



Challenges and opportunities at the confluence of semiconductor manufacturing (SM) and applied math (AM): The SM-AM Agora





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Are You Smarter than a 5th Grader?





Insulators, Conductors and Semiconductors

The Nobel Prize in Physics 1956



William Bradford Shockley Prize share: 1/3



Prize share: 1/3

Walter Houser

Walter Houser Brattain Prize share: 1/3

Three American physicists, John Bardeen, Walter H. Brattain, and William Shockley, were honored last month in Stockholm, where they were jointly awarded the 1956 Nobel Prize in Physics for "their investigations on semiconductors and the discovery of the transistor effect".

Semiconductors power the world

"semiconductor industry is an irreplaceable enabler of **tens of trillions of dollars** of annual economic activity worldwide"



Wearable

Medical



Automotive







Silicon is the building block of Integrated Circuits/semiconductor chips

ICs contain billions of components: resistors, capacitors, transistors



Wafer and integrated circuit die ntegrated circuit's element Integrated circuit chip Wafer Samsung Semiconstory

Transistors: logic gateway





n-mos

p-mos

Four terminals: gate, source, drain, body

IC classification



Memory chips

Microprocessors (CPU, GPU)



ASIC

System on Chip



System On Chip

Analog chips



C-MOS: dominant technology for constructing IC



The CHIPs Act

~\$50 Billion for workforce, reshoring, R&D

Chips were invented in America

But most chips are made outside of the U.S.



Logic chip production by country, 2021

Memory chip production by country, 2021



The CHIPs Act

CHIPS for America Vision



Economic Security

This act enables us to build more resilient supply chains for important components.



National Security

This act enables us to bring the most sophisticated technologies back to the U.S.



Future Innovation

Chips are key to the technologies and industries of the future, so we need to be at the forefront. This act will ensure long-term U.S. leadership in the sector.



The Center for Semiconductor Manufacturing

https://csm.arizona.edu/



Mission and Vision

Mission

To coordinate and facilitate an institutional focus on meeting the needs of commercial and defense stakeholders and securing the needed external resources to develop multidisciplinary R&D solutions and workforce training programs that are responsive to semiconductor sector needs.

Vision

To connect and mobilize the University of Arizona's community of faculty and students to develop advanced technology solutions and workforce training programs for semiconductor manufacturing that advance sustainable economic development, national security and to expand the number of well-paid jobs in Arizona.

The Center for Semiconductor Manufacturing



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Challenges and Opportunities

• Chiplets, SoC and heterogenous integration

"Companies are now talking of "chiplets" comprising smaller "building blocks" to be mixed and matched much like **Lego Blocks** creating new flexibility in design and production. Intel, TSMC, Samsung, Arm, Qualcomm, and others have come together to establish standards for building these chips. Mediatek and Nvidia recently announced a collaboration on chiplets."

- Post-silicon technologies: low-D materials, high band-gap semiconductors
- Beyond CMOS: new avenues using photonic , spintronic and bio ICs
- Al-specific chips: "AI chips include graphics processing units (GPUs), field-programmable gate arrays (FPGAs), and applicationspecific integrated circuits (ASICs) "
- Hardware security

- electron to devices (e2d): Multiphysics, multiscale algorithms (materials & manufacturing)
- Al for generative design of ICs
- Computer vision for defect detection
- New computing paradigms (neuromorphic, quantum and quantum analog)
- New approaches for hardware security

'Neu' computing paradigms in the Post-Moore era: Xiaodong Yan

Challenges in traditional computing arise in leveraging big data applications

Ever growing pressure for data size



Seagate and IDC Global Datasphere

Energy cost in data manipulation

- Data transmission
- Data processing



Vidal J, Climate Home News, 2017

von-Neumann Computing

Human brain



1.4 M Watts (>500 times average household power consumption), 8192 processors, 10⁹ synaptic events/sec (10⁹ flops)

v.s.



