Atomic Layer Deposition of Titanium Oxide for Integrated Applications

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Titanium oxide is a material of recent interest for various applications. Especially the high refractive index of TiO_2 of 2.4 at 633 nm [1] enables TiO_2 as material of choice for surface relief grating structures. However, the fabrication of nano-scale TiO_2-based gratings is accompanied by various challenges. Haase et al. demonstrated the technological integration via nano-imprint lithography and subsequent dry etching. [2] Alternatively, a double patterning approach overcomes these challenges.

Another relevant property of TiO_2 is its high relative permittivity ranging from 16 to 100. [3] This makes TiO_2 an interesting material for storage applications as in MIM (metal insulator metal) or MIS (metal insulator semiconductor) capacitors. The low band gap of the material – and in consequence the low breakdown resistance – can be addressed by the combination of TiO_2 with another dielectric material with higher band gap, such as Al_2O_3. [3,4]

This material combination is further an excellent material stack for moisture barrier layers. Both materials, Al_2O_3 and TiO_2, are quite inert and won't be affected by external moisture influence. Multi-layer stacks are used to encapsulate quantum dots for example. [5]

All these mentioned applications require homogeneous coatings of a dense TiO_2 film in small dimensions and also in challenging geometries. This includes the coating of sidewalls of 3D structures within nanometre dimensions. The technology of choice for these applications is the atomic layer deposition (ALD). This deposition method separates the reactive species for the deposition and uses the surface adsorption of the precursor in order to create a self-limiting coating. This will be oxidised in a following step completing one single cycle. With increasing number of cycles, the film growths conformally on almost any geometry.

Within this work, we'll present the integration of ALD-based TiO_2 films for different applications. The process was developed by use of TDMAT (Tetrakis(dimethylamido)titanium) as precursor and ozone as oxidising agent.

We demonstrate the conformal coating of trench structures with an aspect ratio of 64:1. The trenches with a width of 500 nm – hard mask opening of 350 nm – and a depth of 32 µm had been coated with a TiO_2 film. (Figure 1). The film on top of the hard mask has a thickness of 20 nm. The vertical sidewalls on the top of the structure also contain a 20 nm thick film. Same film thickness could be achieved in the bottom of the structure (see Figure 1 lower right). The 3D integration ability has been used to fabricate free standing TiO_2 gratings. Figure 2 shows the final integration on a silicon substrate. These had been fabricated by coating a structured sacrificial SiO_2 layer with vertical sidewalls.

This coating of 3D structures is a key requirement to fabricate MIS and MIM capacitors. In order to optimise this the electrical performance of the ALD film was characterised (see Figure 3). Figure 3 a) shows the effective κ value of the dielectric in the MIS structure. The baseline is Al_2O_3 with a value of 3.2. The amorphous TiO_2 film of 5 nm reaches a κ value of 5.7 while the crystalline TiO_2 film of 10 nm reaches a κ value of 10.4. The layer stack of 5 nm Al_2O_3 and 5 nm TiO_2 reaches an effective κ value of 7.5, while the (10 + 10) nm layer stack reaches an effective κ value of 9.9. TiO_2 is a semiconducting material and suffers a substantial leakage current due to its intrinsic conduction. A low bias of 0.1 V (20 MV/m) will lead to a leakage current density of 10^{-7} A/mm² in a 5 nm thin film. Increasing the film thickness to 10 nm will reduce the leakage current density – under the same electric field – to just 10^{-8} A/mm². In contrast, a 5 nm Al_2O_3 film has a way better performance as the leakage current density is in the order of 10^{-14} A/mm² for the same conditions. The combination of both films can achieve the low electrical leakage of Al_2O_3 in combination with the high κ value of the TiO_2. This enables a high performative platform for device integration using high-capacity modules.

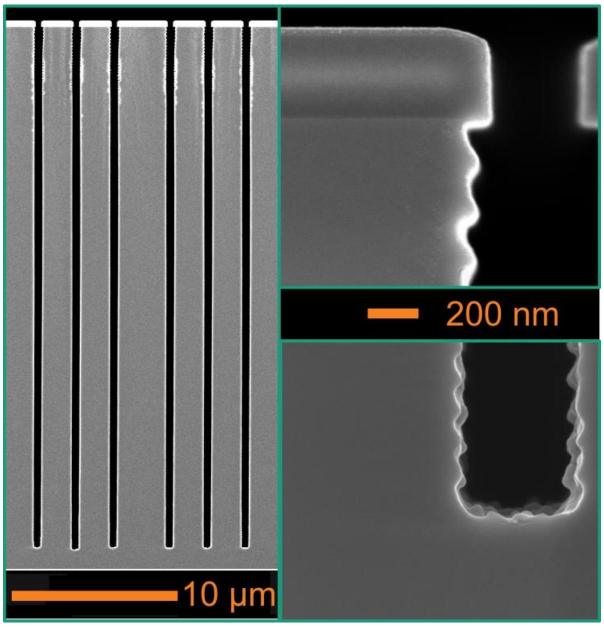


Figure 1: Scanning electron microscope images of trench structures coated with TiO_2.

