TCAD Calibration: Challenges and Opportunities

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The following topics will be discussed in this presentation: the various uses of TCAD, why calibration is so difficult, whether TCAD is "predictive" yet, and the sensitivity of electrical parameters to variations in the physical structure. This presentation will also include a call for TCAD needs from a user perspective.

Role of TCAD

TCAD can be used on a wide class of problems. Table I lists some examples, rank-ordered by the accuracy required for the application. At the top of the list is “predictive” TCAD, which many consider to be the ultimate goal. But as will be discussed later, it may be an unobtainable goal due to rapid changes in technology. In general, the top three items in Table I get most of the attention, while much useful work is done in the bottom three categories. The question that needs to be asked is whether predictive TCAD is worth the effort, since it is time-consuming and expensive to calibrate simulators to a very high level of accuracy.

Application	Accuracy Required	Comments
Predictive TCAD	Very High	Elusive Goal
Advanced Process Control	High	Provide Macro Models
Process Centering	High	Mature Product
Inverse Modeling	High	Extracting Coefficients
Early Exploration	Medium	Reduce Splits
Failure Analysis	Medium	Test Probable Causes
Learning/Insight	Low	High ROI

Table I: TCAD application, rank-ordered by accuracy required.

Why Calibration is So Difficult

Calibrating a set of TCAD simulators is extremely difficult. One reason is that the TCAD engineer typically is simulating a complete process flow (not just a single process step), followed by a device analysis. If the threshold voltage doesn’t match the experimental value, he needs to check the assumptions in both the process and the device simulators. as well as the electrical measurements and the test structure layout. In short, he must be knowledgeable across a wide range of areas.

Table II shows some of the areas where expertise is needed in order to calibrate a set of TCAD simulators. First, and non-trivial, is that you must know the process flow in detail. Second, there are many equipment specific subtleties that are not yet comprehended by process simulators. For example, the wafer temperature during ion implantation can affect the point defect generation and thereby the diffusion in later processing [1]. RTA modeling is complicated by the fact that there are pattern sensitivities to the wafer temperature, and few good methods to even measure the wafer temperature [2]. Electrical results can be highly sensitive to RTA temperature, and a 1 volt variation (out of 220) in the AC line voltage resulted in a 6 degree change in RTA temperature [3].

Specialization	Example Problems
Process/Device	Must know complete flow and process/device physics.
Fab Equipment	Implant temperature affects TED; "local" RTA temperature.
Electrical Test	Electrical versus optical oxide thicknesses (QM effects).
Analytical	SIMS knock-on; SRP probe pressure.
Metrology	Uncertainty in poly length and oxide thickness.
Simulation	Model limitations; grid dependence.

Table II: Knowledge required for TCAD calibration

It is often assumed (incorrectly) that when measurements and simulations disagree, that the simulator must be wrong. In fact, there are errors and uncertainties associated with both electrical and physical testing that are often poorly understood by the TCAD engineer. The bi-annual workshop on the *Measurement and Characterization of Ultra Shallow Doping Profiles in Semiconductors* discusses the issues associated with SIMS and SRP analysis [4]. As examples, the SIMS profile can be affected by the energy of the ion beam, and SRP results are sensitive to probe pressure [5]. Perhaps one of the largest sources of error in TCAD calibration comes simply from the fact that it is very difficult to accurately measure poly linewidth and oxide thickness to the necessary resolution. Many important MOSFET electrical characteristics are first-order related to these two parameters (e.g., a 1% change in either Lgate or Tox will result in approximately a 1% change in Idsat). The desired control on Idsat is ± 10% (3-sigma), or *less*. For 0.25 µm gate lengths with 5 nm gate oxides, 1% variations in these key parameters imply metrology requirements of only 2.5 nm for the poly length and .05 nm for the oxide thickness (much less than a monolayer).

Another major source of calibration error is due to the model and grid choices made by the TCAD engineer. The results can be so sensitive to the grid that the grid should be "calibrated" before any other coefficient. Figure 1 shows the sensitivity of Idsat to the fineness of the surface grid for two different mobility models. In this idealized MOSFET, the data points on the extreme right had the first surface grid line 128 Å below the oxide/silicon interface. For each additional data point, another surface grid line was added half the distance to the interface (e.g., 128, 64, 32, 16 Å). In comparing the two mobility models, one could obtain the result that Tasch predicted higher, lower, or the same current as the Lombardi model. It should be mentioned that these are the models *as implemented by the vendor*, and may not be the same as originally designed. The TCAD engineer has to make the trade-off between CPU time (fine grid) and instability in Idsat (coarse grid). Many casual TCAD users are not aware of these issues, and grid sensitivities are rarely discussed in any TCAD publication.

