Multiscale Simulation and AI-Driven Approaches for Comprehensive Understanding of Advanced Materials and Semiconductor Processing

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Computational modeling is now indispensable to materials science and semiconductor manufacturing, yet standard techniques—Density Functional Theory (DFT), Molecular Dynamics (MD), the Finite Element Method (FEM), and Technology Computer-Aided Design (TCAD)—operate on isolated time and length scales. Each excels within its niche but inevitably omits critical physics that emerge when atomic reactions, mesoscale microstructures, and device-level fields interact. These blind spots, amplified by numerical instability and physical complexity, restrict our ability to predict real process–structure–property relationships. We demonstrate that coupling multiscale simulations with AI-driven data curation overcomes these limitations and yields a cohesive description of material behavior, processing conditions, and device performance.

The talk focuses on chemical-vapor-deposited Ga_2O_3, a wide-band-gap semiconductor whose five polymorphs and diverse out-of-plane orientations challenge process control. Multiphysics FEM reveals how carrier-gas flow, precursor depletion, and thermal gradients develop inside commercial CVD reactors, but it cannot capture the surface chemistry governing which phase nucleates. By embedding Classical Nucleation Theory informed by DFT-computed surface energies, adsorption barriers, and cluster stabilities into the FEM solution, we predict local nucleation rates and explain why specific polymorphs dominate under given precursor partial pressures and substrate temperatures. MD simulations, accelerated by machine-learning interatomic potentials trained on DFT data, extend the analysis to lateral growth fronts, resolving defect incorporation, strain relaxation, and orientation competition in real time. By orchestrating DFT, MD, nucleation theory, FEM, TCAD, and AI within one framework, this study charts a path toward predictive, adaptive process design for complex semiconductors and other multicomponent materials.