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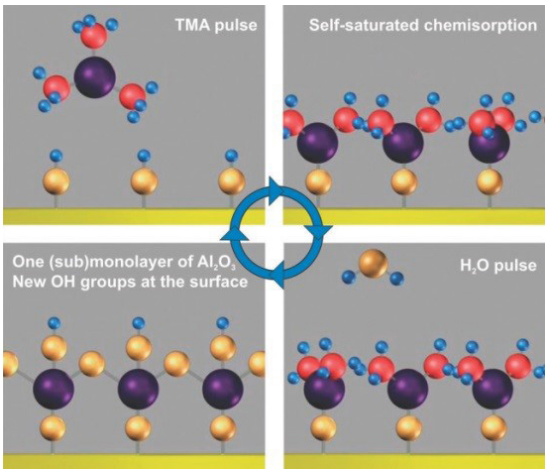
MULTI-SCALE MODELING AND EXPERIMENTAL INVESTIGATION OF AN ATOMIC LAYER DEPOSITION PROCESS

Modélisation multi-échelles du procédé Atomic Layer Deposition



Film growth evolution during a single Atomic Layer Deposition cycle

Atomic Layer Deposition (ALD), is a deposition technique, based on the sequential exposure of substrates to reactants, during which self-terminating reactions take place on the substrate surface. The reactant exposures are separated by a purging period. Each sequence of reactant exposures constitutes an ALD cycle. In theory, each of those cycles produces a monolayer of the targeted film. The uniformity and growth control of ALD produced films are the main advantages of the process.

However, in industrial reactors, the actual film evolution during the first ALD cycles is not as predicted. Influence of the substrate to the deposited film, in terms of composition and film growth evolution is observed during those cycles.

This thesis aims to construct a computational model for a commercial ALD reactor, in order to study the chemical mechanisms and phenomena taking place during the first cycles of the Atomic Layer Deposition of Aluminum oxide (Al_2O_3) films on hydrogen (H) terminates silicon (Si) substrates, using trimethyl aluminum ($Al(CH_3)_3$ as a precursor and water vapor (H_2O) as an oxidant source. The computational results will be compared to experimentally grown Al_2O_3 films, deposited in an industrial reactor, situated in LAAS, Toulouse, France. The thesis aims on a multi-scale model for the ALD reactor, that couples transport phenomena in the reactor 's main volume, with the chemical reactions and species interdiffusion taking place on the feature scale on the substrate. The goal is to obtain optimal process conditions and substrate pre-treatment techniques, in order to overcome the shortcomings observed during the first ALD cycles.