Transient Transport and Reactant-Wafer Interactions: Adsorption and Desorption

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Rapid processing implies processing under transient conditions. In many processes, this includes reactions between gas phase reactants and the wafer surface. These interactions almost always begin with adsorption (and desorption in many cases). We present a three-dimensional extension of a recently developed transient transport and reaction model and numerical implementation for low pressure processes. Atomic layer deposition (ALD) is used to demonstrate the model's ability to account for rapid transients [1–5]. At the wafer surface, the transport model is given by the Boltzmann transport equation for gas dynamics, which has no tunable parameters [6]. The surface reaction model is based on reversible Langmuir expressions and is capable of providing non-linear models [7]. The dimensionless kinetic parameter values for adsorption, desorption, and reaction are chosen for demonstration purposes [5].

ALD is designed to deposit a solid material on the substrate one atomic or molecular layer at a time, in a self-limiting fashion. To accomplish this, a representative ALD process consists of repeating a sequence of reactant flows and reactor purges. In the first step of a cycle, a gaseous species (A) is directed into the reactor, and (ideally) one monolayer adsorbs onto the surface. After purging the reactor, a second gaseous reactant (B) is directed through the reactor, which reacts with the adsorbed molecules of A. To keep average deposition rates at reasonably high levels, high switching frequencies of reactants and purges are desired.

Studies have been performed for ALD in a two-dimensional idealized feature, [4, 5]. Figure 1 shows how the fraction of the wafer surface covered by adsorbed A behaves over four cycles of ALD, each cycle of duration 1000 ms. This results in the monolayer deposition predicted in Fig. 2 for the representative choice of coefficients used. These simulations demonstrate the highly transient nature of ALD on the feature scale. We present recent results of this model for three-dimensional simulations for the rapid transients during ALD on the feature scale using the adsorption step as example.

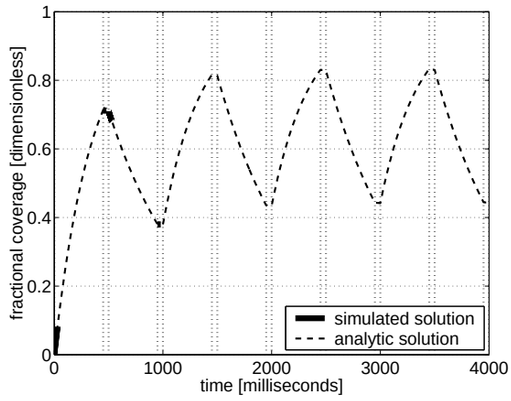

Figure 1: Fractional surface coverage of adsorbed A for four ALD cycles.

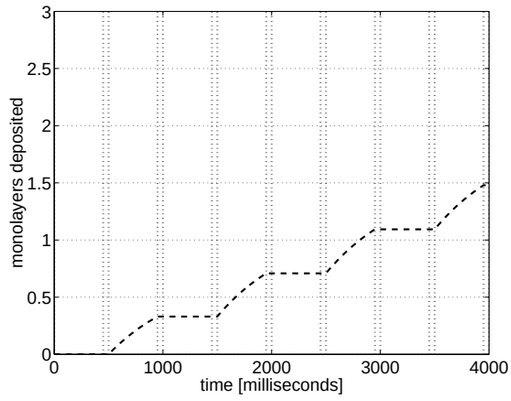

Figure 2: Monolayers deposited for four ALD cycles.

References

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