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CFD analysis of an ALD reactor: gaseous species distribution and cycle time

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A three-dimensional Computational Fluid Dynamics (CFD) model is built for a Cambridge Nanotech® ALD reactor, considering the Atomic Layer Deposition process of aluminum oxide (Al_2O_3), using trimethyl aluminum (TMA, $Al(CH_3)_3$) and water vapor (H_2O) as precursors and argon as inert gas.

The developed model investigates the transport phenomena during the reactant pulses of the ALD cycle, while no reactions are taken into account. Due to the lack of measurements of the reactants inlet flows into the reactor, a model for the precursor feeding system is also built. Its results are used as transient inlet boundary conditions of the reactor model.

Results about the gas flow field, temperature and species distributions inside the ALD reactor are obtained during each pulse. A good agreement between the experimental and calculated pressure pulses at the reactor exit is observed, which allows validating the approach.

The simulations show the effect of the reactor loading door, resulting to flow regimes that affect the gaseous species distribution close to the substrate surface. As illustrated in Fig. 1, it is shown that for the side of the wafer close to the loading door, the gas phase reactant concentration above the substrate is always lower.

Finally, the ALD purging steps of a complete cycle are simulated. The results show that the purging steps can be reduced to a time period smaller than the operated one, thus minimizing the ALD total cycle time.

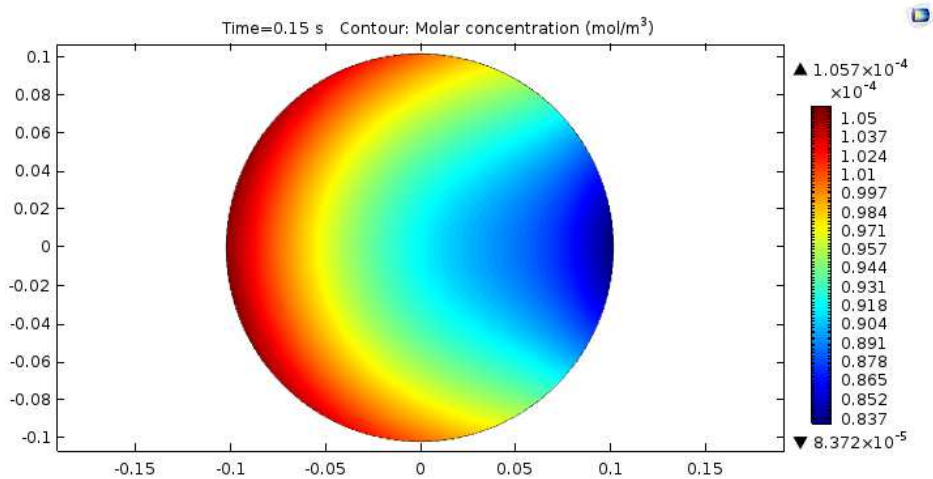

Figure 1: Snapshots of the molar concentration profile of TMA on the substrate surface for 150 ms after the beginning of the TMA pulse (the loading door is located at the right part of the wafer)