Applied Materials Invited tutorial for MLCAD https://mlcad.org/symposium/

Accelerating Semiconductor Industry Innovation with AI/ML

Part 1: Introduction

Exponential progress in Artificial Intelligence (**AI**) owes much to remarkable advancements in semiconductor technology. The semiconductor roadmap is guided by the **PPACt** metrics: low **P**ower, high **P**erformance, reduced **A**rea, low **C**ost, and rapid **t**ime to market. Typically, it involves years or even decades of meticulous refinement of semiconductor innovations traversing from Concept & Feasibility (CnF) stage to High Volume Manufacturing (HVM). This multifaceted endeavor is a sequence of four key steps - Materials discovery, Process optimization, Device engineering and Chip design. In this tutorial, we will explore transformative shifts in semiconductor industry driven by cutting edge AI/Machine Learning (ML) methodologies which can accelerate PPACt.

Part 2: ML for Semiconductor Materials Engineering

Materials engineering involves identifying combinations of materials, seeking structurally or compositionally similar alternatives to existing elements, and creating a seek out combination using insights from the periodic table and literature reviews. The stability of these materials is assessed using thermodynamics analysis, atomistic simulations, with feedback by performing laboratory synthesis and subsequent integration into a high-volume manufacturing fab. However, this conventional approach faces limitations when dealing with complex materials and intricate process flows.

With the advancement of data driven approach, we can utilize publicly available databases such as Materials Project, which starts from a materials Gnome effort an extensive materials data repository where researchers can now access materials properties including stability, band gap, elastic constants, and geometric structures. Leveraging the extensive geometrical information availability, a graph neural network approach (which is based on spatial connectivity) distills a staggering 1 billion material combinations into 2 million new crystals, of which 500,000 have been validated as stable materials. MatterGen is a generative AI diffusion model empowering researchers to design materials with specific chemistry symmetry and scalar property constraints, opening new avenues for tailored material creation. Bridging the gap between materials and manufacturing, we will demonstrate two test cases by applying AI/ML driven use cases, one is efficient materials stack engineering by predicting band alignments, second one is intelligent chemical precursor design to enable low-k materials for back end of line (BEOL).

Part 3: ML for Semiconductor Process Plasma Engineering

Plasmas are used for a variety of applications during microelectronics fabrication. With the advance in microelectronics technology, 3D device architectures and atomic layer precision have come to the forefront in the semiconductor industry. The primary challenges during the manufacturing of these devices include wafer-scale uniformity, selectivity, and feature profile control. Fabrication of 3D and nanoscale device require high selectivity during vertical etch, lateral etch, and deposition. Although atomic layer deposition and etch enable high selectivity due to self-limiting reactions, process throughput remains a challenge. Capacitively coupled plasma, inductively coupled plasma, and microwave plasma sources are widely used to provide the desired ion and neutral species fluxes and energies to the wafer. RF pulsing has emerged as an effective means of controlling the neutral to ion ratio and ion angular and energy distribution function.

Modeling plays an important role in the design and development of new plasma systems. Plasma sources are typically modeled using physics-based fluid, kinetic, and/or hybrid plasma models. Investigation of plasma behavior using physics-based plasma models can be computationally expensive due to model complexity resulting from multi-dimensionality, non-linearity, multi-physics, complex chemistry, and/or fine spatio-temporal resolution. This precludes the integration of such models for important scenarios where the computations need to be done rapidly and repeatedly. To overcome these challenges, deep learning based non-linear model order reduction methods are developed for plasma applications. The deep learning model can provide understanding of plasma behavior in a rapid manner. Machine learning model needs further development depending on type of problems to address fast design evaluation, real time control and process optimization. Physics-informed machine learning model trained with experimental data can potentially be developed to realize digital twin in the semiconductor industry.

Part 4: ML for Semiconductor Process Optimization

Bridging the gap between materials and manufacturing, AppliedPRO® is a software and library of algorithms for process recipe optimization to meet the simultaneous process requirements across the entire wafer. The software is tailored to semiconductor use-cases and designed to be primarily used by semiconductor fab process and yield engineers to make critical decisions with confidence during process development. AppliedPRO combines predictive modeling and neural network to handle process behaviors and generates digital process maps that accelerate materials and recipe development, reduce variability, and widen process windows. The neural network-based model designed to work alongside the process engineer during process development, enabling the capabilities to handle large number of process knobs during early R&D phase.

Part 5: ML for Semiconductor Device Engineering

Predictive device modeling relies on well-informed models of thin film materials and their properties, including phases, grain boundaries, vacancies, and relaxations. These models must be closely linked to process parameters such as growth techniques, substrate, temperature, and reactivity. Additionally, they should be connected to the output of the equipment used for materials engineering. To achieve this, we have developed a modeling ecosystem called Ginestra®, which analyzes equipment output using spectroscopic techniques. We combine predictive modeling and Machine-learning (ML) to augment semiconductor device development. By leveraging this Material to Device approach, we can evaluate the impact of transport of charge and atom transport, stress-induced material changes, phase transformations and individual species' behavior. This comprehensive evaluation allows us to predict materials properties, defect relaxation, charge redistribution, domain distribution, nucleation, and bond breakage, all of which contribute to device reliability and variability. The Ginestra modeling framework consists of two interconnected parts: one covering charge (e/h) and material transport and the other addressing stress-induced material modifications. These components are critical for modeling device aging and reliability phenomena based on underlying physics. The framework handles discrete contributions of charge, atomic species, and defects (such as interstitial ions and vacancies), simulating their generation and diffusion processes. Additionally, it accounts for the recombination of material and electronic species within the film. We will show how the combination of the Ginestra modeling framework and ML algorithms allows for enhanced prediction capabilities of material and/or geometrical device properties directly from electrical measurements both at device and wafer levels.

