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Experimental investigation and CFD-based analysis of an ALD reactor depositing alumina from TMA and water

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The requirements of the microelectronic industry, producing high quality electronic devices, has led to the integration and miniaturization of the electronic devices towards smaller sizes, leading to an intensified need for deposition of ultra-thin nanometric films. In this context, the Atomic Layer Deposition (ALD) process [1] has emerged as the appropriate process to produce such films. Due to the self-limiting nature of the deposition reactions involving two precursors alternatively fed, the process is characterized by its high film thickness control, uniformity and composition purity.

The ALD process is complex since it combines transport phenomena occurring inside the reactor chamber and surface chemistry on the substrate [2]. Indeed, the duration of each precursor feeding and of each intermediate purge must be finely tuned for the optimal operation of the process. Hence, an in depth understanding of the involved mechanisms is of major importance.

Experiments of alumina deposition using trimethyl aluminum (TMA, $\text{Al}(\text{CH}_3)_3$) and water vapor (H_2O) as precursors and argon as inert gas have been performed in a commercial Ultratech® ALD reactor. Results show that even for established recipes, the thickness variation of the deposit reaches 2.5 to 3% on a 200 mm silicon wafer substrate after 550 ALD cycles, and a clear influence of the reactor geometry appears.

A three-dimensional Computational Fluid Dynamics (CFD) model is developed, in order to investigate the various phenomena involved and aiming at improving the deposition uniformity. The model comprises two sub-models: one for the precursor feeding system, to compensate for the lack of measurements of the reactants inlet flows into the reactor; the other for treating the reactant pulses of the ALD cycle in the reactor. The outcome of the former is used as transient inlet boundary condition of the latter. The simulations show the effect of the loading door argon flow, resulting to a non-isothermal substrate surface, where the computed maximum temperature difference is above 20°C. Results about the gas flow field, temperature and species distributions inside the ALD reactor are obtained during each pulse.

Improved understanding of the phenomena involved in the reactor requires coupling the transport model with a surface model accounting for the chemical reaction mechanisms taking place on the substrate. A preliminary chemistry model is developed and its results are compared with experimental measurements.

[1] S.M. George, Chem. Rev. 110 (2010) 111–131

[2] Puurunen, R.L., J. Appl. Phys. 97 (2005), 121301