20 Watts, 10¹⁵ synapses, 10¹¹ neurons, 10¹⁶ synaptic events/sec Area efficiency...



Can we make our computing hardware as efficient as the human brain?

von Neumann architecture







350,000 gallons of water a day

a human: 3.5 gallons a day



(b) Neuromorphic computing architecture

Neuromorphic computing: an efficient computing paradigm inspired by the brain and realized by emerging semiconductor devices



Moiré Synaptic Transistor with Room-Temperature Neuromorphic Functionality

X. Yan, Z. Zheng, V. K. Sangwan, J. H. Qian, *et al.*, *Nature*, **624**, 551 (2023). <u>Collaborators</u>: S. E. Liu, K. Watanabe, T. Taniguchi, S. Y. Xu, P. Jarillo-Herrero, Q. Ma



Semiconductor Chips for Neuromorphic Computing: Computing-In-Memory





Hardware Neural Network

'New materials in the Post-Moore era: Brian Kim

Next-generation 2D/quantum materials and devices



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Advanced device platform



Novel materials platform



Novel moiré systems



AI–Driven Materials Discovery and Design Patrick Lohr

Accelerating Materials Design



Schleder, G. R. *et al.* From DFT to machine learning: recent approaches to materials science–a review. *J. Phys. Mater.* **2**, 032001 (2019)

The Materials Project Database





Lawrence Berkeley National Laboratory

https://next-gen.materialsproject.org

The Materials Project Database

The Materials Project by the numbers



https://next-gen.materialsproject.org

Graph Neural Networks (GNNs)



Structure–Property Relationships



Merchant, A. *et al.* Scaling deep learning for materials discovery. *Nature* **624**, 80–85 (2023)

<u>GNNs for Materials Exploration (GNoME)</u>





Merchant, A. *et al.* Scaling deep learning for materials discovery. *Nature* **624**, 80–85 (2023)

Material Stability





Merchant, A. *et al.* Scaling deep learning for materials discovery. *Nature* **624**, 80–85 (2023)

Thin-Film Semiconductors (My Work)





Automated Synthesis (A-LAB)



Szymanski, N. J. *et al.* An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* **624**, 86–91 (2023)

Automated Synthesis (A-LAB)



Back to Basics

Lens Optics

Monte Carlo

Interface Molecular dynamics

Level 1-3:

Packaging

module

ght efficiency

Source: W. van Driel TUD, Phillips

Level 0



Level 6:

processes

(We

.

Level 5:

Large

Level 4:

vstem

Chapter 14: Modeling and Simulation

For updates, visit http://eps.ieee.org/hir

Semiconductor Manufacturing: A deep dive



• Typically several hundred to thousands of steps to complete a modern device!

Wafer Manufacturing

- Czochralski (CZ) Method
 - High purity silicon and selected dopant are melted in large crucible
 - Seed crystal of known crystal orientation is dipped into melt pool
 - Seed and crucible are counterrotated while seed is slowly drawn upward from melt surface
 - Silicon solidifies into large cylindrical ingot which is sliced into wafers which are polished and processed further



Chemical-Mechanical Planarization (CMP): Need for multiphysics modeling for process optimization

- CMP is used to remove excess material and planarize/polish wafer surface after different processing steps
- Uses both mechanical force (pressure, abrasives) and chemical means (etch chemistry) to remove material
- Wafer is placed into carrier and pressed into polishing pad while slurry (etchant + abrasive) is dispensed onto pad
- Both the wafer carrier and pad are rotated during planarization
- Slurry chemistry and abrasives are tailored to material being removed



Wafer Cleaning: accounts for 30 % of processing steps









- high yield (>> 95%) required for manufacturers to remain competetive
- Cleaning steps used to remove contamination and prepare surface for next step
 - Form native oxide (hydrophilic), Si-H termination (hydrophobic), etc.
- Wet Cleaning
 - Single wafer or batch process using aqueous chemistry
- Dry Cleaning
 - **Plasma-based** clean steps to remove contamination
- Supercritical CO₂ Clean
 - Good for high aspect ratio structures

