Deposition: One Layer at a Time

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As device sizes continue to shrink below 90nm, the semiconductor roadmap suggests that atomic layer deposition, or ALD processes will be required for a variety of applications, such as the deposition of barriers for copper interconnects, the creation of tungsten nucleation layers, and the production of highly conducting dielectrics. In the ALD process, two or more precursor gases flow over a wafer surface in an alternating manner, so that the gases can react with the sites or functional groups on the wafer surface. When all of the available sites are saturated, the reaction stops and an inert gas flow purges the excess precursor molecules from the region. The process is repeated, as the next precursor gas flows over the wafer surface. A cycle is defined as one pulse of precursor 1, purge, one pulse of precursor 2, and purge. This sequence is repeated until the final thickness is reached. These sequential, self-limiting surface reactions result in one monolayer of deposited film per cycle.

ALD is a stable process over a wide range of temperatures, and as a result there is a linear relationship between the thickness of the layer deposited and the number of deposition cycles. Because of the periodic pulsing of reactants and purge gases in short intervals, the ALD process is challenging to simulate using CFD. The modeling strategy for one cycle should include convective and diffusive transport of reactants to the surface, transient boundary conditions to account for pulse sequences, adsorption of the monolayer of the first precursor on the wafer surface, and subsequent surface reactions with the second precursor gas.

One important application for ALD is the deposition of a TiN (titanium nitride) diffusion barrier using $TiCl_4$ (titanium tetrachloride) and NH_3 (ammonia) precursors. Since the properties of barrier films are related to their nucleation and growth mechanisms, a detailed surface chemistry model is needed to characterize adsorption, desorption, and heterogeneous surface reactions on the wafer surface. The self-limiting surface reactions used in the model are:

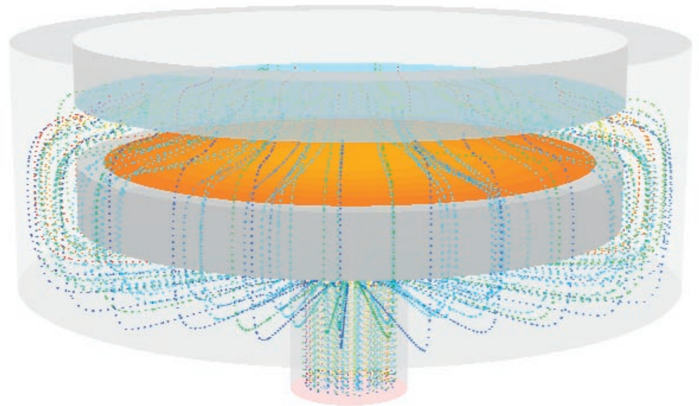
$$NH_2(a) + TiCl_4(g) \rightarrow TiCl_2(a) + 2HCl(g) + N(s)$$

$$TiCl_2(a) + 2NH_3(g) \rightarrow 2NH_2(a) + 2HCl(g) + Ti(s)$$

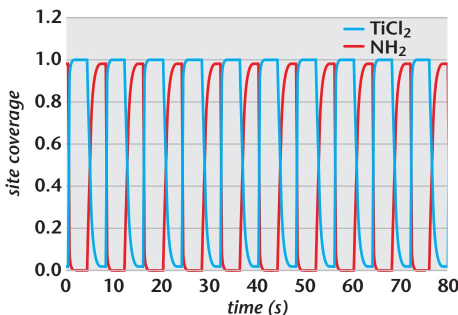
Where *(a)* is an adsorbed site/surface species, *(g)* is a gas phase species, and *(s)* is the deposited solid or bulk species.

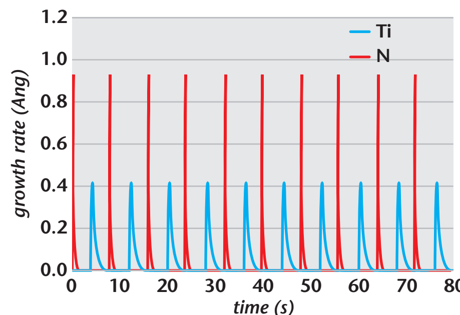
The TiN growth in a typical ALD reactor was investigated in FLUENT 6.1 by looking at the number of Ti atoms in the TiN layer per unit area, as a function of the number of deposition cycles. Transient simulations indicated that the gaseous concentration of $TiCl_4$ increases during the first pulse, as does the adsorbed site species $TiCl_2$. After the purge, an NH_3 pulse is initiated and reacts with the site species $TiCl_2$. No cross-contamination between the pulse cycles was observed, suggesting that the purge time could be reduced. The model also predicted that the growth rates are uniform over successive ALD cycles.

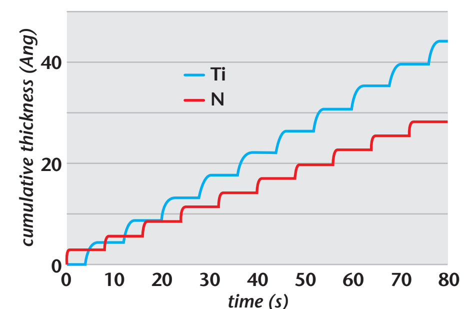
The results shed light on different growth regimes: a transient regime where film thickness for one deposition cycle increases towards a constant value, and a saturated regime where film thickness for a given deposition cycle is constant. The simulations also suggested that growth rate has a linear relationship with the number of deposition cycles. The CFD model provides a framework for investigating the influence of geometrical parameters and different precursor doses on film thickness. The results implied that the NH_3 dose significantly affects the TiN film growth. For low ammonia dosing, the growth rates are significantly lower than those associated with high ammonia doses. ■



A typical ALD reactor along with pathlines colored by velocity, and TiN growth rate on the wafer







Fractional coverages of $TiCl_2$ and NH_2 (left), growth rate for Ti and N as a function of pulse time (middle), and predicted film thickness at the wafer center over 10 cycles (right)

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