Optimization of the Growth of Atomic Layer Deposited Ta_2O_5 Thin Films for Large Area Electronics

X. Chen[1*], K. Niang[1], B. Bakhit[1, 2], Y. Jeon[2]. J. Driscoll[2] and A. Flewitt[1]
[1]Dept. of Engineering, University of Cambridge, Cambridge, UK.
[2] Dept. of Materials Science and Metallurgy, University of Cambridge, Cambridge, UK.
**E-mail: xc363@cam.ac.uk*

Tantalum oxide, Ta_2O_5, has been extensively studied as a promising high-*k* dielectric in semiconductor devices (1), as a capacitor dielectric in memory devices (2), and as an antireflection coating in solar cells (3). Ta_2O_5 has been deposited using various technologies including e-beam evaporation (4), sputtering (5), and atomic layer deposition (ALD) (6, 7). Among these, ALD is particularly attractive technique due to its ability to precisely control stoichiometry as a result of the self-limiting growth process. In addition, ALD tends to produce thin films with high conformality and good uniformity over a large substrate areas. This work focusses on optimization of ALD Ta_2O_5 for large area electronic applications where an amorphous morphology is favored as this allows excellent device-to-device uniformity, and substrate deposition temperature is limited by unconventional substrates such as glass and plastic.

Ta_2O_5 is grown by ALD from pentakis(dimethylamino)Ta (PDMAT) and water using a Savannah system from Cambridge Nanotech/Veeco. We have investigated various ALD process parameters such as the pulse time, purge time, substrate temperatures, and various post-deposition annealing temperatures. We have also investigated the physical, electronic and optical properties of the deposited thin films using various characterization techniques.

We show that the ALD Ta_2O_5 can be produced within a large process window and with good uniformity. At 200 °C, the saturated growth rate is ~ 0.6 Å/cycle, and thickness uniformity of ~ 95% is obtained across a 4-inch diameter wafer. The as-deposited Ta_2O_5 thin films are amorphous and require a post-deposition annealing at ~ 700 °C to become polycrystalline with a textured surface. We will correlate the morphology of the as-deposited thin films with their optical and electrical properties such as dielectric constants and breakdown voltages.

References:

(1) D. A. Deen et al., "Atomic Layer Deposited Ta_2O_5 Gate Insulation for Enhancing Breakdown Voltage of AlN/GaN High Electron Mobility Transistors," *Applied Physics Letters* **2011**, *98*, 023506.

(2) Y. Yang et al., "Complementary Resistive Switching in Tantalum Oxide-based Resistive Memory Devices," *Applied Physics Letters* **2012**, *100*, 203112.

(3) S. Yun et al., "Non-Pt Counter Electrode Catalysts Using Tantalum Oxide for Low-Cost Dye-sensitized Solar Cells," *Electrochemistry Communications* **2012**, *24*, 69-73.

(4) Y. Kang et al., "Comparison of Resistive Switching between Tantalum Oxides Deposited by Atomic Layer Deposition and E-Beam Physical Vapor Evaporation," *ECS Transactions* **2013**, *53*, 65-70.

(5) C. Mannequin et al., "Identification and Roles of Nonstoichiometric Oxygen in Amorphous Ta_2O_5 Thin Films Deposited by Electron Beam and Sputtering Processes," *Applied Surface Science* **2016**, 385, 426-435.

(6) S. Song et al., “Comparison of the Atomic Layer Deposition of Tantalum Oxide Thin Films Using $Ta(N^{t}Bu)(NEt_2)_3$, $Ta(N^{t}Bu)(NEt_2)_2Cp$, and H_2O,” *ACS Applied Materials & Interfaces* **2017**, *9*, 537-547.

(7) W. J. Maeng et al., “Atomic Layer Deposition of Ta-based Thin Films: Reactions of Alkylamide Precursor with Various Reactants,” *Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures* **2006**, *24*, 2276.

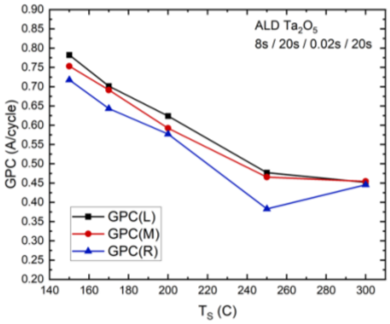

Figure 1. The growth per cycle of Ta_2O_5 as a function of the substrate temperatures.

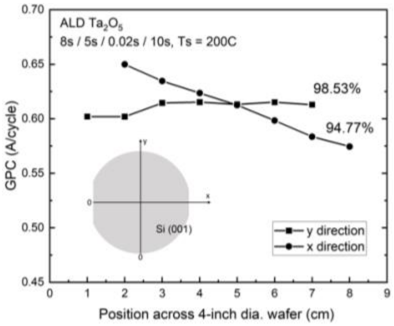

Figure 2. The thickness uniformity of the Ta_2O_5 across x- and y-directions of a 4-inch diameter wafer

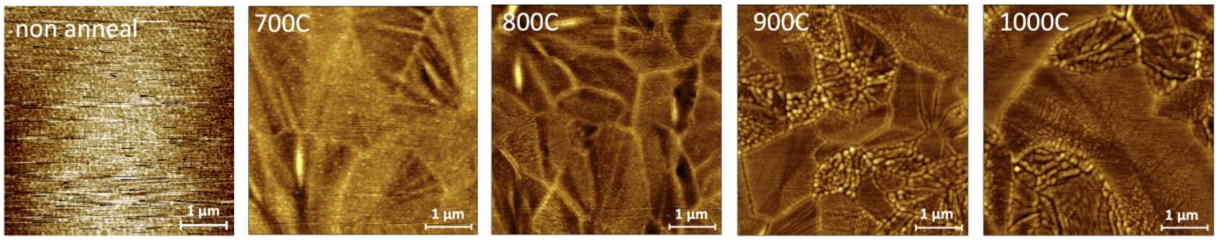

Figure 4. The surface morphology of the as-deposited and after annealing at various temperatures