Wafer Cleaning: accounts for 30 % of processing steps

Defect density D0 (< 0.09 /cm²)



AI-leading the way

1. Advanced Process Control (APC): Data-drive real-time monitoring & control

2. Machine Learning for Predictive Maintenance: Downtime minimization via predicting potential failures

- **3. Smart Manufacturing and Industry 4.0:** Data-driven decisions for operational efficiency
- **4. Defect Detection with Computer Vision:** Identifying defects during manufacturing
- 5. **Statistical Process Control (SPC):** maintains consistency and reduces variability

Thermal Oxidation





- Forms insulating regions between devices and can protect wafer surface during other processes
- Wafers are loaded into a "boat" and placed into furnace
- Furnace is heated in "dry" (O₂-only) or "wet" (O₂ + steam) conditions and exposed Si oxidizes
- Temperature, time, and conditions are adjusted to achieve desired oxide thickness

Photolithography

- Wafer is coated in a photoactive film that reacts to particular wavelengths of light
- Wafer is exposed with light passed through a patterned photomask to transfer the image to the photoresist to create a positive or negative image
- Resist layer is "developed" to remove unwanted resist and leave desired image structure to be used in subsequent processing step (etch, deposition, etc.)







Traditional Photolithography

EUV Photolithography

ML in Lithography Hotspot Prediction



Fig. 5. Example results for the test dataset. Real and predicted hotspots are indicated by blue bounding boxes in SEM G.T images and by red and yellow bounding boxes in generated SEM images which are final outputs of model, respectively. G.T represents ground truth. In segmentation prediction maps, yellow bounding boxes represent false positives (potential hotspot regions) in segmentation prediction map.

Kim, Jaehoon, et al. "Hotspot Prediction: SEM Image Generation With Potential Lithography Hotspots." *IEEE Transactions on Semiconductor Manufacturing* (2023).

- High feature density can lead to defects in lithography, or "hotspots", that can transfer to subsequent process steps
- ML algorithms takes in design level layout diagrams and corresponding SEM images and learns to predict where real hotspots or potential hotspots will occur and generate a predicted SEM image

Etching









- Material is removed from areas of a wafer using "wet" or "dry" etching methods
- Wet etching introduces a wafer to a chemical solution formulated to attack the desired material
 - Isotropic in non-crystalline materials
- Dry etching utilizes plasma chemistry to attack a specific material (allows for directional etching)
 - Anisotropic etching, good for small features
- Prior lithography steps allow for specific patterns to be etched into layers on the wafer

Finite Element Analysis in Wet Etch Processing



Derek Bassett et al 2015 ECS Trans. 69 159

Figure 6: Etch profiles for simulations with varying outer liquid flow velocity showing mole fraction of Si(OH)₄. The left image is at t = 0 s, the middle image is at t = 830 s, and the right image is at t = 1660 s when etching of the SiN is complete. This is an example case for all the SiN layers etching at the same rate, indicating a reaction-limited etching process.

- FEM analysis allows for predicting etch profile progression and concentration profiles of byproduct under various conditions
- Predictability can help avoid structural defects and make the process engineer's life much easier

Modeling Plasmas & Etch Equipment (Monica Titus)



culty/economou/tsf_00_review.pdf

0

52403_2021.pdf

Modeling material evolution (Monica Titus)

Molecular Dynamics (MD) and Hybrid Models illustrate etch, mixing, deposition, adsorption, implantation, and desorption affects, among others, on substrate materials. The generation of mixing layers, contaminants, and surface roughness, help process engineers mitigate undesired effects or target desirable results by appropriate hardware and chemistry selection.

Hybrid Simulations: Global Plasma Model + Particle-in-Cell Monte Carlo





MD Simulations

Example of Hybrid simulations incorporating global plasma models with PIC-MC simulations to demonstrate specie distribution, uniformity, and profile evolution during atomic layer deposition and etching conditions.

