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Fraunhofer Institute for Integrated
Systems and Device Technology IISB

TCAD: From process roots at IISB to industrial standard tools

Dr. Jürgen Lorenz
IISB Annual Symposium 2023
October 12, 2023, Fraunhofer IISB, Erlangen, Germany

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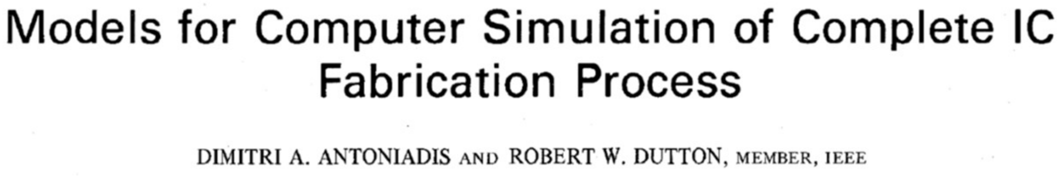
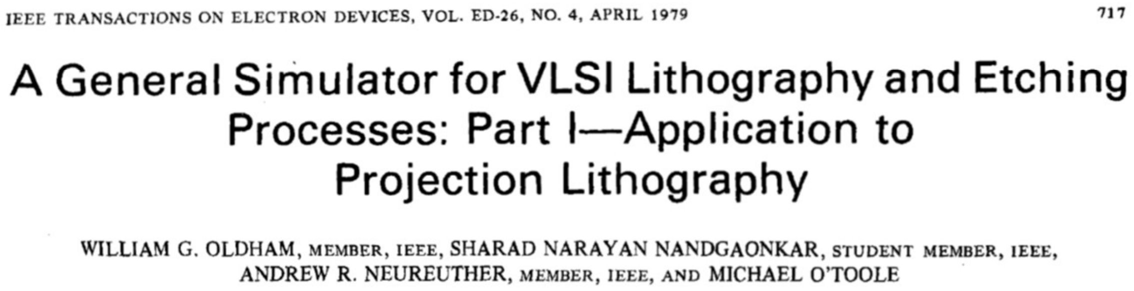
The late 1970s ….: First 1D programs in USA @ Stanford and Berkeley – and at Fraunhofer IFT



Models for Computer Simulation of Complete IC Fabrication Process

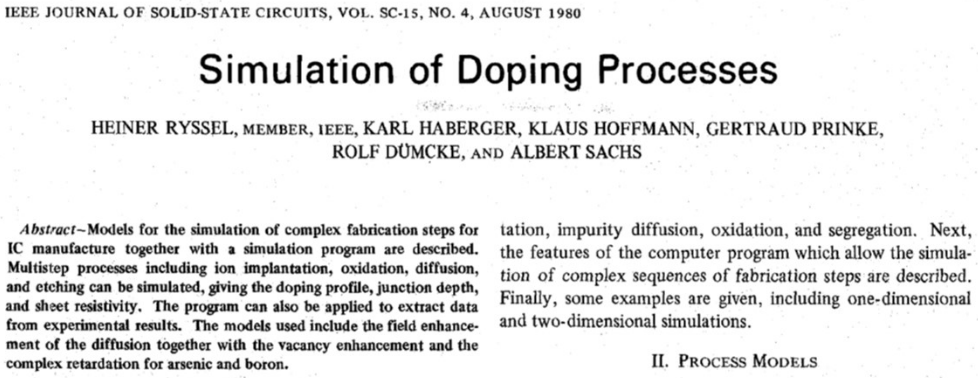
DIMITRI A. ANTONIADIS AND ROBERT W. DUTTON, MEMBER, IEEE



IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. ED-26, NO. 4, APRIL 1979 717

A General Simulator for VLSI Lithography and Etching Processes: Part I—Application to Projection Lithography

WILLIAM G. OLDHAM, MEMBER, IEEE, SHARAD NARAYAN NANDGAONKAR, STUDENT MEMBER, IEEE,
ANDREW R. NEUREUTHER, MEMBER, IEEE, AND MICHAEL O'TOOLE



IEEE JOURNAL OF SOLID-STATE CIRCUITS, VOL. SC-15, NO. 4, AUGUST 1980

Simulation of Doping Processes

HEINER RYSSEL, MEMBER, IEEE, KARL HABERGER, KLAUS HOFFMANN, GERTRAUD PRINKE,
ROLF DÜMCKE, AND ALBERT SACHS

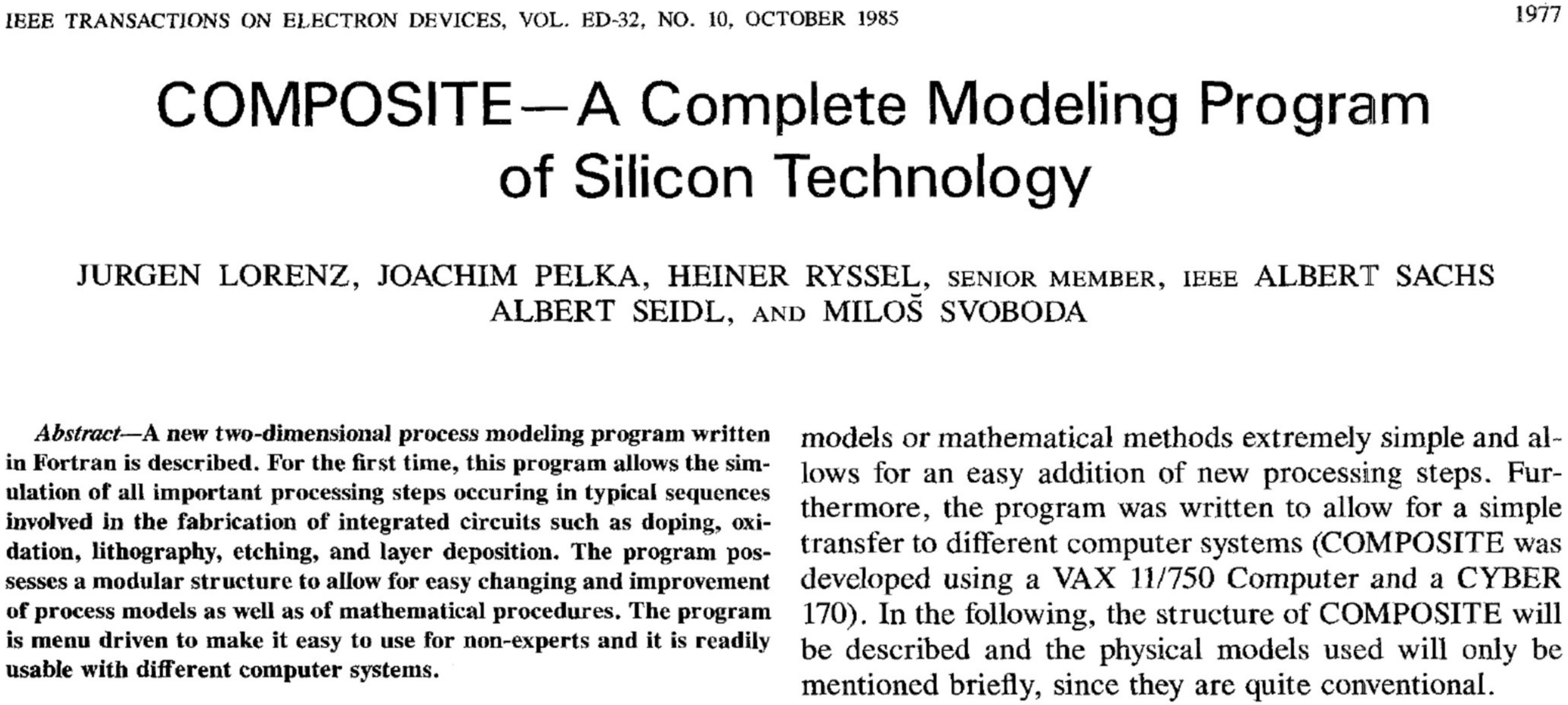
Abstract—Models for the simulation of complex fabrication steps for IC manufacture together with a simulation program are described. Multistep processes including ion implantation, oxidation, diffusion, and etching can be simulated, giving the doping profile, junction depth, and sheet resistivity. The program can also be applied to extract data from experimental results. The models used include the field enhancement of the diffusion together with the vacancy enhancement and the complex retardation for arsenic and boron.

