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The Application of TCAD in Industry

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1. Introduction

The industrial need for TCAD is clear. Experiments have become extremely time-consuming and escalating equipment costs have steadily reduced the number of experimental wafers that can be processed. Since the complexity of IC processes continues to grow, computer-based experiments using TCAD are essential for countering this experimental shortfall if progress is to continue.

Unfortunately, using TCAD for this purpose is less than straightforward. The popular notion of "virtual fabs" suggests one can simply substitute TCAD simulations for experiments, but the reality is far less ideal. Current process modeling and simulation capabilities cannot replace experiments except in very limited applications. The physics and chemistry of many of our fabrication processes are poorly understood. Where physical models do exist, internal model parameter values are often unknown due to lack of experimental data and characterization methodologies. IC processes are also evolving, making the modeling task a moving target. There is no equivalent to circuit simulation in the process simulation world. Instead, what we have are a collection of *partial modeling* capabilities with varying degrees of predictability. The diverse nature of the user base and their computing environments further complicates application of TCAD.

The key to making use of TCAD is matching available capabilities to specific applications to multiply information from available experimental wafers. The art of using such partial capabilities is the focus of this paper. The following sections will describe applications of TCAD in four areas: technology selection, process optimization, process control, and design optimization.

2. Technology Selection

An historic application area for TCAD is *initial design of new IC technologies*. Depending on the predictability of the imbedded models, TCAD tools can be used to eliminate or narrow technology development options prior to starting experiments. For example, device simulations using target device profiles can determine whether specific device designs can meet performance and density goals. They can also be used to estimate the importance of second-order physical effects (like punchthrough, velocity-overshoot, etc.) and help define size and voltage scaling targets. When combined with approximate process models, TCAD tools can also gauge the manufacturability of a "paper" technology.

2.1 Global Models

The key ingredient for all of these applications is *model predictability*. To be useful, the accuracy of the TCAD models must be sufficient to resolve the technology decisions under consideration. What is needed are *global models*, models whose predictability has been verified across many different technologies.

Ideally, global models are first-principles models, imbedding as much physics and basic understanding as available. Unfortunately, such models are almost always complex, involving interactions of a multitude of physical effects. For example, consider the modeling of short-cycle, low temperature impurity diffusion. The relevant physics includes modeling interactions of dopants with each other, dopants with defects of varying charge states (interstitials and vacancies), and the clustering and diffusion of both dopants and defects. It also requires modeling initial defect distributions and their dependence on processing history. Unfortunately, the fundamental reaction and interaction rates are mostly unknown. Furthermore, they cannot be determined from an analysis of post-diffusion experimental impurity profiles, since the number of modeling parameters is far greater than that needed to fit available experimental profiles.

This has led to the concept of *globally-calibrated models*. These are models that are global in formulation, with model parameters simultaneously fitted to data from the widest range of technologies possible. The rationale for this process is the following assumption: *when model parameters are adjusted to expand the range of technologies simultaneously fitted by the model, key modeling parameters move towards their fundamental values, generating a more predictive model.*

Although the absolute validity of this concept depends on the particular model, data used, and number and type of modeling parameters - experience has shown this process to be very effective. Whether such models are merely effective extrapolation vehicles of prior data, or models with increasing physical validity, is academic if the models can meet application needs. The methodology for application and refinement of local models is depicted in Fig. 1 below.

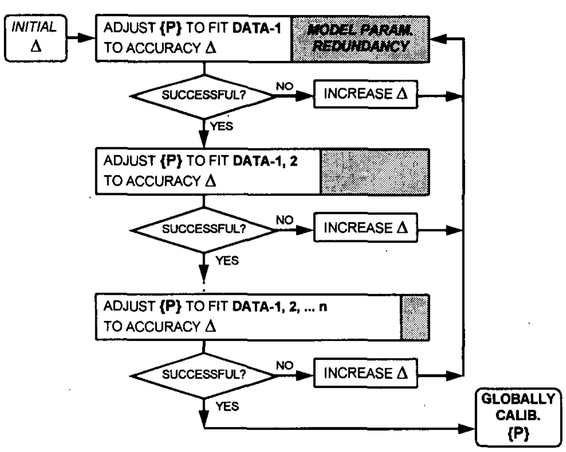

Fig 1. Global model calibration methodology ({P} represents the model parameter set).

2.2 Application of Global Models

The usefulness of such models is intimately tied to the application: determining directions for the technology development. As stated early, the accuracy of such models need only be sufficient for making initial technology decisions. Precise modeling is not needed and inaccuracies in the 30% range are often acceptable, since equipment selections are still to be made and process flows have not yet been developed. These reduced requirements are fortuitous, since imperfections in the underlying model formulations often limit the overall fitting accuracy that can be achieved in a global calibration.

