20 years of SISPAD:

Adolescence of TCAD and Further Perspective

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***Abstract*— SISPAD and Technology Computer Aided Design (TCAD) are relatively new compared to semiconductors. The history of using computers to design technology dates to the 60's and the first conferences devoted to the field started in the late 70's. As the field matured, the various conferences combined. TCAD has both benefited from and contributed to Moore's Law. New frontiers in nano-devices, sensors, reliability, and alternate materials are still active areas of research.**

Keywords—TCAD, device simulation, process simulation, conference history

I. Introduction

On the occasion of the 20th anniversary of the first SISPAD conference, I've been asked to reflect back on the history of the conference. This is a somewhat daunting assignment, as many excellent researchers have contributed to the field and meeting. I am sure I will have left out many who have contributed greatly to the field and the meetings. The Moore's Law driven advances in computing power have greatly aided the advances in our field, while at the same time advances in TCAD have enabled those advances in technology. For the most part, I'm going to stay close to my own area of expertise, process modeling while discussing some of the history scientifically. This means I am necessarily going to overlook contributions in other vital areas, but I will leave those to others with more expertise than I to address.

One of the earliest key papers was Scharfetter and Gummel's "Large Scale Analysis of a Silicon Read Diode Oscillator"[1]. This title obscures the most lasting contribution of the paper, which was buried in the Appendix "Semiconductor Device Analysis Computer Program", part I, "Mathematical Model", section D "Solution Procedures." In this obscure little section lies the Scharfetter-Gummel method for discretizing particle current. Acknowledging the numerical instability brought on when large drift and diffusion currents cancel one another, they propose treating the current along the edges as a differential equation with constant field and mobility. This basic idea has been extended to two and then three-dimensions and has remained the workhorse of commercial device simulation to this day. Scharfetter and Gummel made a breakthrough that enabled the growth of the TCAD field. It also illustrated several issues that plagued the field and continue to do so.

First, the paper appeared over a decade after the device was proposed. TCAD tools have always struggled staying abreast of technology trends. Despite this, there have always been contributions to the cutting edge of technology derived from modeling and simulation.

Second, the computational aspect got buried under the application. Frequently, publication of software and algorithm papers has been difficult and there has been a bias against papers solely describing a software tool without novel device data. It was clear early that there needed to be venues for this type of work.

Third, the role of structure and the need for accurate doping is discussed. The doping profile of their sample device was evolved to meet electrical performance goals, but no discussion followed of what a realistic profile might be or how to achieve it in manufacturing.

II. Historical Perspective

A. Early Days and Continental Conference Precursors

The earliest meetings I am aware of are the Numerical Analysis of Semiconductor Devices (NASECODE) meetings. The first NASECODE meeting was held in Dublin at Trinity college in June 1979 and was organized by Prof. JJ Miller. The second meeting added "and Integrated Circuits" to the title and was held in 1981 again at Trinity College Dublin. These meetings continued through NASECODE XI held in 1993.

The late 70's saw an explosion of interest in process modeling. Simple Fick's law descriptions of doping didn't hold. More complex things were happening during annealing. Implant profiles weren't simple Gaussian distributions and channeling tails were an important area of interest. The dominant isolation technology was Local Oxidation of Silicon (LOCOS). Shapes were very hard to predict, in particular with changes in temperature, gas flow, and nitride thickness. This was a critical problem because the shape of resulting oxide dictated layout design rules. The first version SUPREM [2] was released in 1978.

In North America, two meetings were held in Boston in November of 1982 and 1984 under joint sponsorship of the Society for Industrial and Applied Mathematics and the IEEE Electron Device Society. Wolfgang Fichtner and Don Rose were the organizers. Special issues of the IEEE Transactions on Electron Devices were published in September 1983 and October of 1985. I had the pleasure of attending the Boston 1984 meeting. Papers were presented using a transparency projector, and several of the participants wrote notes on blank slides as they talked.