tation, impurity diffusion, oxidation, and segregation. Next, the features of the computer program which allow the simulation of complex sequences of fabrication steps are described. Finally, some examples are given, including one-dimensional and two-dimensional simulations.

II. PROCESS MODELS

Process Simulation: A Glimps on History

The beginning of full two-dimensional process simulation – at Fraunhofer same time as at Stanford USA



IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. ED-32, NO. 10, OCTOBER 1985 1977

COMPOSITE—A Complete Modeling Program of Silicon Technology

JURGEN LORENZ, JOACHIM PELKA, HEINER RYSSEL, SENIOR MEMBER, IEEE ALBERT SACHS
ALBERT SEIDL, AND MILOŠ SVOBODA

Abstract—A new two-dimensional process modeling program written in Fortran is described. For the first time, this program allows the simulation of all important processing steps occuring in typical sequences involved in the fabrication of integrated circuits such as doping, oxidation, lithography, etching, and layer deposition. The program possesses a modular structure to allow for easy changing and improvement of process models as well as of mathematical procedures. The program is menu driven to make it easy to use for non-experts and it is readily usable with different computer systems.

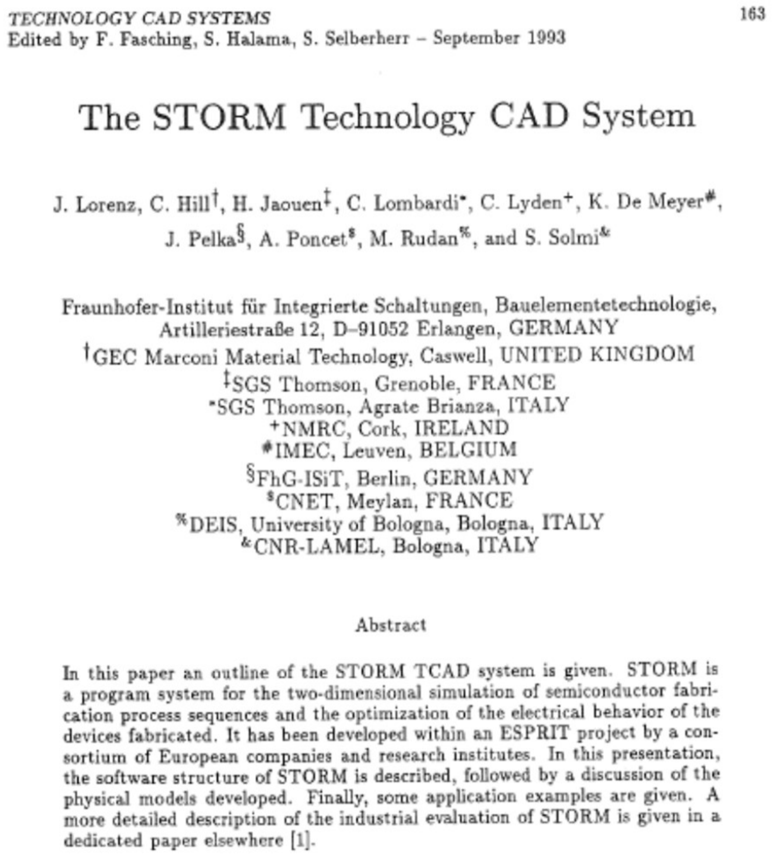
models or mathematical methods extremely simple and allows for an easy addition of new processing steps. Furthermore, the program was written to allow for a simple transfer to different computer systems (COMPOSITE was developed using a VAX 11/750 Computer and a CYBER 170). In the following, the structure of COMPOSITE will be described and the physical models used will only be mentioned briefly, since they are quite conventional.

Process Simulation: A Glimps on History

Progress in simulation depends on broad and good cooperation ….

History of cooperative European projects started late 80s …

- STORM project (2D process and device simulation) (CNET, FhG-IISB & ISiT, … ..)
- DESSIS: 3D device simulation (ETHZ, Univ. Bologna, …)
- PROMPT / PROMPT II: 3D process simulation (FhG-IISB, ETHZ, ….)
- DESSIS and PROMPT were cornerstones for 3D device and process simulation and for the Zurich-based software house ISE AG – later bought by Synopsys
- FP5 MAGIC_FEAT (FhG-IISB,ISE,..) on 3D meshing for process simulation
- SUPERTHEME / SUPERAID7: Process variations (FhG-IISB, GSS, ….) – GSS was later bought by Synopsys



TECHNOLOGY CAD SYSTEMS 163
Edited by F. Fasching, S. Halama, S. Selberherr – September 1993

The STORM Technology CAD System

J. Lorenz, C. Hill[†], H. Jaouen[‡], C. Lombardi[•], C. Lyden[+], K. De Meyer[#],
J. Pelka[§], A. Poncet[$], M. Rudan[%], and S. Solmi[&]

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[%]DEIS, University of Bologna, Bologna, ITALY
[&]CNR-LAMEL, Bologna, ITALY

