Modeling of Transport and Kinetic Processes in an Atomic Layer Deposition Reactor

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Atomic Layer Deposition (ALD) has received increased attention lately because of its ability to produce ultra-thin, and conformal film structures using sequential self-limiting surface reactions. Simulation of an ALD process is difficult because of periodic pulsing of reactants and purge gases in short intervals. A comprehensive model for ALD should include gas phase transport, transient boundary conditions, adsorption/desorption and surface reactions. The current work focuses on predicting deposition rates of thin film diffusion barriers - deposition of TiN in an ALD reactor using $TiCl_4$, and NH_3 as reactants. Adsorption, desorption, and surface reaction steps are characterized using heterogeneous reaction mechanisms. The simulation results will also shed light on effect of geometrical and process parameters on precursor adsorption on the wafer surface, whether the precursors completely purge over the specified purge time, and finally TiN growth rate dependence on pulse times.

In the present investigation, the growth is characterized by looking at the titanium and nitride depositions in the ALD TiN layer per unit area, as a function of increasing number of deposition cycles. Figure 1. shows the distribution of TiCl4 concentration inside the reactor as a function of pulse time. The simulation results provide insight whether $TiCl_4$ is completely purged or not over the specified time. Figures 2a. and 2b. show the concentrations, and fractional coverage of $TiCl_4$ and NH_3 at wafer center over 10 cycles. Figure. 3 show the cumulative deposition of titanium and nitride in a TiN layer over 10 cycles. The rate parameters for surface chemistry models need to be chosen to provide the agreement between the simulation results and experimental data. Finally, the model provides a framework to investigate growth rates of different materials such as oxides and nitrides using ALD process.

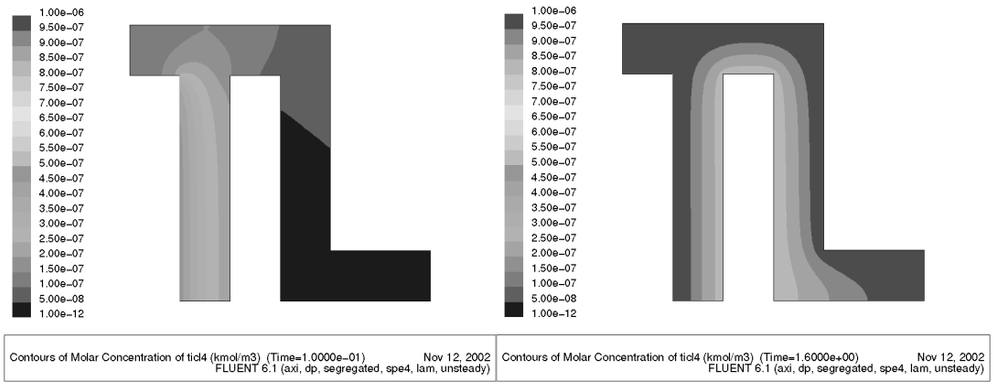
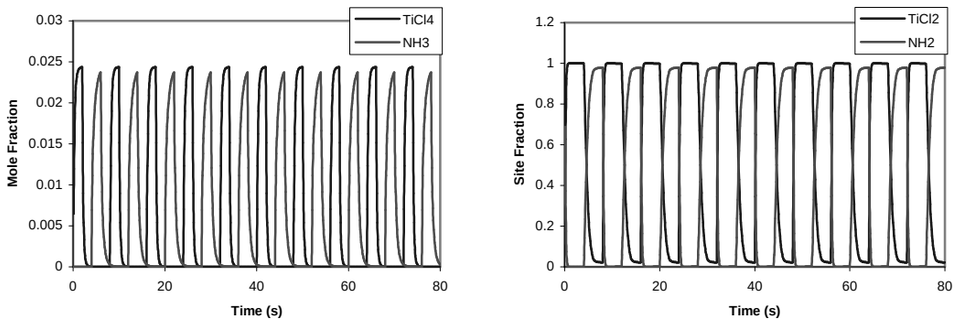


Figure 1. Contours of TiCl4 concentrations at different pulse times



2a *2b*

Figure 2. (a) Concentrations and (b) Fractional coverages of TiCl4 and NH3 at the wafer center over 10 cycles

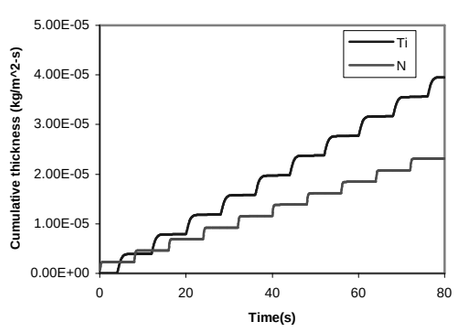


Figure 3. Cumulative deposition of titanium and nitride in a TiN layer over 10 pulse cycles