I attempted to find the first use of TCAD in a paper using IEEE xplore. Of course, there is a possibility that other literature featured it first. Within IEEE, the first reference to

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TCAD is in an invited plenary paper by R.W. Dutton of Stanford at the International Electron Devices Meeting in 1986 [3]. Dutton's paper reviewed the developments from the 60's forward and discussed challenges ahead. Quoting that paper:

> Technology CAD can play essential role in achieving both flexibility and simplicity. Namely, the growing power of TCAD tools will allow them to carefully assess process design and its implication on design rules. In addition, through the use of these tools it will be possible for both process developers and circuit/device end-users to communicate and optimize technologies to meet both performance and production objectives. New tools that meet these objectives are beginning to emerge.

This remains as valid today as it did in 1986.

In the mid-80's fierce debates were raging over the dominant point defect type controlling diffusion. In addition to difficulty predicting the shape of oxide regions, it was becoming obvious that growing an oxide changed the rate of diffusion of impurities, a phenomenon known as oxidation enhanced diffusion. Predicting implant profiles was a concern, particularly with the large computation times required for Monte Carlo approaches.

B. Continental Conferences

In Japan, there must have been a VPAD meeting in 1981. I only know this because Bob Dutton's plenary for 1991 VPAD references that as the 10^{th} anniversary of the conference. I believe the 1981 meeting was associated with the VLSI Symposium sponsored by the IEEE Electron Device Society and the Japan Society of Applied Physics. The meeting was held in the fall in Maui.

The oldest separate VPAD proceedings I could identify is from 1988. There were several talks on diffusion of impurities, defects, and implantation. Another theme of this meeting was hot carriers and mobility. Several talks focused on circuit modeling were also presented. VPAD eventually associated permanently with the VLSI Symposium as a workshop with the larger meeting when the VLSI Symposium was held in Asia.

In North America, a similar tack was taken. The Boston meetings were replaced by NUPAD. The first NUPAD was in 1986 in Santa Clara, CA and was organized by Bob Dutton as was the second in San Diego. The IEEE Electron Device Society and Circuits and Systems Society sponsored these meetings. From 1991 forward, the NUPAD and VPAD meetings alternated years, both being associated with the VLSI Symposium.

I attended all of the NUPAD meetings since I could manage domestic travel easily. I chaired the 1994 meeting at the Hilton Hawaiian Village. During one break, we had fresh pineapple carved right in front of us. The meeting room windows looked out at the pool, and by the end of the day I could see more attendees at the pool then at the talks.

In Europe, K. Board and D.R.J. Owen hosted two SISDEP meetings at Swansea, Wales in 1984 and 1986. The Swansea site was appropriate, as the famous O.C Zienkiewicz who pioneered the finite element method starting in the 40s was at Swansea from 1961 to 1988. He established a numerical analysis school there, as well as the first big journal of numerical analysis, IJNME, and the classic textbook "The Finite Element Method" [4].

The 1986 SISDEP meeting featured a paper presented by Conor Raffery and I on SUPREM-IV, the first two dimensional version of the SUPREM codes. Nearly all codes written prior to SUPREM-IV were FORTRAN based. We made the choice to write SUPREM-IV in C. This was a radical choice at the time and not popular with all of our industrial partners. It was a different time for computing. SUPREM-IV was designed to handle point-defect based diffusion models, nonlinear LOCOS growth, and the interaction between these through point defect injection from the oxide growth. Simulations of LOCOS steps and isolation diffusion would frequently take several days on desktop computer and overnight on the available supercomputers. Similar simulations complete in minutes on my laptop today.

In process modeling, the 80's saw a shift of concern from oxidation-enhanced diffusion to Transient Enhanced Diffusion (TED). It was becoming clear that reducing the annealing temperature and time was not producing shallower junctions. Counter to intuition, in fact, sometimes a lower temperature was producing a deeper junction. The 80's saw an explosion of work on the interaction of implant damage with the implanted dopant.

C. Merger – Early SISPAD

These three conferences were increasingly presenting a challenge to researchers. VPAD and SISDEP were in the same year and frequently only months apart, making it very difficult to attend both and hurting the productivity of both meetings. IEDM had strong modeling and simulation sessions that further diluted the overall attendance and quality. Discussion began to try and hold a unified meeting addressing concerns of all three regional entities.

