CROSS-FLOW ALD: STRATEGIES FOR OPTIMIZATION OF ALD PROCESS RECIPES AT WAFER SCALE

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Motivations

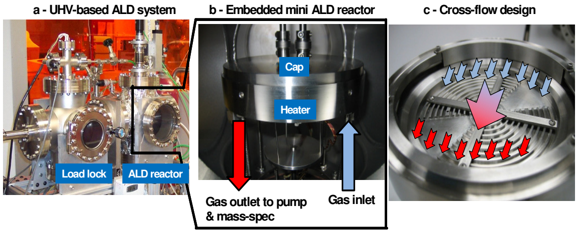
✓ The optimization of ALD process recipes is often challenging as interdependent variables, e.g., dosage, purge, temperature or pressure, must be optimized for a given reactor design in order to achieve the thickness, uniformity and conformality control at the atomic level while providing the desired materials properties (electrical, optical, compositional, etc.). These challenges become even more critical as we consider a shift towards ternary and quaternary materials systems or the application of ALD to production-size substrates where uniformity requirements present a stringent test for ALD process performance.

✓ Using in situ-chemical sensing and ex-situ across-wafer uniformity measurements, we propose a strategy to characterize the Al_2O_3 ALD process space in the context of a cross-flow wafer-scale (100 mm) system and determine the effect of reactant dosage and purge times on process and materials properties.

✓ This work is to provide a framework for combinatorial materials synthesis of ternary and quaternary systems using ALD.

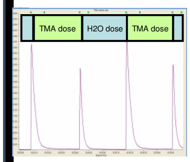
Cross-flow ALD reactor design

- ✓ UHV-based with load-lock for rapid wafer throughput and minimized contamination
- ✓ 0.2 L embedded reactor for <1s residence time and small wall-to-wafer surface ratio
- ✓ 100 mm wafer-scale substrate heater with cross-flow design
- ✓ Gases sampled downstream to reactor into 300 amu MKS mass-spectrometer



Real-time process sensing via mass-spectrometry for chemical diagnostic and process optimization

Mass 16 QMS spectra during ALD cycle



Mass 16 integration over varying H_2O and TMA dose conditions

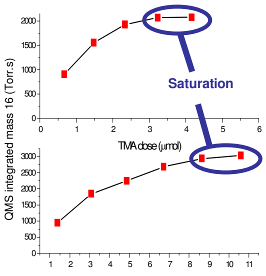
TMA half-cycle

(a) $-OH + Al(CH_3)_3 \rightarrow -O\text{-}Al(CH_3)_2^* + CH_4$

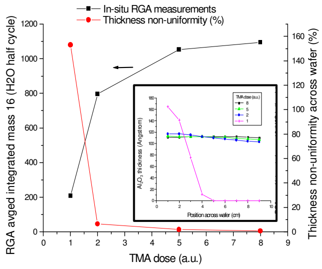
(b) $2\text{-}OH + Al(CH_3)_3 \rightarrow (\text{-}O\text{-})_2Al(CH_3)^* + 2\,CH_4$

H_2O half-cycle

$\text{-}O\text{-}Al\text{-}(CH_3)_n^* + n\,H_2O \rightarrow (\text{-}O\text{-})Al\text{-}(OH)_n^* + n\,CH_4$



In-situ characterization of ALD saturating doses



Thickness uniformity vs. by-product generation

✓ Saturating doses of TMA and H_2O are estimated within one single run using mass-spectrometry by integrating the QMS signals corresponding to the by-product generation during each half cycle (i.e., CH_4).

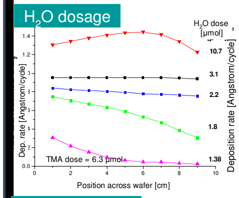
✓ Integrated by-product QMS results can be correlated to the uniformity across the wafer.

✓ QMS-based sensing can also be used to monitor the process chemistry, evaluate nucleation kinetics in real-time, or perform process fault detection.

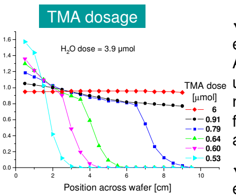
✓ This approach provides a valid strategy to rapidly evaluate the contours of the process space leading to optimal dose conditions.

Uniformity vs. reactant dosage / purge

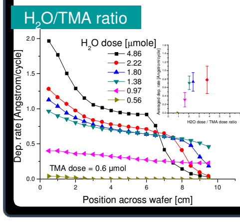
H_2O dosage



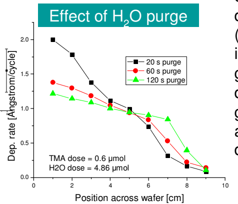
TMA dosage



H_2O/TMA ratio



Effect of H_2O purge

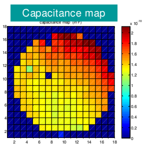


✓ The cross-flow design emphasizes when the ALD reaction is unbalanced as it amplifies non-uniformities resulting from reactant depletion across the wafer.

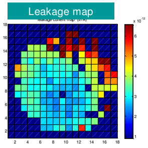
✓ Excess of water, either from unbalanced dose conditions (H_2O/TMA dose ratio) or insufficient purge generates sharp gradient discontinuities with higher growth rates at the inlet and increased depletion downstream.

Materials properties vs. reactant dosage

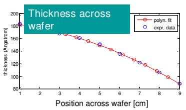
Capacitance map



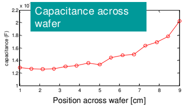
Leakage map



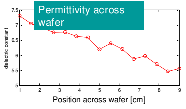
Thickness across wafer



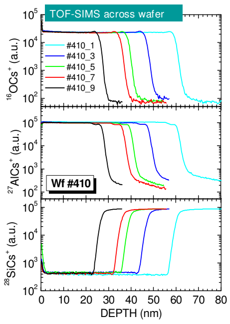
Capacitance across wafer



Permittivity across wafer



TOF-SIMS across wafer



✓ Capacitance and leakage current maps indicate a potential degradation of electrical properties upon reactant depletion, with up to 20% decrease of permittivity across wafer.

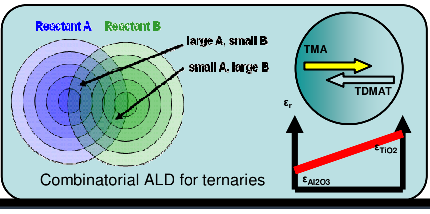
✓ TOF-SIMS and XPS measurements across the wafer reveal no change of composition with dose.

Conclusions and Future Work

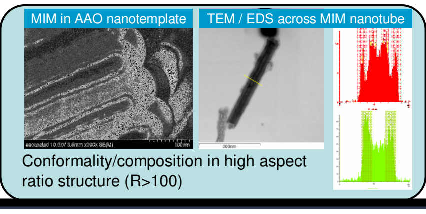
➢ Optimal ALD growth (growth rate, uniformity, film properties) could only be achieved within a well-defined region of the process space. Mass-spectrometry proved a versatile tool to characterize its outline by giving approximated saturation conditions directly. Growth rate and uniformity are strongly affected by the water dose and associated purge due to water's ability for multilayer physisorption.

➢ The ability to control thickness gradients across the wafer provides a platform for combinatorial ALD approaches for process and materials optimization in multicomponent systems.

➢ We are also investigating the effect of dose depletion in high aspect ratio nano-structures for binary and ternary systems.



Combinatorial ALD for ternaries



Conformality/composition in high aspect ratio structure (R>100)

Acknowledgments

This work has been supported in part by the UMD NSF-MRSEC as a seed grant under DMR 05-20471, the Laboratory for Physical Sciences and MKS Instruments.