Example of MD simulation incorporating particle physics and chemistry to demonstrate etch of Silicon under various chemistries and the thickness of the mixing and damage layer that results.

Doping

- Group III or Group V elements are added to silicon to enhance conductivity by introducing excess electrons or holes (forming source/drain regions, n- or p-wells)
- Ion implantation
 - Dopant ions are introduced from an ion source and are accelerated through an E-field toward wafer surface to deposit a dose of dopant atoms
 - Depth profile of dopant determined by current, accelerating voltage, and time
- Diffusion Doping
 - Wafers are loaded into furnace similar to that in oxidation and dopant gases are introduced to chamber
 - Dopant diffuses into exposed areas under high temperature conditions





Ion Implantation Optimization via Machine Learning



Lang, Christopher I., et al. "Intelligent Optimization of Dosing Uniformity in Ion Implantation Systems." *IEEE Transactions on Semiconductor Manufacturing* 35.3 (2022): 580-584.



- Using ML to account for beam shape and intensity and ensure uniform spatial dosage
- ML increased uniformity include spatial variation of implant time across wafer

Deposition



- Physical Vapor Deposition
 - A solid source of material is thermally evaporated or sputtered and the resulting vapor condenses on the wafer to form a thin film
- Chemical Vapor Deposition
 - Wafers in a reaction chamber are introduced to precursor gases that react and deposit a solid film on the surface
- Atomic Layer Deposition
 - Special-case cyclic CVD process using typically two precursors
 - Precursor A introduced to form monolayer on wafer, then precursor B introduced to form another monolayer on top of first (A,B,A,B...)
 - Used for very thin layers of dielectrics (like high-k gate oxides) and some metals

Metallization





- Electrochemical deposition is used to deposit copper in metal layers on wafer (other metals can also be deposited with ECD)
- Low-k dielectric is deposited onto wafer and patterned to form areas for metal lines between devices
- A barrier layer (TaN/Ta) and a Cu seed layer are deposited, then wafer is introduced to Cucontaining solution
- As current is passed through the electrochemical cell, wafer acts as the cathode and Cu is deposited

Packaging

- Packaging is important to optimize thermal/electrical/ mechanical environments for given application
- Individual die are cut from wafer and attached to substrate
- Electrical connections between substrate and die are made by wirebonding
- Die is encapsulated and electrical terminations on package are formed
- More sophisticated packages can include multiple stacked die attached together through vias and BGAs or wirebonds (System-in-Package)







Packaging: from 2D-2.5D-3D



is-2d-2-5d-3d-packaging-ofintegratedchips/#:~:text=2D%20IC%20P ackaging%3A%20Components %20are, improved%20perform ance%20and%20power%20eff

Thermo-mechanical models for 'packaged systems'





Thermal profile of a 'single' transistor (cadence.com)

FEM model of a 3D stack IBM J. RES. & DEV. VOL. 52 NO. 6 NOVEMBER 2008

How do we dissipate the heat?

Hardware Security in the Age of AI and Emerging Semiconductor Devices

Soheil Salehi

Assistant Professor of Electrical and Computer Engineering (ECE), The University of Arizona Director of <u>Privacy-preserving</u>, Intelligent, and <u>Secure Computing Lab</u>oratory (PRISM Lab) Email: <u>ssalehi@arizona.edu</u>; Website: <u>https://soheilsalehi.com/</u>