There were several competing concerns. Timing of the meeting, the new name, hosting of the first meeting, sponsoring societies, and publication of proceedings all had to be settled and compromises founds. An international steering committee was formed with three representatives from each region. The initial committee was made up of H. Bennett and R.W. Dutton, and myself from the U.S., M. Fukuma H. Nakayama, and A. Yoshii from Japan, and K. De Meyer, H. Ryssel, and S. Selberherr from Europe.

The committee was able to successfully reach consensus, and SISPAD met for the first time in 1996 in Tokyo, Japan in September. Takuo Sugano was the organizing chair for that meeting. In 1997, John Faricelli and I organized the meeting in Cambridge, MA, and in 1998 the meeting was held at Leuven, Belgium organized by Kristin De Meyer and Serge Biesemans. All meetings were successfully both financially and technically, and this pattern of rotation has been kept for the last 20 years.

The 1996 Plenary included four talks: Nano-Electronics, Majority and Minority Mobility in GaAs, Inter-Valley Phonon Scattering in Strained Si, and Tunneling through Gate Oxides. All four could be referenced in the 2016 meeting talks. Most of the early meetings could have their papers grouped into 4 main areas: device and carrier transport modeling, manufacturing equipment and process modeling, application of tools, and numerical methods (with a particular emphasis on grid generation). The American years specifically had technical program subcommittees in each of these four areas to evaluate submitted papers.

Most of the first day of the 1996 meeting was process modeling papers. Oxide growth shapes were less of concern by 1996, but implantation and defect driven diffusion was a vital component. By this time, papers were being presented on computing implantation in 3D and how to compute amorphization depth and damage threshold.

The topic of transient diffusion and its effects dominated the discussion during that first session. At this time it was understood that the damage from the implant anneals out quickly, but creates an transient enhanced diffusion (TED) while present. One key paper was on the reverse short channel effect, observed electrically in devices but caused by the lateral diffusion of point defects from the source / drain implant damage [6].

D. The Online Journal

Coincident with the start of SISPAD as a unified meeting in 1996, an online journal was started [5]. This journal was envisioned as place where many of the papers from the meeting would be published. The idea was to be entirely online with no paper version. The hope was that some emerging tools might be utilized to have interactive papers. For example, you could envision changing the implant energy and seeing the profile change in real time. I was the initial and only editor.

The journal closed in 2001. It never really got traction and sufficient submissions to be sustainable. It was probably ahead of its time. One issue for academics was the lack of an archival reference for tenure and promotion packages. Most institutions now have ways to include web publications, but this was not true in 2000. No one really took advantage of features that differentiated it from a hard-copy print journal. Including a java applet to compute the values of a circuit model, for example, would have distinguished the papers.

E. SISPAD Matures, Focus Meetings

SISPAD quickly became the premier meeting focused on semiconductor process and device simulation and modeling. The unification paid dividends with excellent programs, increased submissions, and attendance increases. There was healthy turnover in the organizing committees. Most meetings became healthy enough to have parallel sessions on different topics.

Looking back at 10 years ago to the meeting in Monterey, California in 2006 gives a good perspective on how the meeting involved. The plenary session included talks on tools for emerging technology, nanometer scale devices, modeling as a part of the semiconductor environment, and active and passive RF compact modeling. Sessions continued to focus on transport (particularly in strained materials), nano devices, noise modeling, and compact models.

Process modeling largely focused on defects and diffusion. TED was still an important talk, but things had expanded to look at transient activation driven by defects as well. Defects were a critical part of modeling diffusion and activation, and of particular growing concern was the role of extended defects. Of new interest was the emergence of different approaches – nearly half of the process modeling papers discussed the use of ab-initio tools for computing defect and dopant states. As an example, Intel presented a paper on ab-initio calculations of defects under shear stress in silicon [7]. Complexity of the models exploded – in some cases 20 partial differential equations representing the behaviors defects, clusters, and dopants were being solved to predict diffusion and activation. This was only possible because of the insights provided by first principles ab-initio calculations.

