ALD Fundamentals: Growth and Characterization
Room HB Plant Ballroom - Session AF2-WeA

Modeling for ALD Processes II

Moderators: Simon D. Elliott, Schrödinger, **Michael Nolan**, University College Cork

4:00pm **AF2-WeA-11 Validation of the Direct Simulation Monte Carlo Method for the Numerical Modelling of ALD Conformality**, ***Paul Nizenkov***, *Asim Mirza, Stephen Copplestone, Julian Beyer,* boltzplatz - numerical plasma dynamics GmbH, Germany*; Simone Lauterbach, Marcel Pfeiffer,* Institute of Space Systems, University of Stuttgart, Germany

Atomic layer deposition (ALD) processes span a wide range of length scales and operating pressures, from nano-scale semiconductor features to micrometer-scale structures in MEMS. This means that diffusion processes can range from free molecular flow to the transitional Knudsen regime, where conventional fluid models may require empirical corrections to accurately predict film conformality.

Direct Simulation Monte Carlo (DSMC) offers a reliable approach to the simulation of rarefied gas dynamics on a molecular level. The method has been extensively validated against experimental measurements in different applications including turbo-molecular pumps, spacecraft re-entry aerothermodynamics, and vacuum systems in general. Its ability to accurately resolve gas flow across a wide range of Knudsen numbers, makes it ideally suited for ALD applications spanning multiple flow regimes.

We apply the DSMC method using the open-source plasma simulation framework PICLas to simulate Al_2O_3 ALD conformality from TMA/H_2O in lateral high-aspect-ratio channels. The method is validated against experimental thickness profiles from Arts et al. (2019), then employed to evaluate the extended slope method by Gonsalves et al. (2024) in the transitional regime. DSMC enables seamless multi-scale coupling between reactor-level transport and feature-scale deposition, providing a framework for determining sticking coefficients across industrially relevant conditions. Additionally, PICLas offers the capability to investigate plasma-enhanced ALD processes in the future.

4:15pm **AF2-WeA-12 Multi-Scale Model for Optimization of HfO_2 ALD in High Aspect Ratio Structures**, ***Ivan Petras***, *Andrey Smirnov, Yury Shustrov,* Semiconductor Technology Research d.o.o. Beograd, Serbia

ALD is characterized by two self-limiting steps and purging. Each step requires a certain time to ensure complete coverage of the surface by precursor and complete removal of excess precursor from reactor volume and surfaces during purging. DRAM capacitors have a complex structure, so it is important to form high-k thin film conformally with excellent step coverage to reduce leakage current. Thus ALD is a key technology for scaling of deep trench DRAM capacitors, where film thickness required is low. HfO2 ALD presents a challenge for conformal deposition in high aspect ratio (HAR) structures due to specific processes such as narrow temperature window due to precursor properties or film quality. In this sense, multi-scale models with coupled reactor- and feature-scale simulations can be applied for reducing process development costs and achieving conformal trench coverage. Focus of this work is aimed at improvement of HfO2 ALD process with consideration of patterned wafers by tuning type of precursor, dosing and purging duration. HfCl4 is known for its thermal stability and ease of use but has the disadvantage of having corrosive by-products, whereas hafnium amides are considered promising due to their high reactivity, non-corrosiveness, and suitability for low temperature processes. An integrated modeling approach was developed with self-consistent coupling of modeling tasks on different scales. Reactor-scale model of Hf-delivery by either HfCl4 or TDMAHf, oxidation and purging include unsteady mass transport with surface chemical reactions. Trench-scale model includes tracing Hf- and oxide precursor species, as well as products of surface chemical reactions.We demonstrate results of process recipe optimization for conformal deposition of HfO2 on patterned wafer within the smallest possible ALD cycle time using multi-scale model. It is shown that optimization of purging is important to keep as few impurities and conformal deposition as possible. Increasing of trench AR leads to remarkably longer time for achieving ALD conformality during precursor delivery, especially for HfCl4 due to secondary effects such as H2O adsorption or etching by HCl by-product. Effect of temperature and H2O purge step duration on resulting film stoichiometry is shown, demonstrating the importance of purge duration due to adsorption of additional H2O. Coating of deep trench surface with each of the precursors has its own characteristics that must be taken into account when optimizing the recipe. Due to its lower reactivity, chloride covers the trench surface more evenly than organometallic precursor. In addition, reactivity of both precursors is sensitive to temperature in different ways. Step coverage dependence on precursor pulse duration is shown for different precursors, pressure and trench AR. Optimal process parameters of HfO2 ALD in HAR trenches are discussed according to temperature range and precursor choice.

4:30pm **AF2-WeA-13 Engineering the Interlayer Materials to Improve Interfacial Thermal Conductance**, ***Saikat Mukhopadhyay***, U.S. Naval Research Laboratory*; Neeraj Nepal, Brian Downey, James Champlain, Shawn Mack, James Lund, Peter Litwin, Virginia Wheeler,* US Naval Research Laboratory

The heterogeneous integration of diverse material components is crucial for developing advanced, multi-functional microelectronic circuits. A significant challenge in this approach is the thermal boundary resistance at material interfaces, which can impede heat dissipation and compromise the performance and reliability of devices. As device sizes shrink and power densities rise, enhancing the interfacial thermal conductance (TBC) has become a critical aspect of thermal management. Recent research on GaN/SiC and AlGaN/Diamond interfaces suggests that introducing an interlayer material can effectively improve TBC.

However, the impact of different interlayer materials and their thickness on TBC is not well understood, and conventional theoretical models like the Acoustic Mismatch Model (AMM) and Diffusion Mismatch Model (DMM) are insufficient as they do not account for the critical role of interfacial states. To address this, our study focuses on the TBC of GaAs/Diamond and GaN/Diamond interfaces, both with and without interlayer materials. We employed advanced transport approaches, including the Non-Equilibrium Green's Function (NEGF) method and Reverse Non-Equilibrium Molecular Dynamics (RNEMD), to accurately calculate TBC incorporating the chemical reconstructions that happen at the interface.

Our calculations find that TBC through GaN/AlN/Diamond is significantly higher than GaN/Diamond. This can be explained in terms of much higher TBC associated with GaN/AlN and AlN/Diamond interfaces compared to the direct GaN/Diamond interface. This motivated a broader investigation using a series of interlayer materials (AlN, TiN, and TaN). We found that all interlayer materials improved the TBC for the GaN/Diamond interface, with TiN yielding the maximum improvement. Additionally, a nearly linear increase in TBC was observed when the TiN layer's thickness was increased from 3nm to 6nm, resulting in a 10% enhancement. Conversely, for the GaAs/Diamond interface, we did not observe a similar improvement in TBC, but the introduction of an AlN interlayer was found to improve the structural stability of the interface. This work provides guidance for future ALD experiments with carefully selected interlayer materials to optimize thermal management in next-generation electronic devices.

4:45pm **AF2-WeA-14 Closing Remarks and Award Presentations**,

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