Threats on Hardware Supply Chain and Al Algorithm



□ Hardware security is questioned due to: WH.GOV mMin Emerging attacks and globalized fabrication supply chain. OCTOBER 30, 2023 Trojan, IP theft, IC Cloning, Counterfeiting, etc. FACT SHEET: President Biden Issues Executive Order on **U** Vulnerability of Transformer models: Safe, Secure, and Trustworthy Dependency on large-scale training datasets Artificial Intelligence Vulnerability to adversarial attacks WH.GOV Complexity of the hardware accelerator NOVEMBER 27, 2023 Lack of transparency FACT SHEET: President Biden □ Threats affecting the integrity of AI accelerator chips: Announces New Actions to Side-Channel and Probing Attacks Strengthen America's Supply Chains, Lower Costs for Families, Reverse-Engineering Attacks and Secure Key Sectors Fault Injection and Focused Ion Beam Attacks Hardware Trojan Attacks Source of Threats: **Algorithm Threats** Algorithm Model **Training Dataset** Training & Inference **Almost Everywhere!** Data Poisoning 품 🛖 SW Trojan Attacke Reverse Engineering Model Poisoning Al Algorithm **Design Integration** Synthesis & Verification Fabrication Testing & Packing Al Chips Design & Training Hardware Threats Architecture Circuits HW Troiai Fault Injection Design Reverse Engineering Side-Channel Analysis Engineer

OASIC: Optimized and Automated Secure IC Design Flow



OASIC: Optimized and Automated Secure IC Design Flow:



Simulation Results:



Power-Area-Security trade-off of obfuscating an AES core with the proposed (a) 8x8 (b) 8x8x8 lockboxes.

- Optimization: Number (N) = {2, 3}, Size (S) = {4, 8}, and Depth (D) = {2, 3}.
- Scalability: Design Size (\uparrow) = Overhead (\downarrow)
- Overhead: Area =<1.15 and Power =<1

Secure AI Hardware Accelerator Design using Post-CMOS





• Digit '9' has the lowest impact and '2', '3', and '8' unaffected.

the device level

ree Lave

FANDEMIC: Firmware Attack Construction and Deployment on Power Management Integrated Circuit and Impacts on IoT Applications





Design framework for attack implementation flow:



1.2

10

Voltage (V)

0.7

1.5

Flow diagram of the sensitivity and threat analysis approach:

- Identify addresses associated with Two-Wire Interface (TWI) peripheral that nRF52 uses for I2C.
- Reverse engineer binary to locate Buck2 configuration.
- Modify Buck2 configuration bytes and checksum.

0003 8DA0: 3A 31 30 42 33 36 30 30

```
original_temp_1.8V_09.hex:
0003 8D20: 30 30 34 32 32 32 31 41
                                                46 38 30 46 0042221A 709DF80F
                                   37 30 39 44
0003 8D30: 33 30 30 30 32 42 30 33
                                   44 30 31 36 34 42 30 31 30002B03 D0164B01
0003 8D40: 32 32 43 39 0D 0A 3A 31
                                   30 42 33 34 30 30 30 31 22C9..:1 0B340001
0003 8D50: 41 37 30 30 32 45 30 31
                                   34 34 42 30 30 32 32 31 A7002E01 44B00221
0003 8D60: 41 37 30 31 33 34 42 30
                                    39 32 32 35 41 37 30 33 A70134B0 9225A703
0003 8D70: 33 0D 0A 3A 31 30 42 33
                                    35 30 30 30 30 44 46 31 3... 10B3 50000DF1
0003 8D80: 31 33 30 33 31 39 34 36
                                    30 32 32 30 46 46 46 37 13031946 0220FFF
0003 8D90: 31 32 46 45 30 35 39 30
                                   30 35 39 42 31 44 0D 0A 12FE0590 059B1D.
0003 8DA0: 3A 31 30 42 33 36 30 30
                                   30 30 30
                                             32
                                                42 30 38
                                                         44 :10B3600 0002B08D
modified_temp_3.8V_1d.hex:
0003 8D20: 30 30 34 32 32 32 31 41
                                    37 30 39 44
                                                46 38 30 46 0042221A 709DF80E
0003 8D30: 33 30 30 30 32 42 30 33
                                   44 30 31 36 34 42 30 31 30002B03 D0164B01
0003 8D40: 32 32 43 39 0D 0A 3A 31
                                   30 42 33 34 30 30 30 31 22C9...:1 0B340001
0003 8D50: 41 37 30 30 32 45 30 31
                                   34 34 42 30 30 32 32 31 A7002E01 44B00221
0003 8D60: 41 37 30 31 33 34 42 31
                                    44 32 32 35 41 37 30 31 A70134B1 D225A701
0003 8D70: 46 0D 0A 3A 31 30 42 33
                                    35 30 30 30 30 44 46 31 F. .: 10B3
                                                                     50000DF1
0003 8D80: 31 33 30 33 31 39 34 36
                                    30 32 32 30 46 46 46 37 13031946 0220FFF
0003 8D90: 31 32 46 45 30 35 39 30
                                    30 35 39 42 31 44 0D 0A 12FE0590 059B1D.
```