Abstract

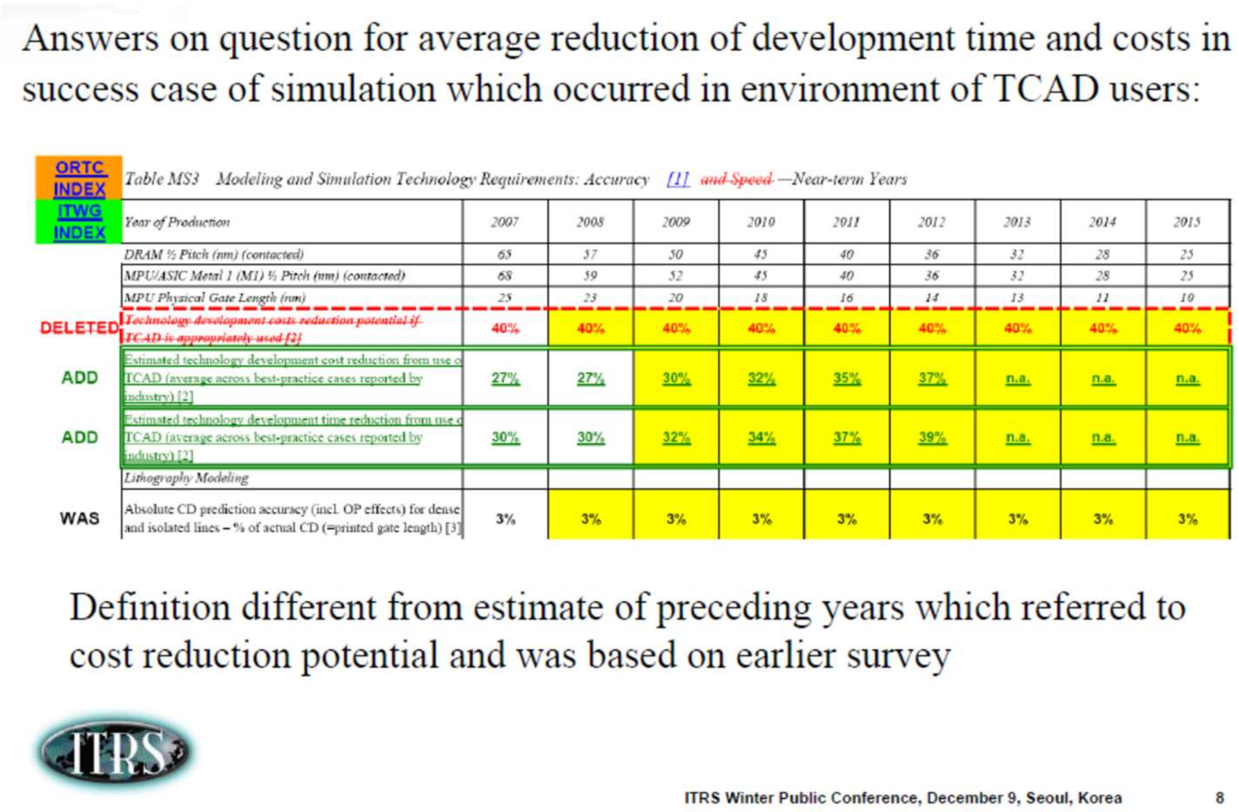
In this paper an outline of the STORM TCAD system is given. STORM is a program system for the two-dimensional simulation of semiconductor fabrication process sequences and the optimization of the electrical behavior of the devices fabricated. It has been developed within an ESPRIT project by a consortium of European companies and research institutes. In this presentation, the software structure of STORM is described, followed by a discussion of the physical models developed. Finally, some application examples are given. A more detailed description of the industrial evaluation of STORM is given in a dedicated paper elsewhere [1].

Process Simulation: A Glimps on History

TCAD arrived in industry as indispensible tool: Development time and cost reduction in ITRS ….

- In the beginnings (1970ies, 1980ies) Technology-Computer Aided Design (process, device, circuit simulation) not considered as important by industry
- Various trends worked for TCAD:
  - Increased complexity of technology and devices → need to complement/replace experiments by simulation
  - Progress in predictivity and efficiency of TCAD, partly enabled by progress in computing hardware
  - Growth of professional support (SW houses)

→ Estimate for cost and time reduction in the ITRS



Answers on question for average reduction of development time and costs in success case of simulation which occurred in environment of TCAD users:

Table MS3 Modeling and Simulation Technology Requirements: Accuracy [1] ~~and Speed~~ *—Near-term Years*

ORTC INDEX ITWG INDEX	*Year of Production*	*2007*	*2008*	*2009*	*2010*	*2011*	*2012*	*2013*	*2014*	*2015*
	DRAM ½ Pitch (nm) (contacted)	65	57	50	45	40	36	32	28	25
	MPU/ASIC Metal 1 (M1) ½ Pitch (nm) (contacted)	68	59	52	45	40	36	32	28	25
	MPU Physical Gate Length (nm)	25	23	20	18	16	14	13	11	10
DELETED	~~Technology development costs reduction potential if TCAD is appropriately used [2]~~	40%	40%	40%	40%	40%	40%	40%	40%	40%
ADD	Estimated technology development cost reduction from use o TCAD (average across best-practice cases reported by industry) [2]	27%	27%	30%	32%	35%	37%	n.a.	n.a.	n.a.
ADD	Estimated technology development time reduction from use c TCAD (average across best-practice cases reported by industry) [2]	30%	30%	32%	34%	37%	39%	n.a.	n.a.	n.a.
	Lithography Modeling									
WAS	Absolute CD prediction accuracy (incl. OP effects) for dense and isolated lines – % of actual CD (=printed gate length) [3]	3%	3%	3%	3%	3%	3%	3%	3%	3%

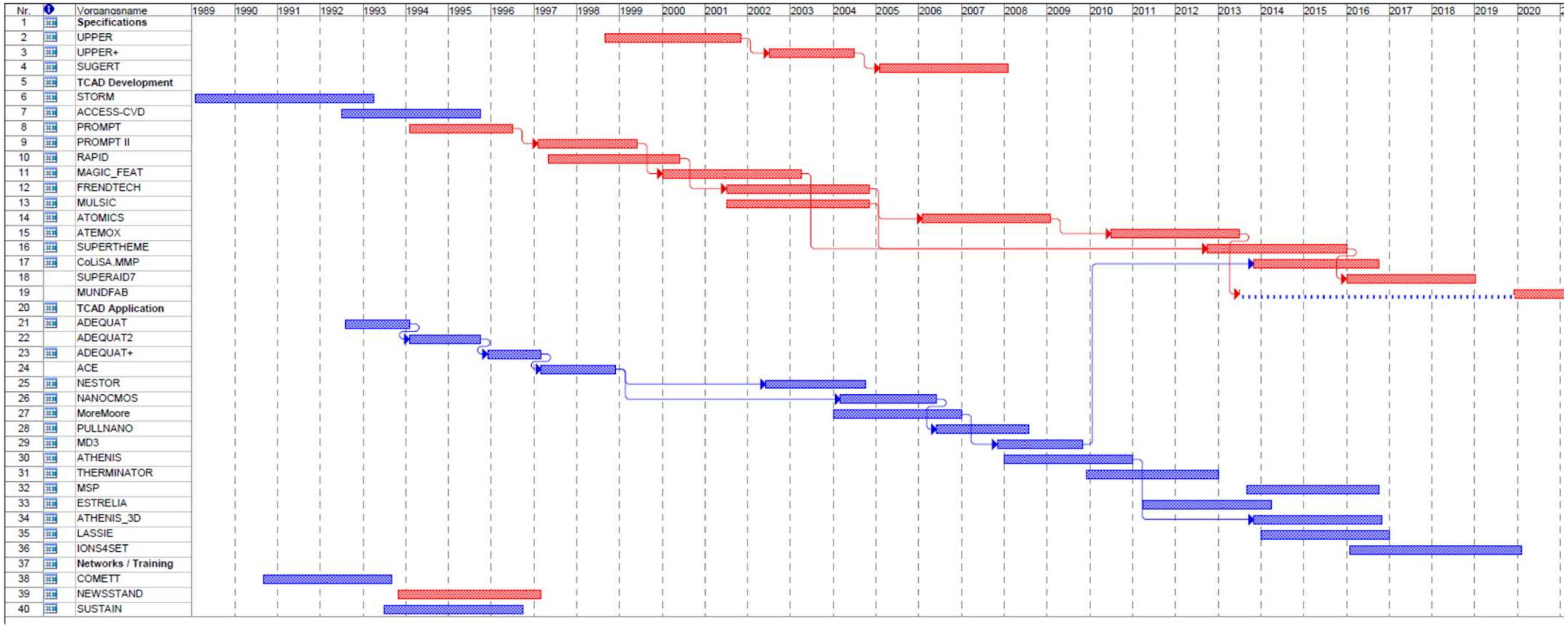
Definition different from estimate of preceding years which referred to cost reduction potential and was based on earlier survey