Although the number of TCAD users involved in technology selection may be small, technology selection applications are critically important - since they determine where hundreds of millions of dollars will be spent in subsequent phases of the technology development.

2.3 Application Environment

Applications of this type require a tool system that facilitates specification and simulation of very general 2D and 3D problems. Such systems will typically include 1D, 2D and 3D simulators, device specification/editing tools, efficient gridders, and flexible visualization tools for analyzing results. It may also include model integration frameworks for constructing hybrid models. High-end, floating-point computing facilities are normally required, since the simulations are often highly CPU intensive.

3. Process Optimization

A growing area for TCAD applications is *development and optimization of IC fabrication processes*. Here, basic technology directions and equipment selections have already been made, and the task is developing the detailed fabrication process and supporting design collateral. It may also include development of test monitors for manufacturing control and special circuit libraries, but these will be discussed later in Sections 4 and 5.

Since basic process equipment and technology directions are already defined, the primary task is tuning process variables and design rules to optimize performance, reliability, cost, and manufacturability. Although experimental data (wafers) are available during this phase of the development, the large number of process variables precludes purely experimental optimization approaches. For example, full optimization of a 5-variable litho step could require 5000 experiments (based on a simulated annealing optimization scheme without statistical variables). A far more effective approach is to use TCAD simulations to perform the process optimization, and use experiments to verify results.

Simulation-based optimizations will only be useful if the imbedded models are accurate, however. Since the task is process refinement, high accuracy and resolution is required and maximum allowable errors are often less than 10%, far less than the ~30% error allowed for technology selection applications.

3.1 Local Models

The key to achieving the needed accuracy is *local modeling*. Since basic process directions and equipment sets are already determined, optimization models need only fit the variable space of the specific optimization problem - not general process problems. This allows us to trade-off model generality for enhanced local accuracy. For example, global models can be made more accurate for process optimization by adjusting their parameters to make the models fit available experimental data for the specific fabrication process. This methodology is called *local model calibration,* and the resulting models are called *local models*.

Local models are especially effective when they are used iteratively with experiments. In this methodology, initial process optimizations are performed with local-model simulations and the results used to target initial wafer split experiments. Subsequent experimental runs verify simulation results and provide data for further refinement of local model parameters. The refined models are then used for the next phase of optimization, and the procedure is repeated until the process is optimized. This methodology, which is illustrated in Fig. 2, compensates for imperfections in the models and the possibility of the occasional incorrect prediction. In this methodology simulation-based optimization provides major benefits as long as they provide correct answers most of the time.

3.2 Applications of Local Models

Using simulation in this manner can significantly reduce wafer requirements since the majority of the optimization is performed using simulation instead of experiments. Experimental leverages of 10X or greater are not uncommon, depending on the application range of the local models.

The power of local models is rooted in their ability to accurately fit existing experimental data for the developing process. This enables them to also predict changes to impurity profiles and device topographies when process variables are changed. When these models are coupled with numerical device simulation, they enable device properties to be optimized as a function of the process variables (this last application may require local calibration of device simulator mobility models).

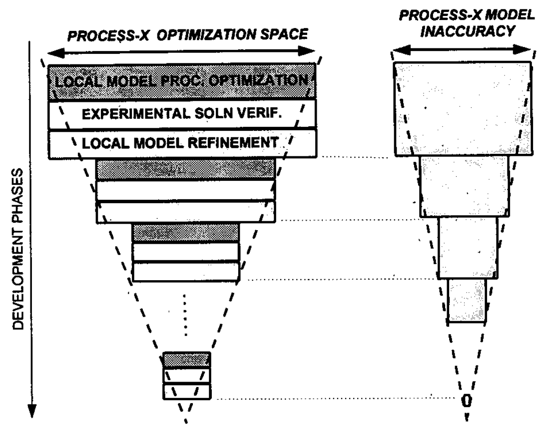

Fig. 2 Iterative local model refinement.

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Example applications include optimization of implant and diffusion processes to minimize capacitances; minimization of device sensitivities to process variations; and manufacturing process window definition. The latter examples require performing simulation-based analyses of manufacturing distributions early in the process development.

The advantages of simulation-based optimization is even greater when process equipment variables are included, since equipment design changes normally require a great deal of time. For example, in one practical lithography optimization problem involving stepper optics, automated simulations examined >1,000 solutions in one day and found three superior solutions. Experimental verification of just *one* of those solutions took 6 months - a simulation to experiment throughput advantage of 200,000:1.