In process modeling, however, competing meetings started to become very important and drew some focus away from SISPAD. In the decade of the 2000's, front-end process modeling became a collaborative effort among and between simulation and modeling researchers, equipment developers, and technologists. Front-end processing symposia held at the spring Materials Research Society meetings started to attract more papers than the SISPAD meetings in this area. Driven by modeling insights into transient activation and diffusion, millisecond, high temperature annealing equipment was being developed and characterized.

III. The Next 20 Years

My crystal ball has been faulty for years. Predicting the trends of device technology has never been harder. Scaling rules made predictions about future devices easier in the 80's and 90's. With the advent of new materials (SiGe, HfO_2, metal gates) and device designs (strained, FINFETS, nanostructures) straightforward scaling of MOS devices has ended. It is very difficult to even predict the channel material of the device 2036. Nonetheless, there are some trends that I think have staying power in simulation.

The plenary talks all highlight fields that will remain exciting and vital in the next 20 years. Several of this year's plenary talks are continuing in the long themes of transport and nano-devices. One I'm particularly excited about is Dr. Juge's talk from STMicrolectronics on device modeling with variability [8]. As devices scale to smaller and smaller dimensions, we are reaching the point where single defects or dopants can alter the response, and helping circuit designers approach will be an area of interest for some time.

I will not presume to list areas of challenge in all sub-fields of the conference. I'll focus on the areas I'm most interested in and that I think will be relevant for the next 20 years.

A. Challenges for Process Modeling

All these new materials create enormous new challenges for process modeling. It is very clear that point defects control diffusion and activation in most semiconductor materials. Point defects in compound materials are considerably more

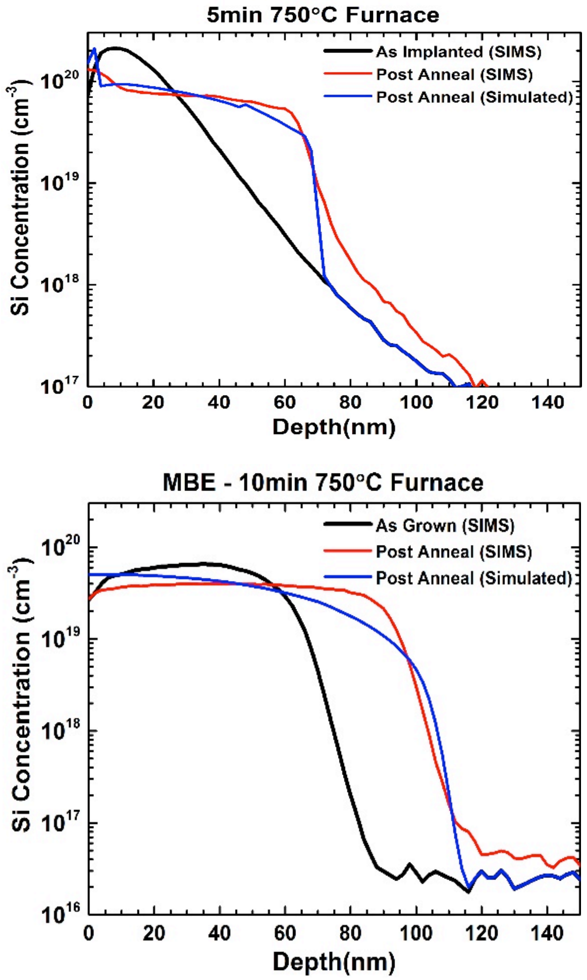

Figure 1 – Diffusion of Si in InGaAs annealed at 750°C. Top - implanted material, bottom MBE grown material.

complicated. III-V materials feature column III and column V interstitials, vacancies on both sub-lattices, and anti-site defects. It was difficult getting silicon defects modeled and there were only two for an elemental compared to 6 for a III-V. Of course, there can be more defect types for III-V alloy compounds, not to mention how atomistic level variations in the alloy could lead to changes in local strain and therefore defect formation and migration energy strain.