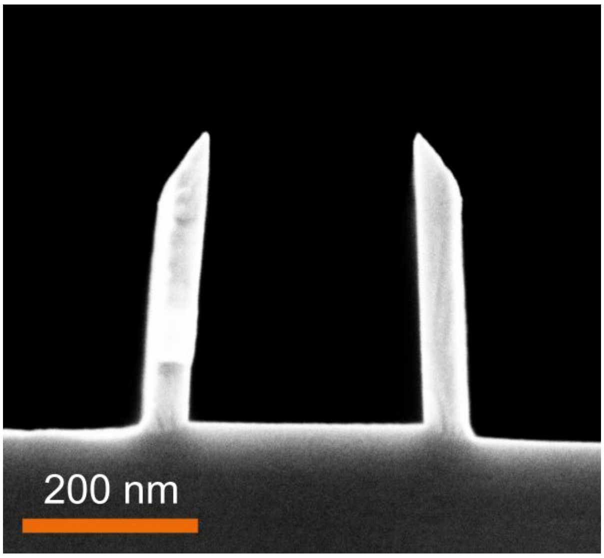
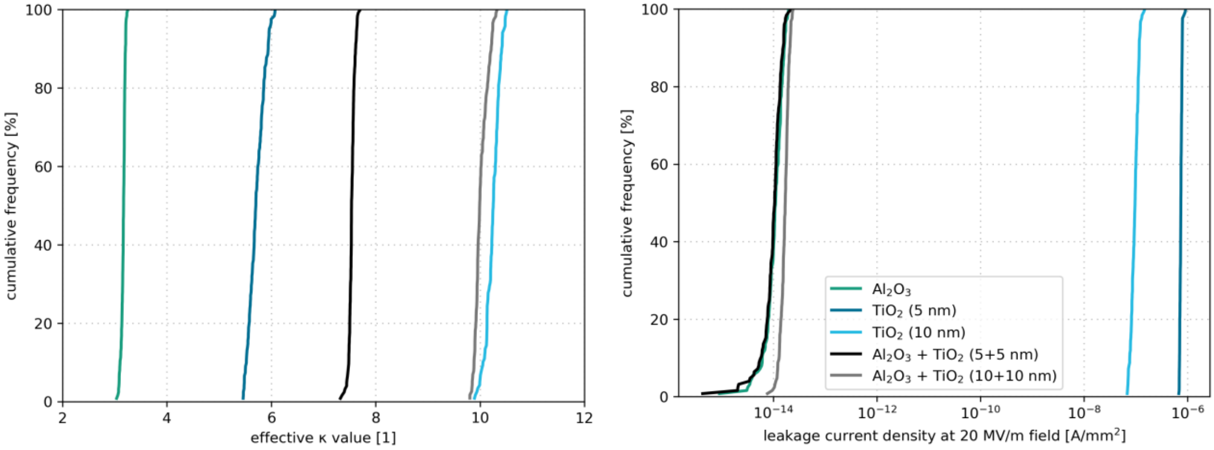


Figure 2: Free standing TiO_2 grating structure.


a) effective κ value

b) leakage current density

Figure 3: Results of electrical measurements of different TiO_2 and Al_2O_3 films: a) effective *κ* value of the dielectric in a MIS structure, b) leakage current in the MIS structure under 20 MV/m electric field.

References

[1] A. Jolivet et al., Applied Surface Science **608**, 155214 (2023).

[2] M. Haase, N. Dittmar, A. Kneidinger, P. Schuster, F. Bachhuber, C. Helke, and D. Reuter, edited by G. Von Freymann, E. Blasco, and D. Chanda (SPIE, San Francisco, United States, 2024), p. 52.

[3] J. H. Hwang et al., , Applied Surface Science **698**, 163044 (2025).

[4] Z. M. Karimi and J. A. Davis, in *2025 IEEE 37th International Conference on Microelectronic Test Structures (ICMTS)* (IEEE, San Antonio, TX, USA, 2025), pp. 1–4.

[5] Y. Weng, G. Chen, X. Zhou, Q. Yan, T. Guo, and Y. Zhang, Nanotechnology **30**, 085702 (2019).

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