PillarHall lateral high aspect ratio assisted unveiling of secondary growth front and background reaction mechanism in atomic layer deposition

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The 3D vertical scaling trend in nanoelectronics necessitates high-aspect ratio (HAR) features and conformal ultra-thin films, crucial for the semiconductor industry today. The lateral high aspect ratio (LHAR) test structure and measurement method is a unique test vehicle for characterizing the conformality for the 3D thin films. The unique feature of LHAR is the ability to quantify the conformality for both ALD and CVD processes. PillarHall® LHAR4 test chips enable accurate and repeatable film penetration depth (PD) profile measurements which help to predict and quantify the step coverage in any HAR features. In the current research we are showing another important aspect of these LHAR structures beyond the already existing applications. Utilization of LHAR in understanding the reaction mechanism of ALD process especially in 3D structures is the major highlight of the current research. We reveal a secondary reaction front (ultra-thin layers, Figure 1) for the TMA+H2O thermal ALD process with the support of LHAR, contrast SEM and imaging ellipsometry techniques. The merit of using imaging ellipsometer is that beyond visualizing the second front, it also facilitates the measurement of film thickness within the second front region. We checked the process at two different deposition temperatures (125°C and 300°C) and with different combinations of pulsing and purging lengths to investigate the influence of these parameters on the observed secondary growth front. The observation of secondary growth front for both temperatures unambiguously ruled out the deposition temperature influence on the observed feature. To investigate the possible mechanistic reasons for the secondary growth front, we have carried out microkinetic modelling of ALD cycles over a range of combinations of precursor pressures, simulating the situation at various cavity depths. As expected, high pressure of both precursors leads to high growth rates up to the primary growth front. At the lower pressures that are present further into the cavity, the model predicts much lower growth rates, along with an increase in the sticking coefficient of TMA (Figure 2). As the depth of a growth front scales with the square root of the sticking coefficient [1], the low-pressure growth front should therefore be deeper than the high pressure one, which matches the experimental observation. Our results indicate that the formation of the second front results from the presence of multiple reaction mechanisms, which are otherwise challenging to distinguish.

Reference

[1] K. Arts, V. Vandalon, R.L. Puurunen, M. Utriainen, F. Gao, W.M.M. Kessels, H.C.M. Knoops, J. Vac. Sci. Technol. A 37, 030908 (2019).

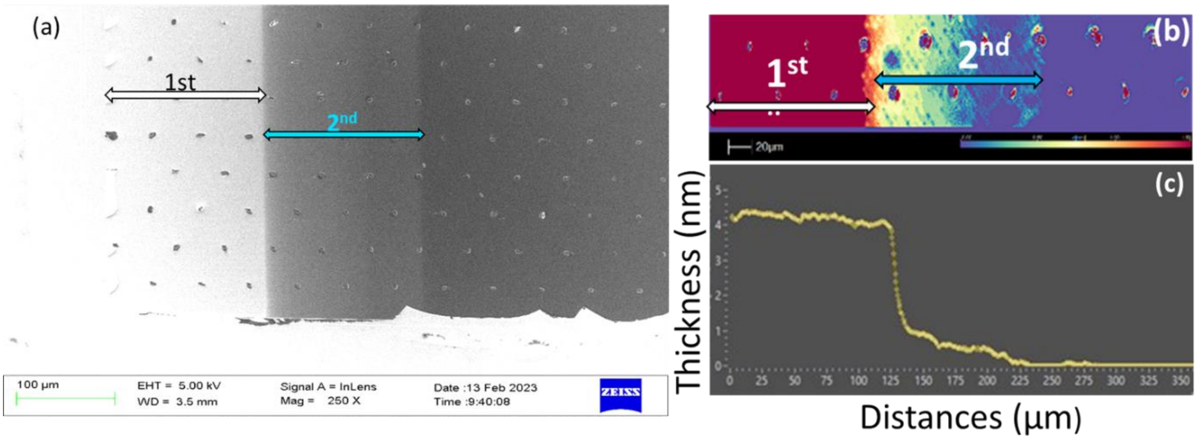

Figure 1. (a) Top-view SEM of an LHAR test structure following the deposition of ≈5 nm thick Al_2O_3 deposition. Contrast map (b) and profile analysis (c) were obtained using an imaging ellipsometer from the same sample. Both primary (1st) and secondary (2nd) growth front are highlighted. The profile analysis reveals the thickness within the second front region. The distance between two pillars is 50 µm.

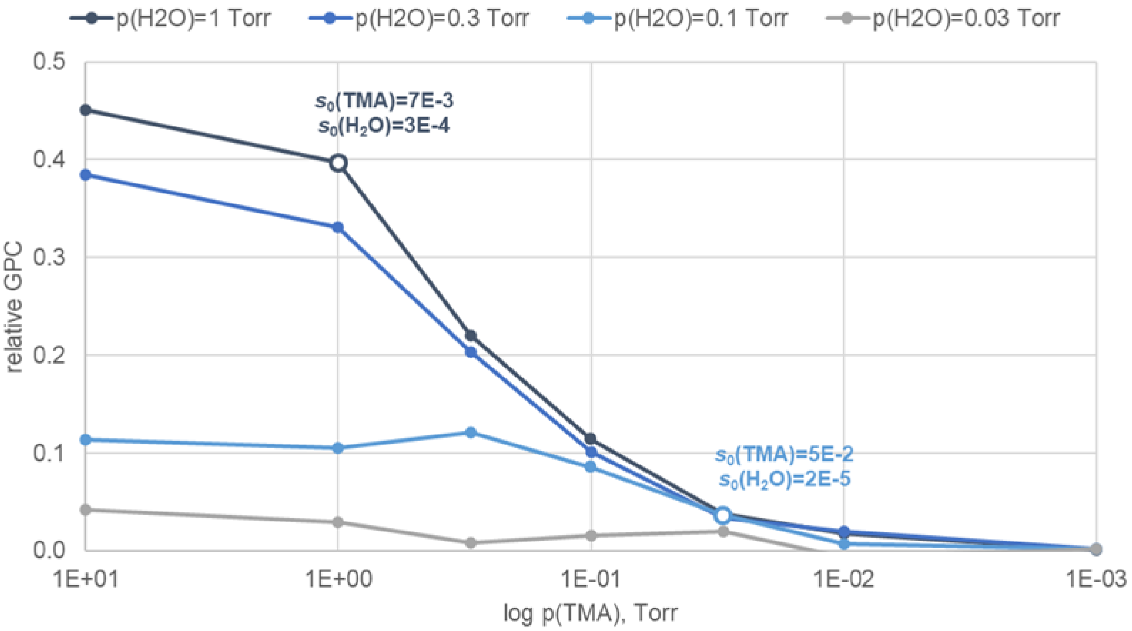

Figure 2. Al_2O_3 growth per cycle from microkinetic modelling based on activation free energies from density functional theory. The model allows sticking coefficients of each precursor to be derived and values are quoted at (i) p(TMA)=1 Torr, p(H_2O)=1 Torr and (ii) p(TMA)=0.03 Torr, p(H_2O)=0.1 Torr.