Part 6: ML for Semiconductor Chip Design

Applied Materials' novel Materials to Systems and Systems to Materials Co-Optimization (MSCO®) platform encompasses materials modeling all the way to system design, allowing for rapid & efficient PPACt evaluations and tradeoff analysis, and down selection of materials, process and device innovations. Standard Cell Libraries are an essential component of MSCO, and our SLiC® (Standard Cell Library Compiler) tool for highly automated production quality library generation is thus vital for rapid MSCO cycles. However, the ever-increasing complexity of advanced technology design rules and extremely large design search space makes it challenging to always guarantee generation of PPACt optimal library cells within reasonable compute times. AI/ML based techniques can help to solve seemingly intractable optimization problems, and we will demonstrate how we use such techniques for the standard cell library generation use case. We will discuss experimental results across multiple library architectures and process nodes and show how AI/ML can enable significant improvements in library quality, coverage and turnaround times and further accelerate new technology development.

Speaker bios

Gaurav Thareja is Head of Logic and Memory Process Integration in the Metals Deposition Products division of the Semiconductor Products Group at Applied Materials, Santa Clara, USA. With a prolific career, he has made significant contributions to semiconductor device processes and materials technology. He is a recognized inventor, holding 40+ US patents, and having authored more than 30 publications and many invited talks. He received PhD in Electrical Engineering from Stanford University and has over 15 years of experience in the semiconductor industry, previously with an AI startup in bay area (Founding team and COO), High performance logic for 7/3/2nm nodes at Intel Process Technology Development in Hillsboro Oregon (Process Integration Lead), Transistor Reliability CAD at Texas Instruments India (Design engineer) and ROM circuit design (Intern) at ST Microelectronics India.

Shruba Gangopadhyay, is Scientist in Applied Materials in the Systems-To-Materials group at Applied Materials. Her current responsibilities include leading the materials simulation effort in materials to device team. She has more than 12 than years of experience working in quantum mechanical aspects of material science and machine learning field. After obtaining PhD from University of Central Florida, Shruba worked as a scientist in IBM, UC Davis, and Mojo Vision. Her research activities span from managing multidisciplinary interdisciplinary projects, serving Journal editor of Frontiers. Dr. Gangopadhyay have published more than 20 papers, numerous invited talks in international conferences. and four unique intellectual properties till date.

Kallol Bera is Senior Director, Plasma Products Modeling. He is leading engineers and guiding plasma product development. He has over 24 years of experience in designing innovative products (chemical vapor deposition, atomic layer deposition, etch, etc.) for Applied Materials using various simulation techniques. His recent interest includes machine learning applications in plasma systems. He has been granted 73 patents, has published > 100 journal and conference papers, presented invited talks, organized conferences, and received several awards. He has served as a guest editor for Applied Physics Letters and Physics of Plasmas jointly. Kallol received Master's degree from Indian Institute of Science, and Ph.D. from Drexel University.

Sravan Nandakumar is a Technical Marketing Manager for AppliedPRO® Software since April 2022. He received his Dual B.Tech/ M.Tech degree in Metallurgical and Materials Engineering from Indian Institute of Technology, Kharagpur with specialization in Machine Learning based approach for new Battery cathode discovery through first principal ab-initio validation. He joined Applied Materials India team in 2015 as an Applications Engineer supporting flagship E-Beam metrology product line. During his time in India, Sravan extensively supported several critical evaluations in Europe and Asia with multiple successful evaluations and repeat purchases. Sravan moved to Applied Materials SCLA in October 2019 as an E-Beam expert with goal of connect process and metrology together for actionable insights. In his 4 years with the group, he took on multiple hats from engineering to product management to product marketing and helped to play a key role in increasing internal adoption of team's metrology competency and AppliedPRO® Software offerings multi-fold. Sravan is a proud recipient of the Applied Marketing Leadership Program Certification in collaboration with UC Berkeley, Haas school of business.

Federico Nardi is Director of Applications Engineering in the Systems-To-Materials group at Applied Materials. He has more than 12 years of experience in managing and leading technical teams in multinational corporations (Intermolecular, SanDisk, Western Digital), spearheading the product development of new technologies and unique TCAD software solutions for electronic device simulations. With his background in Electrical Engineering (Ph.D. from Polytechnic of Milan) he is able to guide the technology development by relating electronic device performances with material science, process integration, circuit design and simulation. He has experience in the development of in-memory computing accelerators and in the exploration of machine learning enhanced TCAD solutions. He created unique intellectual properties (28 granted patents), authored and coauthored more than 35 papers published in international journals and proceedings, presented at multiple international conferences with more than 3000 citations (h-index 22).

Sriram Madhvan is Design Director in the Systems-To-Materials group at Applied Materials, Santa Clara, USA. He and his team are currently focused on researching and developing Machine Learning enhanced flows for Electronic Design Automation and System-Technology co-optimization. He has a Masters in Materials Science from Pennsylvania State University and a Bachelors from the Indian Institute of Technology, Madras and more than two decades of prior industry experience in Design for Manufacturability, foundry design enablement and semiconductor technology development working at GlobalFoundries, AMD and Cypress Semiconductor. He holds 10 granted US patents and has authored and co-authored over 30 technical publications.

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