# Controlling the Deposition Regime in Close Proximity Spatial Atomic Layer Deposition with COMSOL

C. Masse De La Huerta[1], V. Nguyen[1], J-M. Dedulle[1], D. Bellet[1], C. Jiménez[1], D. Muñoz-Rojas[1]

[1]Univ. Grenoble Alpes, CNRS, Grenoble INP , LMGP, F-38000 Grenoble, France

## Abstract

Spatial Atomic Layer Deposition (SALD) is a novel technique that allows the deposition of thin films at a considerably shorter time than the conventional Atomic Layer Deposition (ALD) techniques while retaining its unique assets, i.e. high-quality films at low temperature, precise control over thickness and ability to deposit conformal coatings over large aspect-ratio features or complex substrates. Its principle is based on a physical -rather than temporal- separation of the precursors, which are kept apart by an inert gas region or flow. This can be done using a deposition head through which the gaseous precursors are separated in parallel channels above the substrate, avoiding intermixing of such by inert gas channels. By oscillating the substrate back and forth below the head and, due to the chemical adsorption and subsequent reaction of the gaseous precursors on the surface of the substrate, the conventional ALD cycles are replicated and thin films are grown. To ensure efficient separation of the precursors by the inert gas flows, the head needs to be placed very close to the substrate, i.e. 150 µm. This approach is thus known as "close proximity" setup and ensures a deposition at ALD regime. In contrast, if the substrate-head distance is increased, an efficient separation of gases cannot be obtained and deposition following chemical vapor deposition (CVD) regime is obtained[1]. While this is not an issue for flat, featureless samples, and even contributes to a higher deposition rate, it can be an issue when ALD conditions are needed. In order to have a better control over deposition mode, and to become less sensitive to the gap between head and substrate, the geometrical dimensions of the deposition head as well as the flow distribution and separation of the gaseous precursors have still to be understood and optimized so that the best conditions for deposition are obtained and the usage of precursors is minimized. For this objective, computer simulations help greatly, as they provide information of the flow of the gas distribution and provide paths for their optimization. Here, we present a computational analysis of the SALD system present at our laboratory. The Computational Fluid Dynamics simulations and their coupling with diffusion and chemistry studies made with Comsol Multiphysics® provide insight on the current deposition phenomena taking place in our SALD system. The results offer possible new directions towards the optimization and development of this novel technique and its instrumentation, as well as towards deeper analysis of physical separation and chemical reactions at the surface during deposition.

[1] https://doi.org/10.1016/j.crhy.2017.09.004