ALD Fundamentals
Room On Demand - Session AF2

Precursors and Chemistry: Simulation, Modeling, and Theory of ALD

AF2-1 Comparison of ALD Saturation Profiles Simulated With Two Theoretical Models, ***Jihong Yim***, *E. Verkama, R. L. Puurunen,* Aalto University, Finland

Self-terminating chemistry of atomic layer deposition (ALD) process enables one to grow pinhole free conformal thin films on high-aspect-ratio (HAR) structures. ALD has attracted ever more attention in diverse applications, such as microelectronics and nanostructured catalyst preparation.[1] Yet, it is essential to optimize ALD process parameters for the conformal deposition especially on HARs. Our previous study investigated the effect of experimental parameters on conformality using saturation profiles of archetypical trimethylaluminum-water ALD processes in lateral HARs with an aspect ratio of typically 10000:1.[2]

The investigation on the effect of process parameters on ALD conformality is continued by simulating ALD saturation profiles with two modeling approaches: a MATLAB simulation based on a diffusion–reaction modeling (Model A)[3,4] and a Python simulation based on a ballistic transport modelling (Model B).[5,6] These simulated saturation profiles are compared to each other in approximately the same condition. While the main features of the simulated saturation profiles are similar, differences are found in the value of 50% thickness penetration depth ($PD_{50\%}$) and slope at $PD_{50\%}$, as well as the shape of the tail region.

Sticking coefficient of ALD reactants describes ALD growth kinetics. A recent study by Arts et al.[7] reported a method to back-extract the sticking coefficient value from the slope of saturation profile. By using this method, we back-extract the sticking coefficient values from the saturation profiles simulated by Models A and B and compare those values to the ones initially set for running the simulations. Interestingly, for both Models A and B, the sticking coefficient values set for the simulations differ somewhat from the ones back-extracted.

Acknowledgement

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References:

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6 https://github.com/aldsim/machball (accessed March 4, 2021).

7 Arts et al., *J. Vac. Sci. Technol. A*, 2019, **37**, 030908.

AF2-2 Theoretical Prediction of the Adverse Effects of H^+/Cl^- Byproducts on SiN Atomic Layer Deposition with Dichlorosilane, ***Tsung-Hsuan Yang***, *G. Hwang, E. Cheng,* University of Texas at Austin*; P. Ventzek, T. Iwao , K. Ishibashi ,* Tokyo Electron America

Plasma-enhanced atomic layer deposition (PEALD) has been demonstrated to be a promising technique for controlled growth of silicon nitride (SiN) thin films. The advantages of PEALD may include excellent conformality, precise thickness control, and high quality at relatively low temperatures. In this talk, we will present molecular mechanisms underlying the PEALD of SiN thin films using dichlorosilane (DCS) as the Si source and N_2/NH_3 plasma as the N source. The adsorption and decomposition of DCS have been found to be sensitive to the surface functional groups; especially, the presence of primary amines plays a critical role in the silicon deposition half cycle. According to our recent studies, the byproducts of DCS decomposition, $H^{\delta+}/Cl^{\delta-}$ pairs, may have a significant effect on the film quality and deposition temperature. First-principles calculations predict that $H^{\delta+}/Cl^{\delta-}$ pairs are strongly bound to the H-terminated N-rich surface by forming $–NH_3^+/Cl^-$ ionic complexes. Because of the sizable binding energy (~ 1 eV), it would be difficult to remove $H^{\delta+}/Cl^{\delta-}$ pairs from the surface unless the PEALD temperature is substantially high. This implies that the reaction of DCS with surface primary amines, and in turn SiN ALD, can be significantly suppressed by the presence of $H^{\delta+}/Cl^{\delta-}$ pairs at relatively low temperatures, which has been confirmed by very recent FTIR measurements at 200 °C. In this talk, we will also discuss a potential method to effectively remove $H^{\delta+}/Cl^{\delta-}$ pairs at low temperatures.

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