3.3 Tool Environment

Applications of this type require a tool system that will support automation of predefined simulation methodologies, simulation-experiment comparison, and rapid model recalibration. Such systems may include utilities for editing process flows, device template libraries, tool automation framework, libraries of numerical optimization routines, and application-specific postprocessing tools. Since the majority of the simulations will be 2D, high-end workstations or local compute servers are usually adequate.

4. Process Control

The local models described above can be excellent representations of a chip fabrication process, and can provide far more information than traditional documentation. Such models can imbed not only the process "recipe", but also the effects of those recipes and their variations. Models of this type can be used to aid the transfer of a process from one facility to another (including from development to manufacturing). They can also serve as reference models for diagnosing yield issues and aiding process control in manufacturing.

4.1 Process Reference Models

Such "process reference" models can take a variety of forms. At the base-level they can be the locally-calibrated numerical process models and simulators created during the development of the process. If the methodology shown in Fig. 2 is followed, the resulting local models can be accurate representations of the developed process. When combined with device simulation and appropriate templates, such models can be used to understand process sensitivities, develop measurement methodologies, and diagnose control problems.

While numerically-based local models can aid process transfer, they are more limited for manufacturing control applications. Tools for manufacturing control must be extremely robust, fast, and compatible with manufacturing computing environments. Few numerically-based process and device simulators meet these requirements.

Analytical process models are a better choice for process control. One solution is to use numerically-based local models to calibrate a family of response-surface models (RSM's) and use the resulting RSM's as reference models for manufacturing. RSM's can be created to model the response of electrical test-pattern measurements ("E-tests"), junction depth, dielectric thickness, etc., as manufacturing process variables are changed. While the predictive range of RSM models is narrower than numerical models, they can be adequate for the smaller range of process variations seen in manufacturing. The model calibration hierarchy is shown in Fig. 3.

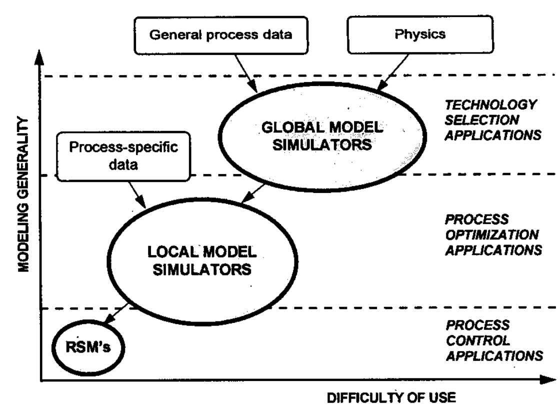

Fig. 3. Model calibration hierarchy.

RSM reference models have several important advantages for manufacturing. They are inherently robust and fast to compute - making them highly suited for interactive tool environments and real-time processing. They do not require complex grids and can be run on computers with minimal memory, making them more compatible with manufacturing computing environments. Their fast speed also makes them suited for statistical simulation and manufacturing distribution modeling.

The ease-of-use of such models can be further enhanced by interfacing them to a knowledge-based "expert system" (see Fig. 4). Such an expert system[2] can serve as the initial interface to the manufacturing modeling system, by providing heuristic diagnoses of the probable causes of a particular problem. The addition of the expert system module also allows other experimental data (e.g., defect data) to be included in problem diagnoses.

4.2 Applications of RSM's

RSM's are most useful during process transfer, when an existing processes is brought up in a new fabrication facility. RSM models can help track down sources of process mismatch and prescribe parametric corrections to bring the process into target. They can also be used to define manufacturing test limits for keeping process excursions from affecting product yield.

RSM and local models can also be used for manufacturing training. When integrated with appropriate graphical user-interfaces, they allow engineers to use a computer to "experiment" and explore

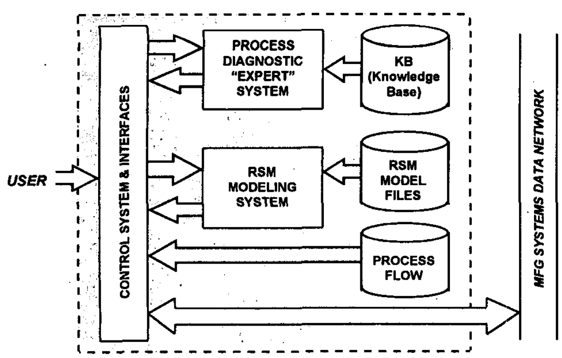

Fig. 4. Model-based manufacturing control system

the effects of process variations. When integrated with layout, they can also be used to visualize device and interconnect structures in specific die regions, facilitating problem diagnoses during low-yield analysis.

4.3 Application Environment

Existing factory automation environments are the preferred operating environment for such applications. These environments are well supported and factory personnel are already familiar with their operation. Such environments are designed to handle large volumes of data and control equipment, and are generally weak for memory-intensive floating point computation. While such systems are not suited for numerical simulation, they are adequate for running RSM models.