ITRS

ITRS Winter Public Conference, December 9, Seoul, Korea 8

Process Simulation: A Glimps on History

Role of IISB in Europe: Coordination of / participation in EU projects



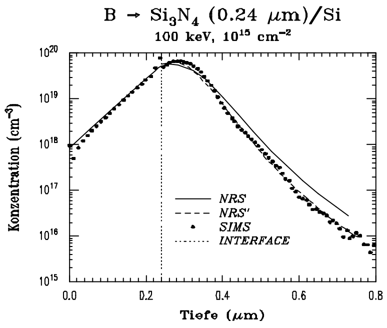
Nr.	Vorgangsname
1	**Specifications**
2	UPPER
3	UPPER+
4	SUGERT
5	**TCAD Development**
6	STORM
7	ACCESS-CVD
8	PROMPT
9	PROMPT II
10	RAPID
11	MAGIC_FEAT
12	FRENDTECH
13	MULSIC
14	ATOMICS
15	ATEMOX
16	SUPERTHEME
17	CoLiSA.MMP
18	SUPERAID7
19	MUNDFAB
20	**TCAD Application**
21	ADEQUAT
22	ADEQUAT2
23	ADEQUAT+
24	ACE
25	NESTOR
26	NANOCMOS
27	MoreMoore
28	PULLNANO
29	MD3
30	ATHENIS
31	THERMINATOR
32	MSP
33	ESTRELIA
34	ATHENIS_3D
35	LASSIE
36	IONS4SET
37	**Networks / Training**
38	COMETT
39	NEWSSTAND
40	SUSTAIN

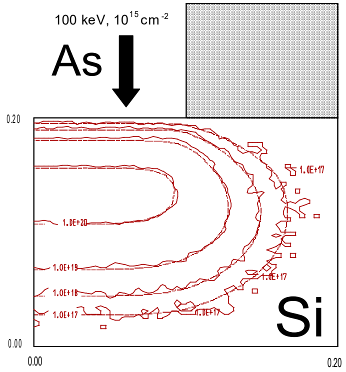
- Participation in 36 projects funded solely by the EC – coordination of 16 of these
- Plus application of lithography simulation in 1 CATRENE, 5 ECSEL and 1 Horizon Europe Project

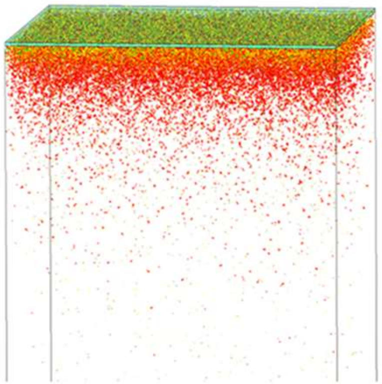
Some Developments in Time-lapse

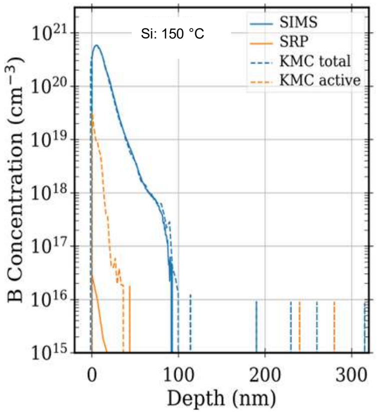
Ion Implantation: From analytical to KMC

- Analytical description standard workhorse for decades
  - IISB 3D multilayer models defined the state-of-the-art (incl. depth-dependent lateral spread and lateral kurtosis) long ago
- Monte-Carlo simulation (amorphous, crystalline, dynamic) originally only for special cases
  - More frequent use due to largely better computer resources, smaller simulation domains and increase of requirements (e.g. more complicated structures; explicit study of variations …)
- Kinetic Monte Carlo to include effects like heated implants, amorphization, recrystallization
  - Current developments in HEU project MUNDFAB (IISB, CEA/Leti, CNR, CNRS, ITME, STM, TU Wien), final review Oct. 5, 2023 – see presentation P. Pichler









Some Developments in Time-lapse

Dopant diffusion: From equilibrium point defects to defect kinetics

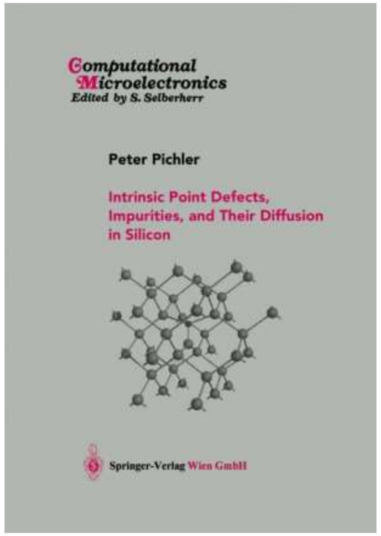
Continuum simulation: Increasingly more driving forces for fluxes considered in diffusion-reaction PDEs

- Dopant gradients + electric field generated by dopants + Fermi-level effect. Diffusion reduced by clustering
- Pair diffusion via vacancies and/or interstitials
- Non-equilibrium point defect distributions, generation/recombination and diffusion of point defects
- Agglomeration of point defects (Ostwald ripening); clustering of dopants and point defects (“BICs”)

Atomistic description (Lattice Kinetic Monte-Carlo) needed e.g. for simulation of laser melt annealing

- Recent investigations and results in HEU project MUNDFAB – see also presentation by P. Pichler

Habilitation thesis of P. Pichler published via Springer in 2012: “Intrinsic Point Defects, Impurities, and Their Diffusion in Silicon”



Computational
Microelectronics
Edited by S. Selberherr

Peter Pichler

Intrinsic Point Defects,
Impurities, and Their Diffusion
in Silicon

Springer-Verlag Wien GmbH

Some Developments in Time-lapse

Oxidation: Shift of emphasis from geometry to morphology

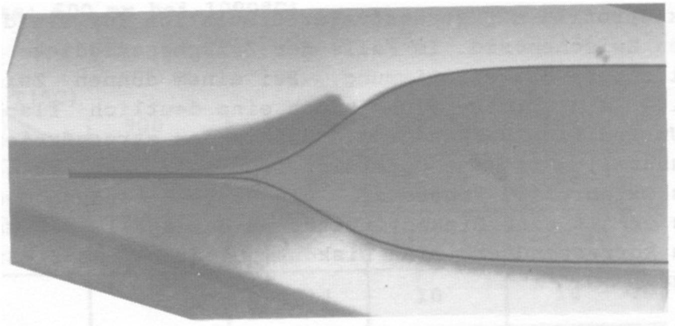
History of continuum models

- 1D Deal-Grove: Diffusion-reaction -> linear-parabolic growth
- 2D first for local oxidation of planar structures (“bird’s beak”): Analytical expression or stress-free diffusion and reaction
- 3D for arbitrary structures: Stress-dependent reaction, diffusion, and oxide flow
  - Numerical problem esp. meshing for dopant diffusion for arbitrary (partly thin) oxide geometries, esp. for dopant flux across interfaces (-> threshold voltage). Among others subject in EC FP5 project “MAGIC_FEAT” – industrialized by ISE AG