30 30 30 32 42 30 38 44 :10B3600 0002B08D

Simulation Results:

٠

- Data corruption by ٠ altering sensor power supplies.
 - Error rate of ~3.75% relative to pressure reading at 2.9V for every change in 0.1V of supply voltage.





Outputs averaged over 100 samples with 100ms period

Config	V_{Supply}	$D[V_{Out}]$	V_{Out}	Pressure (Pa)	% Error
0x10	1.60	545	0.48	618.44	44.04
0x15	1.85	635	0.56	720.99	34.77
0x1C	2.20	710	0.62	805.54	27.12
0x22	2.50	810	0.71	919.40	16.81
0x26	2.70	941	0.83	1068.09	3.36
0x2A	2.90	974	0.86	1105.23	0.00
0x2C	3.00	1043	0.92	1184.12	7.14
0x32	3.30	1161	1.02	1317.43	19.20
0x37	3.55	1211	1.06	1374.38	24.35
0x3D	3.85	1371	1.20	1556.19	40.80

Sensor Outputs vs Supply Voltage

Secure Generative AI Hardware Accelerator Design



Hardware overview of adaptable butterfly accelerator for Generative AI algorithm and Hardware Trojan (HT) vulnerabilities: Sample HT-modified architecture of the butterfly unit with:



HW-V2W-Map for Hardware Vulnerability and Risk Assessment





Flow diagram of the Hardware Vulnerability to Weakness Mapping framework for risk assessment and root cause analysis:

Graphical User Interface for the HW-V2W-Map

- ✓ Demo: <u>https://youtu.be/rdejfpFcqXk</u>
- ✓ Repository: <u>https://gitlab.com/yuzhenglin/HW-V2W-Map</u>



Simulation Results:

Window-based ML-assisted Important HW CWE Prediction

Time Window	Training R^2 Score	Testing R^2 Score	Testing Mean Squared Log Err	Testing Mean Absolute Err	Testing Median Absolute Err
3-year	0.98	0.92	1.95	21.98	6.37
2-year	0.97	0.86	1.78	24.31	6.90
1-year	0.98	0.91	2.14	23.28	6.94

Window-based ML-assisted CVE CVSS Prediction

Model Name	Evaluation Loss	Evaluation F1 Score	Evaluation ROC AUC	Evaluation Accuracy	Evaluation Precision	Evaluation Recall
CWE-CWE	0.18	0.66	0.80	0.62	0.73	0.86
CWE-CWE-Binary	0.44	0.81	0.81	0.80	0.68	0.79
CWE-CVE	0.46	0.84	0.84	0.83	0.84	0.85
CWE-CAPEC	0.51	0.79	0.79	0.77	0.77	0.83

• Predicting the relationship between CWE to CVE and CWE to CAPEC is more accurate than predicting CWE to CWE due to fewer labels involved.

In conclusion

- Enormous R&D and workforce opportunities for 'math' inclined folks
- UA-CSM is poised to spearhead the growth of the semiconductor footprint on campus and in AZ
- More than 30 faculty across campus who would greatly benefit from the AM GIDP program
- Start talking to the faculty if you want to be part of the bandwagon

Acknowledgement: Thanks to the internet for all the nice figures and blurbs