Research Needs for
Device Sciences Modeling and Simulation (DSMS)
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Background, Trend, and Challenges

Technology computer-aided design (TCAD) has become essential to advanced technology development, contributing to solving a diverse range of problems from equipment design and process control to device compact modeling and design variability analysis. The complexity of a modern technology is such that it could not be successfully completed without extensive use of modeling tools in almost every aspect of its development. Process and device simulation tools have become a key enabler for the semiconductor industry to continue to achieve increasing device density and performance with high yield and manufacturability.

This document is prepared for the generation of the Call-for-White-Papers in the DSMS thrust. Within the program structure of GRC SRC, other modeling-related work such as compact modeling or application of readily available modeling tools for device optimization is dealt with in its respective thrust and not included in this call.

According to the Roadmap [1], this discipline can be divided into 11 areas. Of particular interest to this thrust, the areas and their descriptions are:

- Front-end process modeling—Simulation of the physical effects of manufacturing steps used to build transistors and other structures up to metallization. The issues include dopant diffusion and activation, damage kinetics from implant, alternative doping processes, achieving super-sharp doping gradient, segregation and diffusion at interfaces, mechanical stress effects, advanced gate stacks of high-K dielectrics, and epitaxial growth of foreign materials on a Si substrate. One big challenge is accurate metrology and analytical techniques needed to calibrate these models.
- Device modeling—Hierarchy of physically based models for the operational description of active devices. The issues include quantum transport, ballistic transport, effects of stress/strain, contact resistance, 3-D modeling of nm-size devices, power device operation, high-frequency characteristics, analog metrics such as noise, novel devices such as 2-D graphene, 1-D nanowire, and 0-D quantum dot, emerging logic devices based on spin, ionic transport, or electromechanical effects, emerging memory devices based on magnetic, ferroelectrics, and phase change.
- Materials modeling—Physical modeling of properties of materials from atomic to continuum scales to enable process integration and device application. As device dimensions are shrinking to the nm-range, materials modeling is linked more closely to device modeling. The number of materials has continued to increase with each technology. For logic devices, the search for higher mobility includes different forms

of III-V, Si_xGe_{1-x}, carbon nanotube, graphene, etc. For memory devices, material properties related to ferroelectricity, phase change, magnetoresistance, spin, etc. are of high interest.

- Numerical methods—Efforts are needed in all algorithms to improve the models developed in any of the other sections, including grid generation, parallel solvers for systems of (partial) differential equations, and optimization routines for speed and accuracy. As devices tend to go 3-dimensional, automatic grid generation and refinement gets more and more demanding and challenging.
- Reliability/variability—Understanding and modeling of reliability mechanisms and process fluctuation is important in many aspects, such as lifetime prediction, accelerated test strategy, circuit margin, safe-operating area, etc. The phenomena include hot carrier effects, NBTI/PBTI, SILC, TDDB, ESD, tunneling and charge trapping/detrapping, random telegraph signals, 1/f noise, effect of random doping fluctuation and feature LWR, etc. Some of these are particularly critical for nonvolatile memories for endurance, retention, and disturb, especially in light of multi-bit requirements.

Not emphasized in our call is modeling on the following areas: equipment, lithography and resist, interconnect, packaging, and circuit.

Research Topics

The 14 topics in the table are mostly taken from the ITRS Modeling and Simulation chapter as difficult challenges, with some modification by our member companies. These topics are explained below:

1 Interface: gate stack—On channel materials beyond Si. Oxidation, dielectric deposition, interface traps, work-function engineering, leakage.

2 Interface: hetero-epitaxy—Epitaxial III-V and Ge on Si substrate.

3 Doping for advanced materials/structures—Implantation, activation, transient diffusion, strain effects, S/D of super-steep gradient.

4 Stress and defects—Stress distribution, defect formation, annihilation, and diffusion.

5 Synthesis of novel materials—Carbon nanotube, graphene, nanowire, nanodot.

6 Transport beyond-Si devices—Quantum mechanical transport, ballistic transport, strain effects, scattering.

7 Efficient simulation of quantum mechanical transport—Alternative approaches for efficient simulation of QM transport with comprehensive scattering models enabling practical technology performance prediction/analysis.

8 Novel modeling/simulation techniques for memory devices—Spin/magnetic, ferroelectrics, phase change, metallic oxide.

9 Novel modeling/simulation techniques for analog devices—Power, RF, noises, passives.

10 Novel modeling/simulation techniques for functional diversification—Sensors, MEMS, energy harvesting.

11 Heat generation/distribution and effects—including impact on performance and reliability

12 Contact structures and transport—Silicide, M/S interface, barrier heights, beyond-Si semiconductors, connection to atomistic simulations.

13 Reliability

14 Variability effects

Research Priority

Member company representatives were asked to vote on the topics of their preference, with 3 levels of priorities (high/medium/low). Consensus was built on the total of inputs. The scores of priority are included in the table below. It is with these guidelines that we will call for and select proposals. We encourage submissions in the areas of higher priorities which will be weighted more favorably, although all submissions will be considered for special quality and insight.

Reference

[1] International Technology Roadmap for Semiconductors (ITRS), 2010 Edition. Chapter on "Modeling and Simulation". (http://www.itrs.net/Links/2010ITRS/Home2010.htm)

Contributing DSMS TAB members:

Steve Moffatt	Applied
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Lee Hartin	Freescale
Jin Cho	GLOBALFOUNDRIES
Philip Oldiges	IBM
Steve Furkay	IBM
Martin Giles (TAB Chair)	Intel
Mark Stettler	Intel
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Modeling and Simulation: Topics and Priorities

Order by topic

Item #	Topic	Score of priority
1	Interface: gate stack	5
2	Interface: hetero-epitaxy	3
3	Doping for advanced materials/structures	6
4	Stress and defects	5
5	Synthesis of novel materials	2
6	Transport beyond-Si devices	9
7	Efficient simulation of QM transport	4
8	Novel modeling/simulation techniques for memory devices	3
9	Novel modeling/simulation techniques for analog devices	3
10	Novel modeling/simulation techniques for functional diversification	6
11	Heat generation/distribution and effects	3
12	Contact structures and transport	8
13	Reliability	7
14	Variability effects	7

Order by priority

Item #	Topic	Score of priority
6	Transport beyond-Si devices	9
12	Contact structures and transport	8
13	Reliability	7
14	Variability effects	7
3	Doping for advanced materials/structures	6
10	Novel modeling/simulation techniques for functional diversification	6
1	Interface: gate stack	5
4	Stress and defects	5
7	Efficient simulation of QM transport	4
2	Interface: hetero-epitaxy	3
8	Novel modeling/simulation techniques for memory devices	3
9	Novel modeling/simulation techniques for analog devices	3
11	Heat generation/distribution and effects	3
5	Synthesis of novel materials	2