Prediction of Deposition Rates in Plasma-Enhanced Atomic Layer Deposition

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Atomic layer deposition (ALD) offers the possibility of self-limiting, monolayer-by-monolayer deposition. Due to the periodic pulsing of reactants and purge gases, a comprehensive model for ALD should start with the transient nature, and include models for gas phase transport and surface chemistry. We have developed a transient Boltzmann equation based transport and reaction model at the feature scale for atomic layer deposition (ALD) [1-3]. The transport model has no adjustable parameters. Heterogeneous reaction mechanisms are used to express adsorption, desorption, and surface reaction steps. Simulation results show that transport is fast compared to typical pulse times [1-3]. An analytic extension of the simulation results allows us to predict monolayer deposition rates per cycle for any choice of coefficients. We have used the surface reaction model to explain growth rate dependence on pulse times for specific experimental chemistries. Figure 1 shows growth rate dependence on reactant pulse time and predicted film thickness and surface coverage in TiN ALD using TiI_4 and NH_3 as reactants. The experimental data were obtained from Ritala *et al.* [4].

Plasma-enhanced ALD (PEALD) has been investigated [5-7] as a possible method to increase surface reaction rates and improve deposited film properties. In Refs. 6 and 7, tantalum nitride (TaN) was deposited using tertbutylimidotris(diethylamido)tantalum (TBTDET) as a precursor, and hydrogen radicals were used as reducing agents. Films formed using PEALD were found to exhibit better properties (lower electrical resistivity, no aging effects under exposure to air) than those formed using conventional ALD (with NH_3 as a reducing agent) [7]. Figure 2 reproduces experimental data from [7] comparing film thickness per cycle for conventional ALD and PEALD as a function of precursor pulse time. We present the results of simulations used to estimate the parameters values for selected surface chemistry models. Parameter values chosen provide the best fit between simulation results and experimental data. We focus on explaining the difference in film thickness dependencies on TBTDET pulse times in conventional ALD and PEALD shown in Fig. 2, and provide an explanation for the difference in growth rates between the two processes.

References

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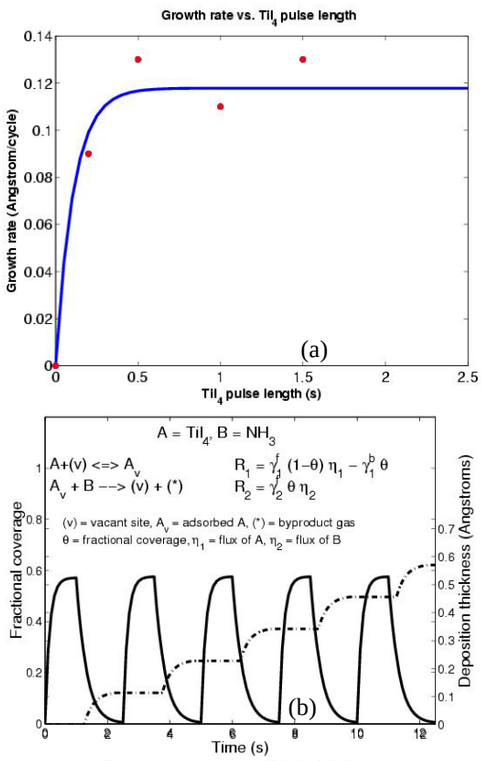

Figure 1. (a) Growth rate for TiN ALD as a function of TiI_4 pulse length (circles: experimental data from [4], lines: modeled growth rates). (b) Predicted film thickness (solid line) and fractional coverage (dot-dash line) over successive ALD cycles.

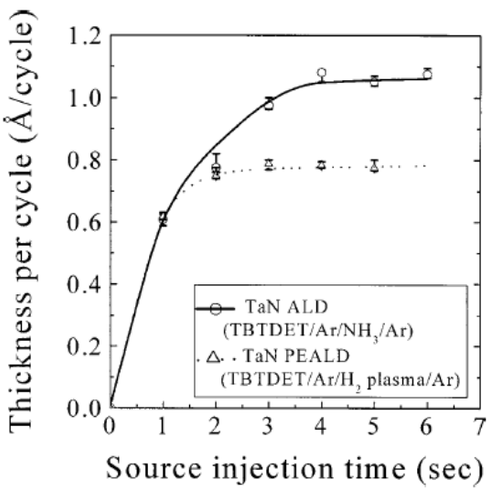

Figure 2. Dependence of deposited film thickness on TBTDET pulse time for conventional ALD and plasma-enhanced ALD (reproduced from [7]).