As an example, Figure 1 shows diffusion after 750°C annealing in InGaAs [9]. There are significant differences in the Si profile between the MBE grown material in Figure 1 top and the implanted material in Figure 1 bottom. Also there are clear non-Fickian profiles artifacts including the relatively flat plateau region and the sharp profile fall off. In the case of the implanted material there is little tail motion compared to the MBE material. There is a very strong concentration dependent diffusion profile indicated by the sharp profile observed. It has the unusual property that annealing makes the profile more abrupt than it was prior to annealing, which has several useful design advantages. This all points to a strong defect diffusion behavior with different defect profiles from implant and MBE growth controlling the profile shape and activation levels.

This trend will only continue. New materials are likely to have dopants grown in, rather than in an implant and anneal cycle. Activation and diffusion, then, will be controlled by the growth defects. Growth conditions will become important in predicting the activation and junction depths.

As novel materials are explored both for channel materials as well to create channel strain, the doping resend will need to be modeled and optimized to allow for the desired contact and link region resistance to be obtained. Understanding the tradeoffs between growth processes, implantation, and annealing will be a driver for modeling.

B. Novel Devices and Applications

Sensor structures provide an interesting modeling opportunity. We've been working on modeling pH sensors in 2D to investigate the trade-offs between sensitivity, power consumption, channel length, and drain bias [10]. Most of the modeling work to date has been in 1D [11], so this offers new insight on the device design and optimization.

Using standard methods for device simulation of AlGaN/GaN HEMT's, we also included differential equations for ions in the electrolyte. This was augmented with two surface reactions that can capture and release hydrogen from the electrolyte layer. In this way, solving for ion motion and capture at defect sites with Poisson's and transport equations is a combination of process and device modeling. This offers some interesting modeling opportunity to extend classic electrical device modeling to include sensor modalities.

Figure 2 shows simulation results of gate lengths ranging from 0.1 um to 3 um at a constant drain voltage of 5V. At either end of the pH scale, the surface reactions saturate and no additional charging is possible with changes in the hydrogen population. Submicron channel lengths have lower sensitivity due to the smaller window opening. Scaling to smaller channels may not be advantageous in design.

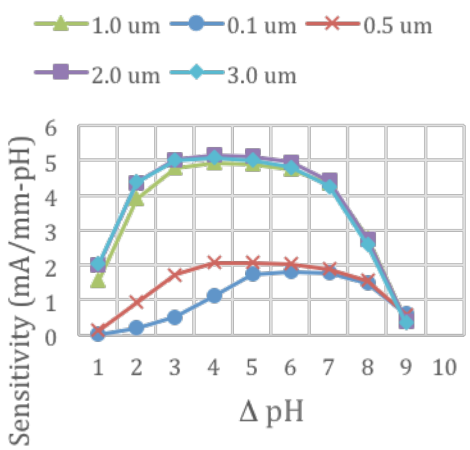

Figure 2. Simulated sensitivity (mA/mm-pH) as a function of pH varying gate lengths from 0.5 um to 3.0 um for a GaN HEMTs pH sensor at a constant, V_{DS}, of 5.0 V.

C. Variability and Reliability

Variability and reliability modeling will be of growing interest. Individual defects or dopant levels can create shifts in nano-devices of the current voltage curves. A single charge contained in a 5nm / side cube of channel represents a density of charge of $8 \cdot 10^{18}$ cm^{-3}. Single defects during fabrication can represent large variability in final device design.

This has important ramifications for reliability and life-time as well. Let's consider the case of radiation tolerance. A single high-energy particle strike could leave behind a single defect state in a device and disable it. The cross-section for this is tiny, so it will still be a somewhat rare event, but thinking about radiation damage may no longer be a case of slow degradation as much as a sudden failure.