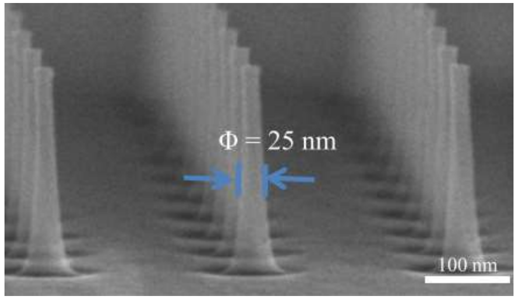
Introduction of STI strongly reduced importance of 3D simulation of oxidation

Emergence of nanowire transistors: fabricated by top-down approach including sacrificial oxidation -> regain of interest in TCAD oxidation simulations

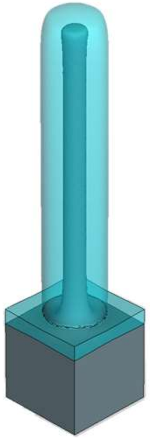
Currently Molecular Dynamics + NN especially for simulation of oxide defects and effects on reliability



Bird’s beak: TEM and simulation w/o stress (IISB)



Guerfi, Y., Larrieu, G. Vertical Silicon Nanowire Field Effect Transistors with Nanoscale Gate-All-Around. *Nanoscale Res Lett* **11**, 210 (2016).

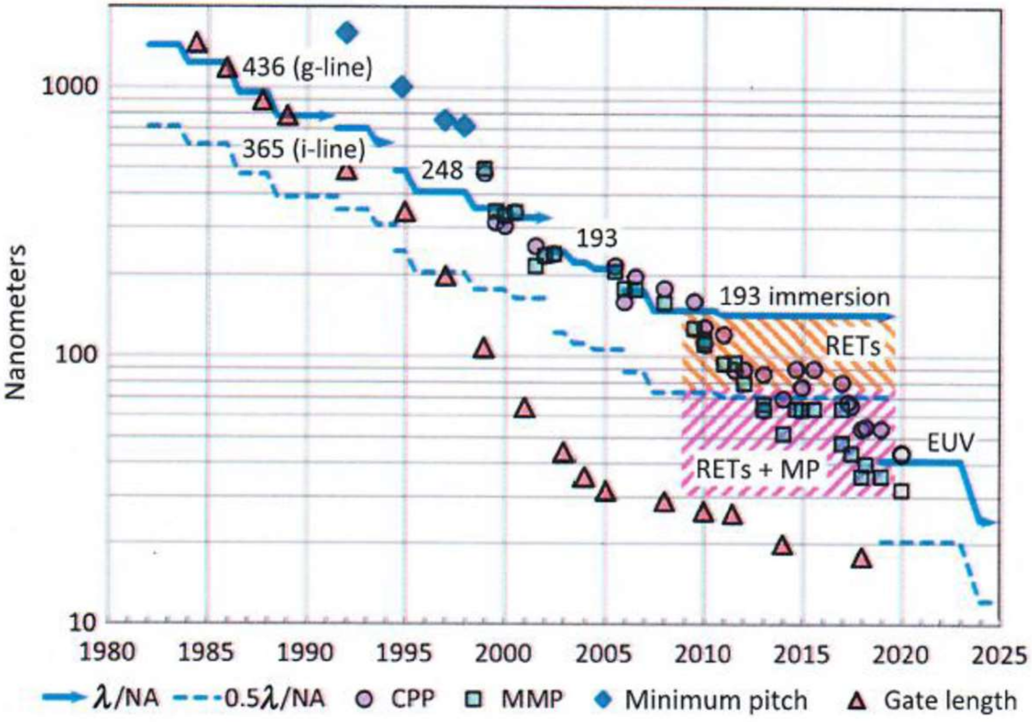


IISB simulation in MUNDFAB

Some Developments in Time-lapse

Lithography: From largely irrelevant to top priority

- Progress in Lithography as predicted by the 1st Rayleigh Criterion $CD = k_1 \cdot \frac{\lambda}{NA}$
- Distortion of structures not relevant as long as feature sizes much larger than this resolution limit
- Importance of lithography simulation drastically increased from about 2000 onwards: Required to help to shrink technology factor k_1 below 0,6



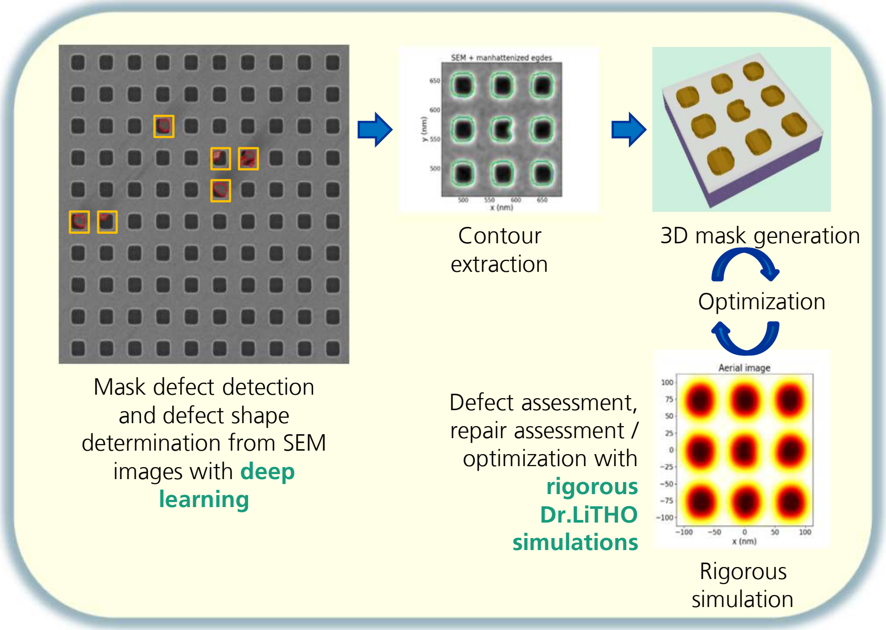
From M.L. Rieger, „Retrospective on VLSI value scaling and lithography",
J. Micro/Nanolith. MEMS MOEMS 18(4), 040902 (Oct–Dec 2019)

Some Developments in Time-lapse

Lithography: Since some years a top priority

Development at IISB **Dr.LiTHO**

- Accurate simulation of imaging (Finite Difference Time Domain, Waveguide)
- Resists exposure and development
- Various methods for speedup by approximation without loss of accuracy
- Additional utilization of AI approaches
- Very close cooperation with industry to address critical aspects (e.g. process windows; novel technological options; defect detection and repair) - first for DUV, since some years primarily for EUV
- See presentation by A. Erdmann and P. Evanschitzky



Mask defect detection and defect shape determination from SEM images with **deep learning**

Contour extraction

3D mask generation

Optimization

Defect assessment, repair assessment / optimization with **rigorous Dr.LiTHO simulations**