5. Design Optimization

The last TCAD application area to be examined is *process-specific design optimization.* This is the optimization of circuit designs for cost, power, performance, and reliability. Although process-independent design techniques have grown, leading-edge products continue to require designs optimized to specific fabrication processes. Technology trends are also increasing the need for process-specific design optimization.

5.1 TCAD Circuit Design Tools

In the past, the chief tool for process-specific design was circuit simulation using analytical *compact models.* These tools could predict the detailed performance of moderate size circuits, and have been used to optimize the critical circuit paths in a chip design.

Technology trends have created additional requirements. The continual shrinking of technology dimensions has pushed device operation dangerously close to reliability and manufacturing limits. Decreasing voltages, increasing clock frequency, declining device margins, have made circuits far more sensitive to noise and interconnect effects. Statistical device variations, within-die variations, and proximity effects have also become important design factors. The widespread use of statistical process control techniques in manufacturing has also made statistical design advantageous. These and other effects have all *increased* the need for process-specific design optimization, well beyond that required for performance optimization of critical paths.

This poses new challenges and opportunities for TCAD application, as new compact models and model calibration techniques are needed for many of these effects. Since many of the effects involve large areas of a chip, combinations of microscopic and macroscopic modeling are needed, including models integrated into higher-level ECAD design tools. Unlike earlier compact models, many of these effects cannot be characterized experimentally, and are dependent on the neighboring layouts and manufacturing statistics. TCAD simulation will play a key role in calibrating such models.

In some situations, more restrictive design rules and *library circuits* may be used to limit the effects of new technology phenomena on general circuit design. Because of their small size and importance, the full range of TCAD simulation tools and models can be applied to the design of such library circuits.

New technology phenomena may also be coupled into the design process through *design limits*. For example, TCAD-simulated limits can be used to implement an hierarchical statistical design methodology[3]. Design limits are also an effective way to account for reliability effects.

The fourth method of TCAD coupling is *callable TCAD routines*. These are TCAD simulation tools that are periodically accessed from the ECAD environment. Such routines have been used to "recalibrate" compact or look-up table models when more accuracy is required or when designs move outside the range of nominal models.

All of these modeling capabilities need to be integrated into the circuit design (ECAD) environment to impact the design process. The possible TCAD integration methods are shown below in Fig. 5.

5.2 Numerical Simulation Support

In all these applications process and device simulation provides the basic capability for understanding, modeling, and characterizing new process-dependent circuit phenomena. For example, lithography and topography simulation tools can be used to model proximity-based within-die variation effects, process/device simulation can predict device distributions from process variations, and 3D-field solvers can be used to characterize interconnect coupling models. In addition, device simulators can be used to predict punchthrough, non-quasi static, and velocity-overshoot effects; and mixed circuit-device simulation tools can be used to aid the design of optimized circuit libraries.

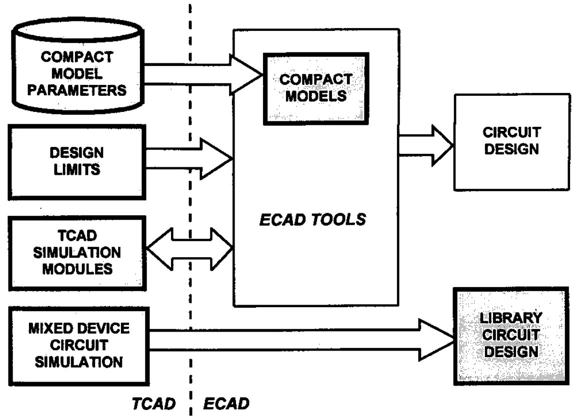

Fig. 5. Integration of TCAD tools into ECAD

When process simulation is used to calibrate compact models, TCAD capabilities for directly coupling process to circuit performance are also created. This enables circuit and process targets to be traded off and optimized during the early phases of a process development, when it is easiest to make changes.

6. Conclusion

The "art" of applying TCAD in industry is understanding the limits of current tools and matching realistic capabilities to specific applications. It is the pragmatic mixing of partial modeling capabilities, heuristic calibration techniques, and flexible application methodologies to solve practical problems.

Although we are still a long ways from making the "virtual fab" a reality, TCAD plays critical roles in the semiconductor industry today. They are the primary tools for initial design of new technologies. They can multiply and leverage information from available experiments to enable better processes to be developed in far less time. They can serve as information repositories to aid the transfer and control of fabrication processes in manufacturing. Lastly, they provide the vehicles for enabling designs to be optimized to specific fabrication technologies. In short, TCAD is, and promises to continue to be, a critical capability for continued progress in the semiconductor industry.

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