ALD Fundamentals
Room Jan & Hubert Van Eyck - Session AF2-TuM

Conformality of ALD

Moderators: Riikka Puurunen, Aalto University, Finland, Myung Mo Sung, Hanyang University

10:00am **AF2-TuM-7 Role of Ions in Film Conformality and Quality during Plasma-Assisted ALD of SiO_2 and TiO_2***, **Karsten Arts,** S Deijkers,* Eindhoven University of Technology, Netherlands*; M Utrianen,* VTT Technical Research Centre of Finland, Finland*; R Puurunen,* Aalto University, Finland*; E Kessels, H Knoops,* Eindhoven University of Technology, Netherlands

This work discusses the impact of ions on film conformality during plasma ALD, in terms of layer thickness and material properties. Ions have been shown to improve the material quality for several plasma ALD processes,[1] yet how and to what extent this works for plasma ALD on high-aspect-ratio structures is difficult to measure and relatively unexplored. Using PillarHall™ lateral-high-aspect-ratio trench structures,[2] where only part of the growth area is exposed to ions, we show how the growth per cycle (GPC) and material properties of SiO_2 and TiO_2 are affected by the locally received ion flux. Our results reveal that ion exposure can be a key factor determining film conformality during plasma ALD of SiO_2 and TiO_2, as the ion flux is inherently anisotropic, while the reactive plasma radicals can diffuse isotropically up to aspect ratios as high as ~1000.[3]

For plasma ALD of SiO_2 using $SiH_2(NEt_2)_2$-, the GPC is affected by ions and decreases significantly when using extended ion doses. Nevertheless, when using moderate ion doses the film thickness is still very conformal. In contrast to the GPC, the material quality is only marginally affected by ions, based on an almost uniform wet etch rate of the SiO_2 film in a buffered HF solution. These results indicate that, in spite of the anisotropic ion flux, plasma ALD can provide highly conformal SiO_2 films for demanding applications.

For plasma ALD of TiO_2 using $Ti(NMe_2)_4$, we show that the GPC and material properties are more strongly affected by ions. For example, at 200 °C crystalline TiO_2 (anatase) with a high GPC and a virtually negligible wet etch rate is obtained with ion exposure, while amorphous TiO_2 with a lower GPC and a much higher wet etch rate is obtained without ion exposure.

In addition to these results, the impact of ions on the refractive index and surface morphology will be discussed, as well as the effect of ion energy and deposition temperature. On the basis of these studies, we will provide insights into the fundamental mechanisms behind the role of ions in film conformality and material quality during plasma ALD.

1. Faraz *et al.*, ACS Appl. Mater. Interfaces **10**, 13158 (2018)

2. Gao *et al.*, J. Vac. Sci. Technol. A **33**, 010601 (2015)

3. Arts *et al.*, J. Phys. Chem. C **123**, 27030 (2019)

10:45am **AF2-TuM-10 ALD Conformality: Effects of Process Parameters on the Simulated Saturation Profile***, E Verkama,* ***Jihong Yim,*** Aalto University, Finland*; M Ylilammi,* VTT Technical Research Centre of Finland, Finland*; R Puurunen,* Aalto University, Finland

Atomic layer deposition (ALD) is widely applied in industrially and in R&D related to applications such as semiconductor processing, microelectromechanical systems, and solid heterogeneous catalysts. ALD has an unparalleled ability to grow uniform, conformal thin films on complex three-dimensional (3D) objects. Experimental and modeling works on conformality investigations have recently been reviewed [1].

This work aims to investigate through theoretical simulations how (i) (simplified) kinetic parameters related to individual ALD reactions and (ii) ALD process parameters more in general influence the saturation profile of ALD films in 3D structures. The 3D structures of interest are rectangular channels, also known as lateral high-aspect-ratio (LHAR) structures, resembling the PillarHall™ structures reported earlier by Puurunen and coworkers. The simulations are made with a Matlab implementation of the Ylilammi et al. 2018 diffusion model [2]. The simulations assume reversible single-site Langmuir adsorption as the chemisorption mechanism, with chemisorption kinetics modeled via a single "lumped" sticking coefficient.

We will present investigations on how the simulated "saturation profile" (thickness vs. distance inside the LHAR structure) or the "scaled saturation profile" (growth per cycle, GPC, vs. dimensionless distance) varies with kinetic constants and process parameters. As expected, reactant partial pressure and exposure time have a major influence on the penetration depth of the film ("50% penetration depth", $PD^{50\%}$). We will also explore the effect of the (lumped) sticking coefficient, equilibrium constant, GPC, the molar mass of the ALD reactant, ALD temperature, LHAR channel height, and total pressure on the saturation profile. An inverse correlation is found between $PD^{50\%}$ and the GPC, explained by a lower binding capacity (atoms per unit surface area) of the surface, which gives a lower GPC. With increasing process pressure, the Knudsen number decreases and the process moves from molecular flow to collisional flow. This is seen as a gradual decrease of $PD^{50\%}$ and a steepening of the slope of the leading edge of the saturation curve.

We believe that these simulations can help experimentalists to understand how different parameters are expected to affect conformality (saturation profile) of ALD processes. The simulations thereby assist one to design meaningful experiments as well as to interpret the results of those experiments. Our aim is to release the Matlab simulation code for open use.

[1] Cremers, Puurunen, Dendooven, Appl. Phys. Rev. 6 (2019) 021302

[2] Ylilammi, Ylivaara, Puurunen, J. Appl. Phys. 2018 (123) 205301

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