Rigorous simulation

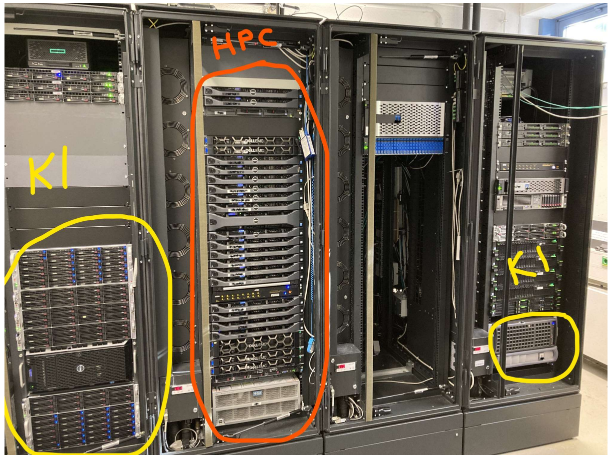
Example of IISB work in ECSEL project PIN3S

Some Developments in Time-lapse

Hardware and algorithms: From 624 kB computer to GPUs and KI

- 40 years ago: Computer without virtual memory, partly punch cards
  - → 1D simulation with few mesh points and simple models (e.g. ICECREM)
- Main computer at IISB (at that time AIS-A) in 1985: VAX 11/750, 8 Mbyte physical memory, about 400 Mbyte user disc
- Adaptive meshing in its infancy
- Now: large processor farms, partly GPUs
  - → Enabled rise/development/application of AI
  - → New trend: Combination of data science and physics –
    Physics-Informed Neural Networks PINNs (department renamed end 2018)

„Memorystick“ in 1985: EAGLE user disc for VAX 11/750 . About 400 MB, about 40 cm * 20 cm * 60 cm, about 100000 DM



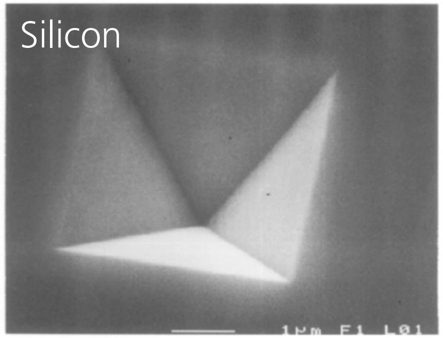
Increased Integration and Extended Scope

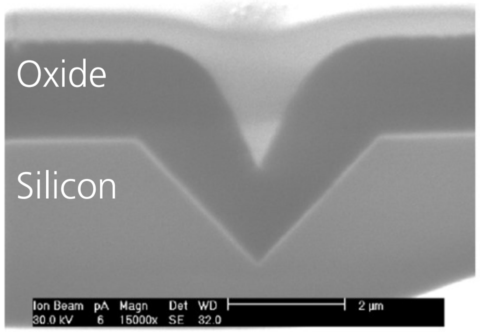
From single process steps to full process + device + circuit

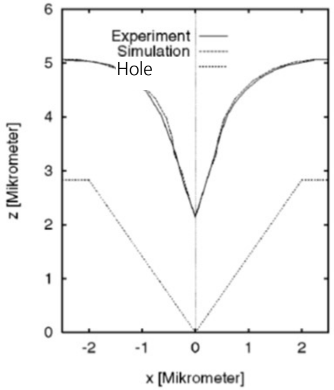
- 1970ies: First 1D programs limited to implantation/diffusion/oxidation: SUPREM (Stanford), ICECREM (Fraunhofer IFT). 2d program SAMPLE (Berkeley) for lithography/etching/deposition
    - No link between dopant and topography simulation or with device simulation
- 1985: First integrated program for doping and topography simulation (COMPOSITE, IISB)
- Subsequently preliminary links between process and device simulation.
- Consolidated coupling between process and device simulation linked with emergence of TCAD suites from large EDA/TCAD companies
- Subsequent trends:
    - Extraction of compact models from process/device simulation
    - Design-Technology Co-Optimization DTCO, System-Technology Co-Optimization (STCO)
    - Study of variability
    - Use of TCAD for development of quantum computing/sensing, use of quantum computing for simulation (see presentation by S. Mundinar and G. Kruse)
    - AI for TCAD (see presentation by A. Roßkopf)

Parameters for Process Simulation

- Atomistic/first principle simulations generally without free parameters
- Several standard parameters /formulas can be harvesting from other areas (e.g. for ion scattering)
- Specific process models (e.g. for dopant diffusion) need extraction of relevant parameters:
  - From theoretical / first principle calculations (e.g. from Monte-Carlo simulations for analytical range models)
  - Standard problem: Separation of effects / extraction of individual parameters independently of others
  - Standard benefit: Frequently parameters extracted from suitable 2D experiment also correct in 3D simulations – e.g. parameters for LTO deposition (two contributing species (sc,1 = 0.05, sc,2 = 0.9), relative contribution of species 1 to growth rate on planar substrates = 0.49)







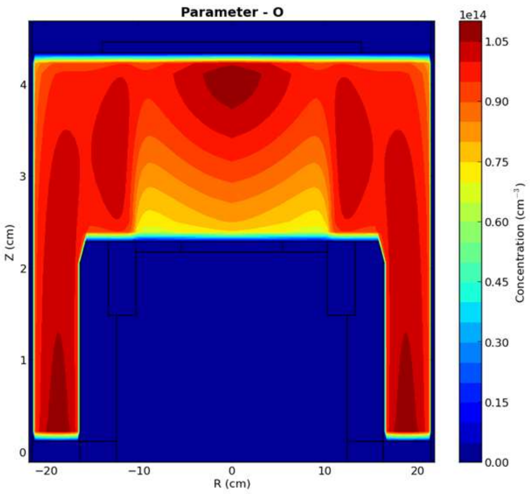
Increased Integration and Extended Scope

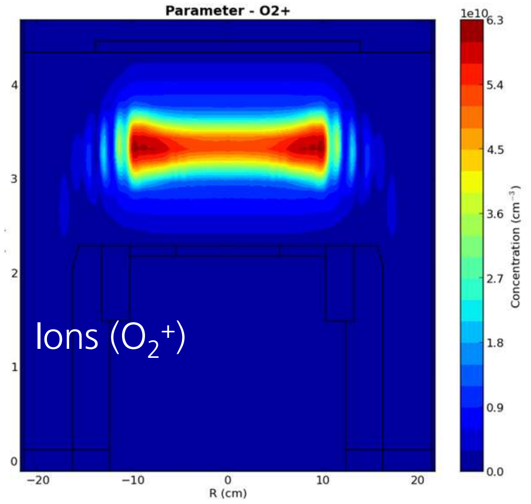
Equipment Simulation: Delimitation from and link with Process Simulation

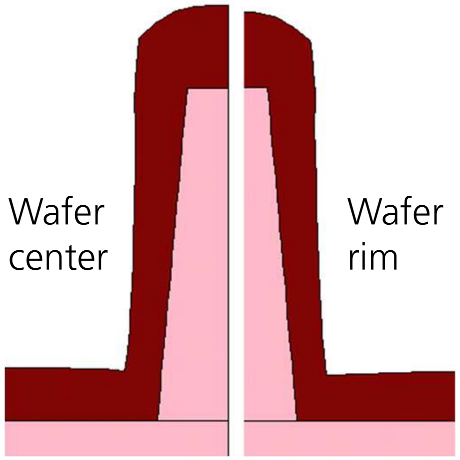
- Simulation of impact of equipment on the wafer
- Input: Equipment geometry, chemistry, physics, sources for particles, energy, …
- Result: Distribution of relevant features (i.e. fluxes) at surface of unstructured wafer, as input for feature-scale simulation
- Benefits: Link of process results to equipment parameters, characterization of (systematic) variations

