution and maintenance capabilities of the program.

The same features (data structuring, modularity, high level input language, programmable graphics) make TITAN a programming environment for new models. The input parser, able to automatically generate data structures, allows the programming task for model management and interpretation to be minimized. The model developer can thus, with very little effort, take advantage of the existing environment - input language, geometry description, graphics processor.

Optimization

Thanks to the generalization of fast computers, allowing a large number of simulations to be run in a couple of hours, automatic optimization can now be foreseen. It can be useful for both model parameter fitting and process parameter optimization. In the latter case, two kinds of problems are classically encountered: in the case of process transfer, starting from an existing satisfactory process and changing a given process step (for example an ion implanter or the thermal annealing conditions), optimization can help retrieve the previous behaviour of the different devices. In general process optimization, the goal is to obtain given characteristics (for example, in MOS technologies, given threshold voltage and sub-threshold characteristics) while minimizing undesired parasitic effects.

These different problems have been tackled in the same general way, by coupling TITAN 6 with the general data processor and optimizer PROFILE [3]. In practice, the target is first defined, as a cost function to be minimized, and the optimization variables (model or process parameters) are marked in the input file for TITAN with question marks (Figure 1a). Starting guess values are given to these variables. Then, PROFILE drives successive runs of TITAN, by replacing each time the optimization variables by real values, following a Levenberg-Maquard algorithm to minimize the cost function.

model parameter fitting

A first range of applications is the model parameter fitting. For this purpose, the target is an experimental curve, or set of curves - either current versus voltage characteristics, or doping profiles, or digitalized experimental profiles. A small programming task may be necessary in the simulator to provide the results on a formatted file, for comparison between simulation and experiments.

For example, Figure 1 illustrates the fit of the deposition model of TITAN to oxide PECVD. This model is a mix of isotropic deposition and hemispherical model; the model parameters are the limiting angles of the gas flux (TETA1 and TETA2), the percentage of hemispherical deposition (ANISO), and the percentage of saturation (SATUR), corresponding, when above 100%, to the transition toward a reaction limited regime. Several experimental shapes define the target. The initial profiles (before deposition) and the deposited profiles (defining the target) are digitalized. The cost function to be minimized by PROFILE is the mean square distance between the experimental points and the corresponding simulated curves. The optimization variables were the half open angle for the hemispherical model (TETAOV2), and the values of ANISO and SATUR. This information is marked by question marks in the input file for TITAN (Figure 1a). The three parameters were voluntarily given starting values far removed from the

expected values. The result is illustrated in Figure 1b. It is a mix of 82% of pure hemispherical model (SATUR=100%, open angle 180°) and 18% of isotropic deposition.

The same method was successfully applied to the determination of a sputter yield curve (Figure 2) and of the parameters of a mobility model. In the latter case, the cost function was the mean square relative error between the simulated and measured currents. All tests carried out so far have shown good results in fitting of parameters, in spite of the noise produced by the discretization. This automatic parameter fitting is particularly interesting for cutting down on human resources when comparing the simulation results to a large number of experimental results for a global validation.

process parameter optimization

The second range of applications is the process parameter optimization. Although the software environment can be the same as for model parameter fitting, several difficulties can be expected, as process parameter optimization implies iterating the complete process and device simulation chain, which means much higher CPU times and possible accumulation of approximation errors.

The simplest problem is the process transfer problem. In this case, the cost function is defined in a natural way as the mean square error on the current characteristic, as in the case of model parameter fitting. Automatic optimization was applied to the transfer of an existing CMOS technology from a research site to an industrial site; the deep implantation machines differed from one site to the other one, so that the well implantation conditions had to be changed. Optimization was successfully used to retrieve the same characteristics for the PMOS, by adjusting the dose and annealing time of the well implant.

In the general process optimization problem, an additional difficulty arises from the necessity of translating the target defined by the process engineer into a computable cost function. At least two methods can be imagined: the first and most natural one is to use parameter extraction after the simulation, and to define the cost function as a mean weighted square error on the extracted parameters; the method for defining the weights must account for the different natures of the target parameters. The second method is to define, from the target parameters, a target current characteristic by using an analytical model. The target elements in this case are of the same nature, so that a natural weighting is possible, but on the other hand the cost function can hardly take into account the relative importance given by the process engineer to one or other of the criteria.

The latter method offers the advantage of requiring very little programming work and was for this reason tested first. The test was carried out on the optimization of a double channel implant in an NMOS device. Good results were obtained on the optimization of the threshold voltage and sub-threshold slope by playing on the two parameters of one of the implants. However, the cost function had to be redefined very carefully to obtain a satisfactory result on the optimization of the four parameters, the two criteria added for this purpose being the minimization of the leakage current and of the junction capacitance; numerical problems like ill-conditionned matrices were encountered. Experiments are under way to check the parameter extraction approach, which is expected to lead in this case to a better defined problem.