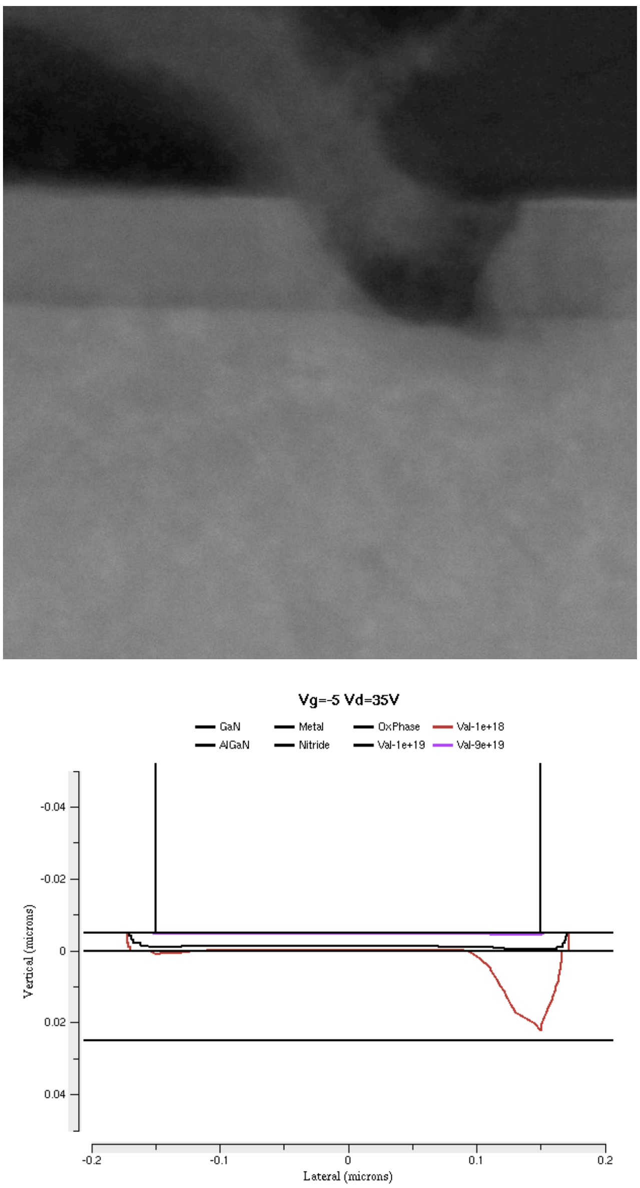

Figure 3 – Comparison of gate sinking profile of TEM measurement and strain-based diffusion model. Top – cross sectional TEM. Bottom – simulated contour of metal

Another interesting area is reliability under operating conditions. Of course, hot electron effects have been important in understanding oxide charging and degradation. In AlGaN/GaN HEMT devices, there are additional behaviors. AlGaN and GaN are both piezoelectric materials and have a strong inverse piezoelectric behavior. This means that high electric fields induce mechanical strain. The mechanical strain, in turn, breaks the diffusion barrier and lowers the diffusion migration energy so that the gate metal begins to move into the channel of the device [12]. Finally, as the gate shape changes, the electric field and distribution changes. Figure 3 top and bottom compare the result of a TEM cross-section and the model prediction of the metal interface. You can see the close match in shape of the two profiles. This is due to the fact that the diffusion strongly matches the strain profile, so the contour shape in the simulation mimics very nicely the strain created by the inverse piezoelectric effect.

This example uses time dependent simulation of the device equations – to get the changing electric field. It solves an elastic material model to get the strain in the material layers, then solves a diffusion equation to get the metal motion from the gate into the semiconductor. Even in 2D, it required nearly 10,000 nodes to do accurately. It is a true blend of device and process simulation. 20 years ago, this type of simulation would have been impossible both because of limitations of codes but also we did not have the computing power available to begin to tackle the problem. Today, these simulations run in about an hour on a laptop.

IV. Conclusions

The complexity of problems that simulation can tackle is far ahead of where it was when SISPAD started in 1996. Moving forward, we can continue to tackle problems with more fundamental physics than ever before. As move beyond CMOS scaling, the problems and solutions offer great opportunity for researchers in this field to solve. SISPAD will continue to be vital in addressing advanced electronics.

Acknowledgements

Far too many people that have made major contributions to the field have been left out of this paper. This is, by definition, a personal perspective on the development of TCAD and the conference. I apologize to all that I have inadvertently left out. Bob Dutton, Conor Rafferty, and Mark Pinto all helped me remember details from the early days of these meetings, and I appreciate their sharing and their friendship.

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