Example:

- Deposition of SiO_2 from TEOS and oxygen, models assumes contributions from oxygen neutrals and ions
- Reactor simulation predicts concentration of ions and neutrals which serve as boundary condition for feature scale simulation



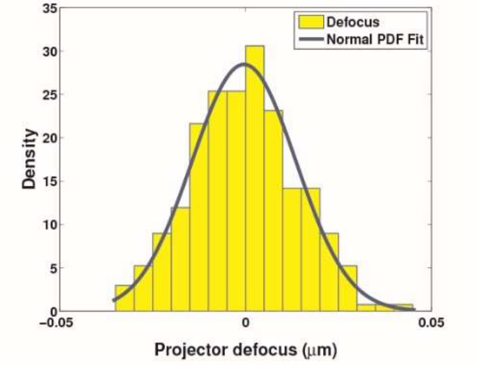




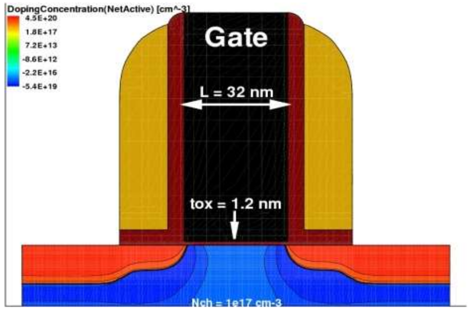
Increased Integration and Extended Scope

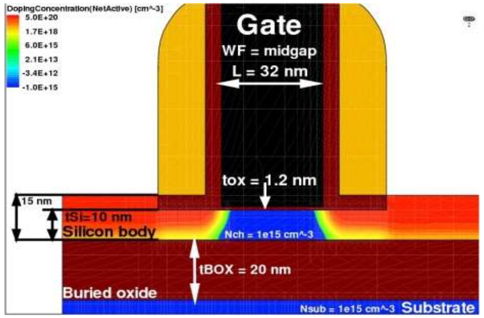
From nominal processes to variations: Historical example of IISB

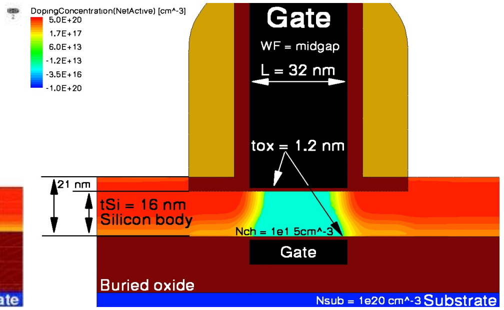
- Simple example for impact of process variations (focus in lithography) on transistors of different architectures



Focus variations
➡ CD-Schwankungen

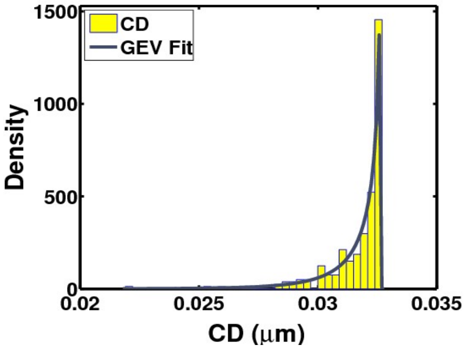


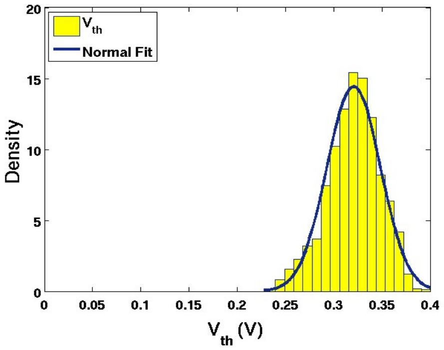


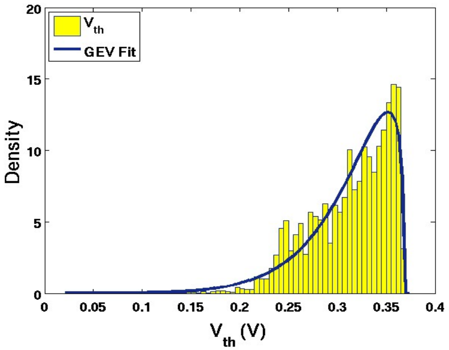


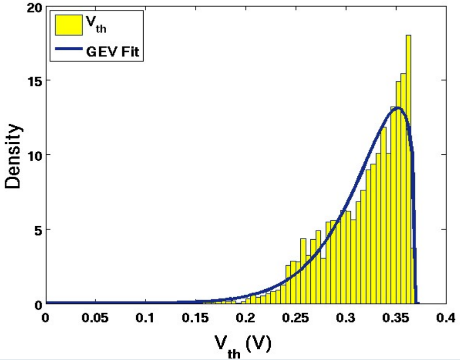
Bulk SOI ***Single Gate FD SOI*** ***DG FD SOI***

differently act as filters for the CD variations caused by the focus variations







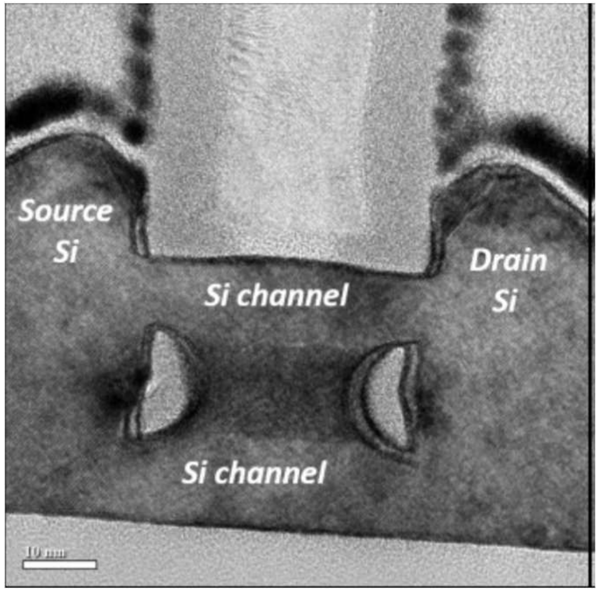


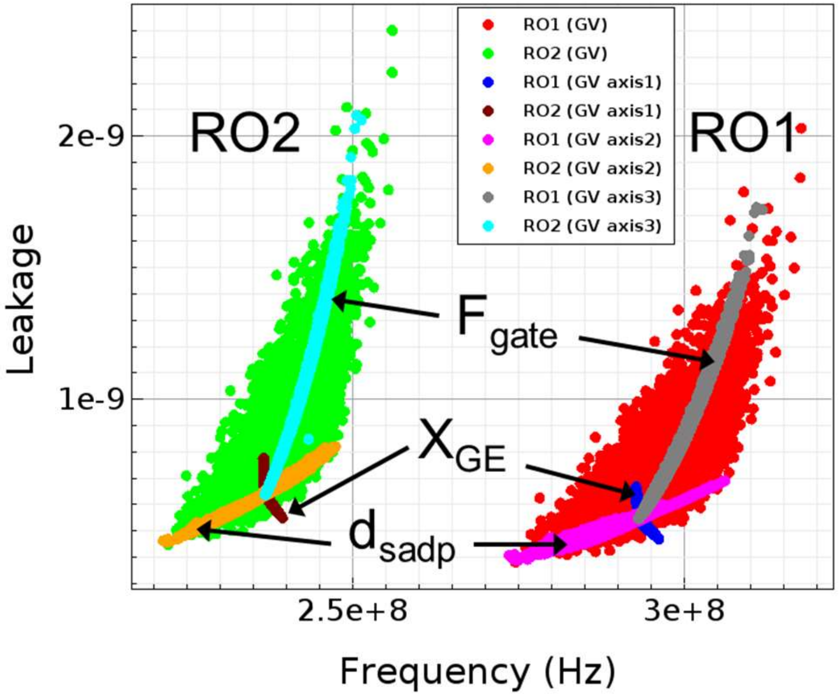
J. Lorenz et al., Proc. Int. Symp. on VLSI Technology, Systems and Applications (2009)

