Mechanism of Alumina ALD

Computing Chemical Reactions at Surfaces

As electronic devices are scaled down, the dielectric films that store charge (e.g. memories or transistors) must be uniform but extremely thin. For example, 5 nm thin alumina films are used as the dielectric in state-of-the-art trench DRAM memory. Atomic layer deposition (ALD) is the leading technology for manufacturing such films in semiconductor fabrication lines. In order to understand how ALD works, we are studying the underlying chemistry at the atomic scale.

Trimethylaluminium (TMA) and water are successful precursors for alumina ALD. How these chemicals react on the surface during growth of the thin film determines the speed of growth, the quality of the film and the level of impurities. We therefore study the adsorption of TMA onto a hydroxylated alumina surface with density functional theory (DFT). We find that TMA fragments only stick permanently to the surface after protons from the surface migrate to TMA and eliminate one or more ligands as CH4. The resulting formation of an Al-O bond is the first step in film growth.

Within the RAPID Marie-Curie project, our ongoing research is into how ALD can favour particular nanocrystal morphologies for alumina, and how this can be altered using oxygen plasma.
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Related Publications

- Simulating the atomic layer deposition of alumina from first principles.
  Authors: Simon D. Elliott, James C. Greer

- Ozone-Based Atomic Layer Deposition of Alumina from TMA: Growth, Morphology, and Reaction Mechanism.
  Chemistry of Materials volume 18 issue 16 pages 3764 to 3773 (2006)
  Authors: S. D. Elliott, G. Scarel, C. Wiemer, M. Fanciulli, G. Pavia