Conclusion

Although the simulation needs seem to be very different in an industrial or research environment, a good compromise can be found by the development of general simulators using robust and evolving pre- and post-processing. Such a tool can be the basis of dedicated industrial simulators by providing adequate documentation, the choice of appropriate models and the suppression of unnecessary features; at the same time, it can form a programming environment for new model developments.

The integration of such a simulator in an optimization loop allows the fitting of model parameters, as well as the automatic optimization of process parameters. However, difficulties may occur when optimizing process parameters: the target and cost function must be defined very carefully, in order to avoid badly stated problems. Human intelligence will therefore remain necessary for optimization by using simulation, but it is believed that automatic optimization can be of great help in saving time and human resources.

references

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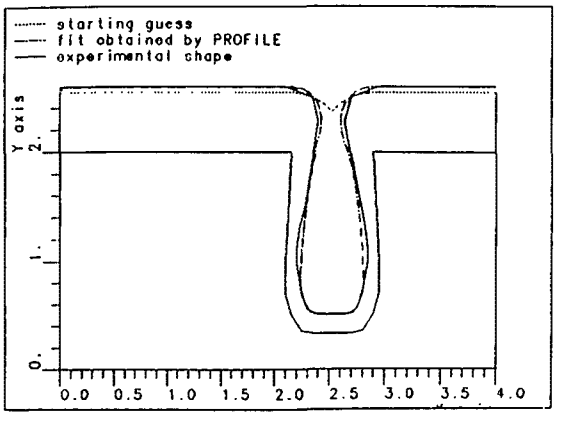
Figure 1: Fit of the deposition model parameters.
Initial: ANISO=10,TETAOV2=10,SATUR=10.
Final: ANISO=82,TETAOV2=90,SATUR=100.

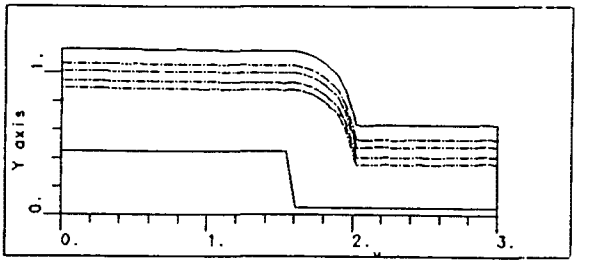
```
Process
STRUCTUR HOMX=11
DEPOSIT  POLY THICK=5
RECESS POLY FILE=PL05030
MODL> DEPO /NAME=TITV ANISO=?aniso? ,
TETA1=90.+?TETAOV2? TETA2=90.-?TETAOV2?,
SATUR=?SATUR?
DEPOSIT  OXIDE THICK=4  modl=TITV
printair filref=pl0503F file=sim05

PROcess
STRUCTUR HOMX=11
DEPOSIT POLY THICK=5
RECESS POLY FILE=PL08030
MODL> DEPO /NOM=TITV ANISO=?aniso?,
TETA1=90.+?TETAOV2? TETA2=90.-?TETAOV2?,
SATUR=?SATUR?
DEPOSIT OXID THICK=2.85 modl=TITV
printair filref=pl0803f file=sim08
```

1a: extract of the input file used for the optimization.

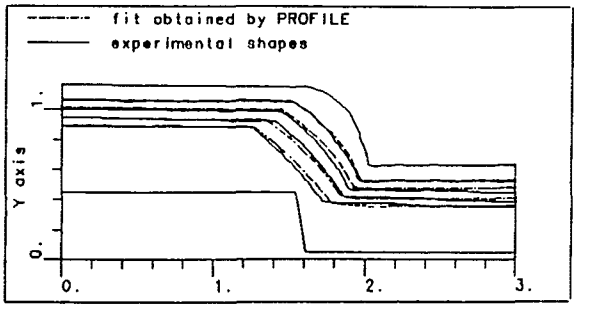


1b: comparison of one of the experimental shapes with the starting guess and with the fit obtained using PROFILE.

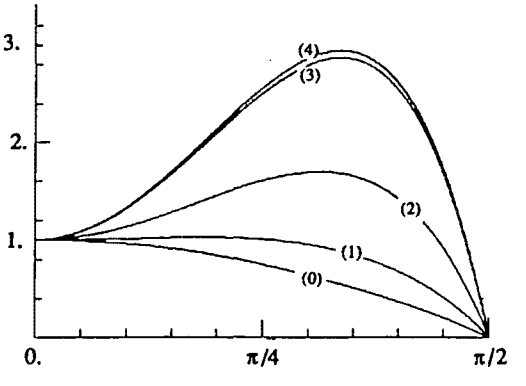
Figure 2: fit of the sputter yield, on profiles obtained by sputter etching of deposited oxide with different etching times.



2a: profiles obtained with the starting guess.



2b: comparison of the experimental shapes with the fit obtained using PROFILE.



2c: successive yield versus angle curves; starting guess: 0 ; final fit: 4.