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MODELING THE CONFORMALITY OF ATOMIC LAYER DEPOSITION: THE EFFECT OF STICKING PROBABILITY

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Atomic layer deposition (ALD) is known to be an excellent technique for conformal coating. In this work, two models, a kinetic and a Monte Carlo model, are developed to predict the deposited film thickness as a function of depth inside a hole. Earlier work by Gordon et al. assumed a sticking probability of 0/100% for molecules hitting a covered/uncovered section of the wall of the hole, thus resulting in a stepwise coverage profile after a single ALD cycle [1]. However, experimental studies indicate a gradual decrease of film thickness instead of a stepwise drop (figure) [2, and references therein]. It has been argued that the gradual slope may be related to (i) the increasing aspect ratio (AR) during deposition and (ii) the sticking probability, which is less than 100%. The first explanation seems reasonable for the case of microscopic trenches, because during each cycle the deposition of new material results in a decrease of the diameter of the hole, and consequently the effective aspect ratio increases during deposition. However, our experiments using macroscopic structures (~0.1x5x20mm) also show a gradual decrease (figure), suggesting that the sticking probability is an important parameter for predicting the conformality. Therefore, in both models, we related the sticking probability s to the surface coverage θ by Langmuir's equation $s(\theta)=s_0(1-\theta)$, whereby the initial sticking probability s_0 is now an adjustable model parameter. For $s_0 \approx 100\%$, the models predict a steplike profile, in agreement with Gordon et al., while for smaller values of s_0, a gradual decreasing coverage profile is predicted. The two models show a good correspondence and follow the same trends as the experimental data (figure).

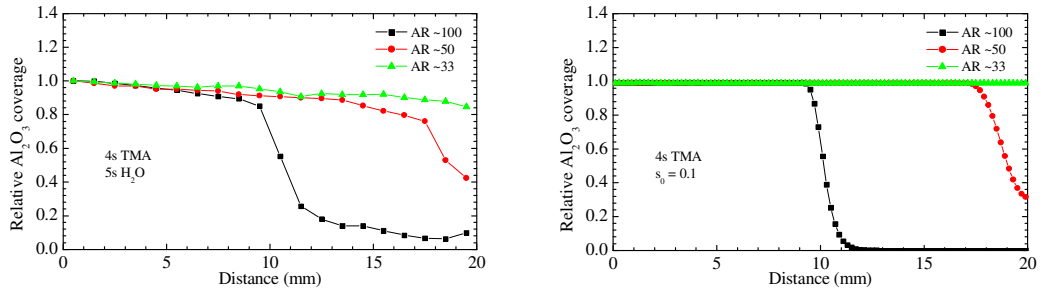

Figure: Al_2O_3 coverage profiles in macroscopic holes using SiO_2 substrates (left),and simulation results for s_0=0.1 using the proposed kinetic model (right) [2].

[1] R. G. Gordon, D. Hausmann, E. Kim, J. Shepard, Chem. Vap. Deposition **9**, 73(2003)
[2] J. Dendooven, D. Deduytsche, J. Musschoot, R. L. Vanmeirhaeghe, C. Detavernier, J. Electrochem. Soc. **156**, P63(2009)