Increased Integration and Extended Scope

From nominal processes to variations: Example from Horizon 2020 SUPERAID7

- 5 nm nanosheets investigated
- 3 systematical variations studied:
  - SiGe mole fraction
  - Fin SADP deposition factor
  - Gate litho defocus
- 2 statistical local variations studied:
  - Random discrete dopants
  - Line Edge Roughness
- IISB topography simulation + S_Process + GARAND + LETI-NSP compact model
- **Impact on IC yield!**



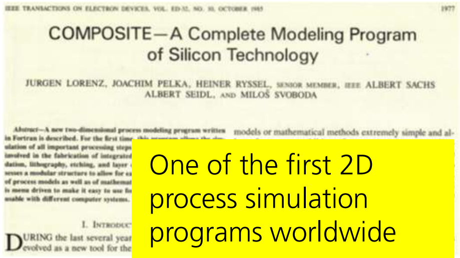


Example for results: Variations introduced by different process parameters for the leakage of two extreme cases ROs (GV axis 1: x_{Ge}; GV axis 2: d_{sadp}; GV axis 3; F_{gate}

From A.R. Brown, …., F. Klüpfel, ….. J. Lorenz, From devices to circuits: modelling the performance of 5nm nanosheets, Proc. SISPAD 2019

Examples for IISB Outreach

Books published and major conferences/workshops organized

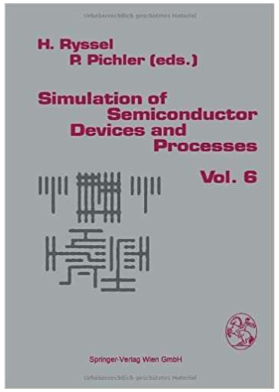


IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. ED-32, NO. 10, OCTOBER 1985 1977

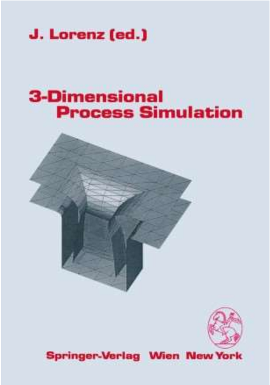
COMPOSITE—A Complete Modeling Program of Silicon Technology

JURGEN LORENZ, JOACHIM PELKA, HEINER RYSSEL, SENIOR MEMBER, IEEE ALBERT SACHS ALBERT SEIDL, AND MILOŠ SVOBODA

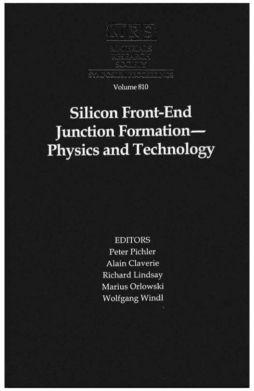
One of the first 2D process simulation programs worldwide



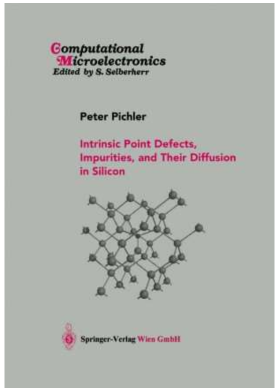
Conference 1995



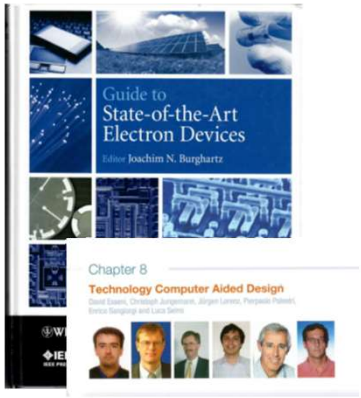
Workshop 1995



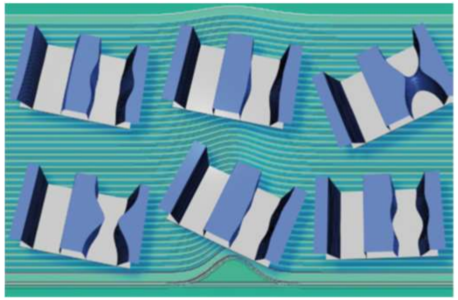
Book 2004



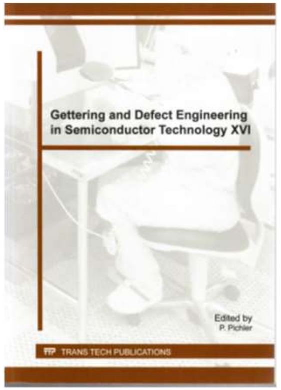
Book 2012



Chapter in book 2013

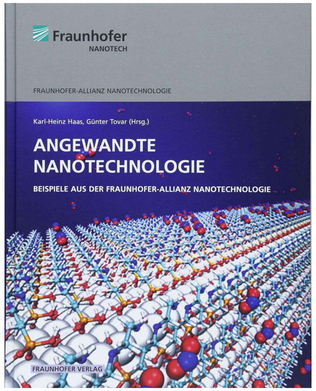


- International Lithography Simulation Workshop: 19th issue June 2024 @ Behringersmühle, Frankonia

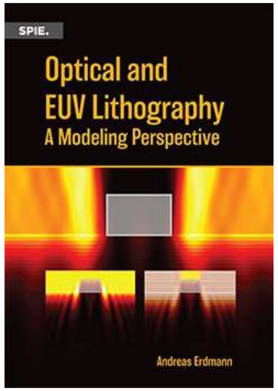


Conference 2015

Conference 2016



2 chapters in book



Book 2021

Chapter in book 2022

Conclusions

- Process simulation (together with device simulation) has developed within the last 40+ years into an indispensable tool for semiconductor industry
- IISB has made central contributions to the development of TCAD: Physical models, algorithms/tools, contributions to and coordination of cooperations and projects
- Many results are in some way implemented or integrated in software frequently used in industry – to some extent “Fraunhofer IISB inside”
- Several examples to be given in subsequent presentations
- Current focus at IISB: Combination of physics and AI (department since end 2018 named “Modeling and Artificial Intelligence”)
  - TCAD application and extension esp. for wide bandgap materials / devices and for quantum computing
  - Development and application of lithography simulation
  - Development, implementation and application of AI approaches for optimization of processes, devices, circuits and systems

Thank you for your attention!

Fraunhofer
IISB

Fraunhofer Institute for Integrated Systems and Device Technology IISB

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