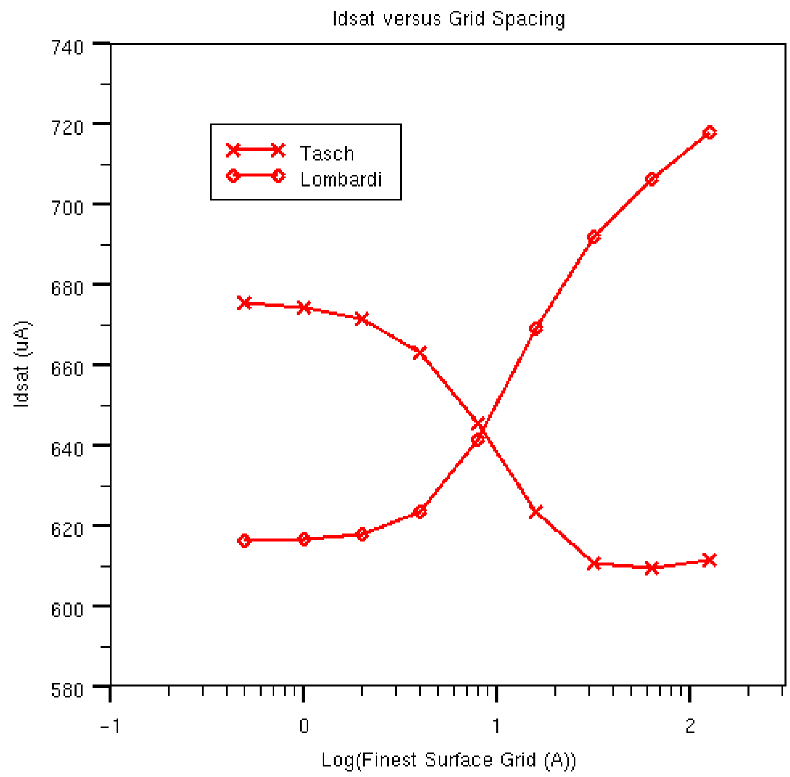

Figure 1: Idsat versus Surface Grid for Two Different Mobility Models

Many examples of “mis-calibration” can be cited - furnace pressures are routinely modified to calibrate oxide thicknesses, and maximum carrier velocity is a common method to tune Idsat. Both of these values should be known, and not have to be adjusted. They are simply ways of accounting for observed differences between measurement and simulation. There is more than one way to calibrate a simulator. In fact, we suffer from an excess of coefficients that can be adjusted, and no generally agreed upon method for calibration. When we speak of calibration, we normally refer to adjusting model coefficients. But from a statistician’s point-of-view, we could just as easily be “calibrating” the input factors or the output responses [6].

The Myth of Predictive TCAD

Is TCAD predictive yet? The answer depends upon the definition of “predictive”. Ideally, you want to be able to simulate a technology as you develop it (or even earlier). The problem arises from the fact that process technology is constantly changing, as is the level of physics necessary to simulate it. A careful calibration of one technology generation does not guarantee that it can predict the next generation [7]. There is the familiar quip about TCAD “simulating yesterday’s technology tomorrow.” Actually, even simulating yesterday’s technology is a significant accomplishment.

As technology development times continue to decrease, the need for rapid transfer of simulation models from research to commercial code increases. Stated another way, the technology developer does not always have time to wait for the TCAD community to develop a model. Despite all the sophistication of today's TCAD, technology developers continue to do much of their development experimentally. A key reason for this is that TCAD is not in a "co-development" mode with technology development. Technology developers today are interested in cobalt silicide, copper interconnects, low dielectric constant (low-k) materials, extremely thin oxide layers, alternate gate oxide dielectrics, and very low energy implants, along with many other examples. Are there TCAD models available, however crude, to investigate the issues associated with these new technologies? What is a needed is a *paradigm shift* in how TCAD models are developed, with much closer cooperation between model and technology developers.

TCAD Needs and Opportunities

There are two major needs from a user perspective - better models and a standard calibration procedure. Implied in better models is more rapid model development, or models for current/future technologies. Other activities that would be beneficial include benchmarking and open software (i.e., the ability to easily use code from multiple sources). These user needs, as well as some more specific calibration needs, are summarized in the following tables.

Top Needs from a User Perspective
More rapid commercialization of new models (co-development of the models as well as more rapid model transfer).
Generally accepted calibration procedures.
More TCAD *users* on steering committees.
More open software (vendors don't want this, but we know what eventually happens to closed software systems).
Round-robin studies / benchmarking. What are the current error bars?
Better equipment-specific models.
TCAD developers need access to state-of-the-art data.

Table III: TCAD needs from a user perspective.

TCAD Calibration Needs
Hierarchy of models and calibration (atomistic, continuum, compact ...)
Need calibration method with any new model.
TCAD-specific test structures / metrics / test-suites.
Ab-initio calculations of key coefficients.

Table IV: Calibration Needs

Summary

TCAD can be used at various stages in the research through manufacturing cycle. There is high leverage early in this cycle, where the models do not have to be perfectly predictive. Often the technology developer finds himself at a fork in the road, and only wishes to know which direction to go, not the detailed directions to his final destination. In fact, predictive TCAD has largely been oversold, with the result that there are as many TCAD skeptics now as there were ten years ago.

Calibration is a highly iterative, difficult and *continuous* process. It is an area where there is much opportunity for pre-competitive collaboration. There still has been no independent benchmarking of TCAD. This is an activity that even the largest companies cannot afford to do thoroughly.

References

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