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

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Outline

- ✓Introduction to SALD
- ✓CFD Comsol Simulation
- ✓CVD Reaction Rate
- ✓Experimental Results
- ✓Conclusions and Future Work

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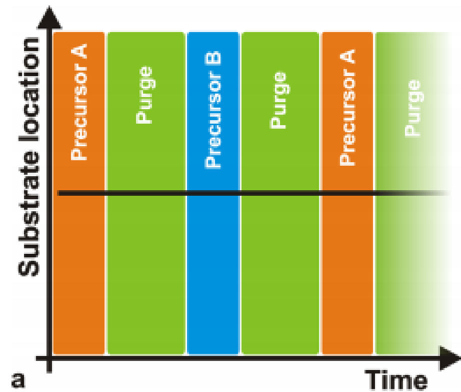
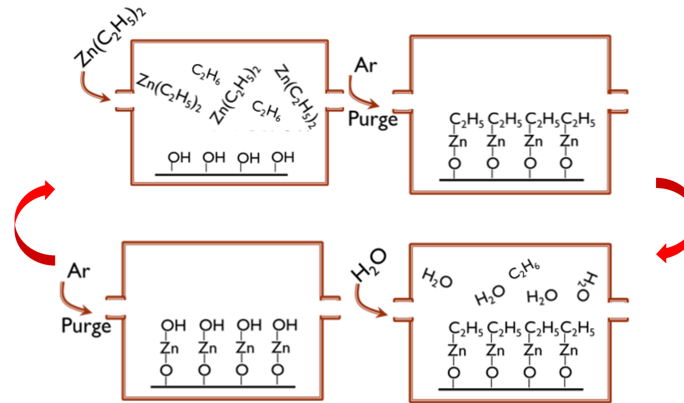
Introduction to SALD – SALD vs ALD



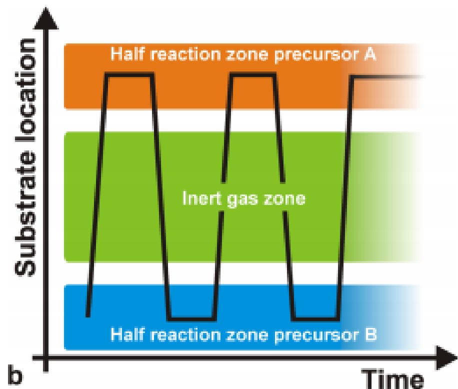


Vacuum

Slow Process

Self-terminating
Surface-liminted **reactions**

Thickness Control
Conformality
Soft Process

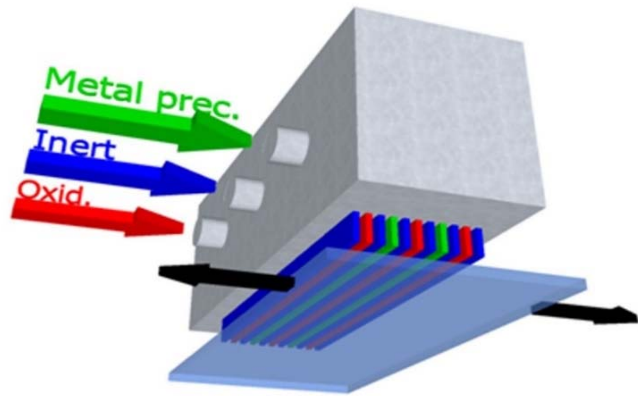


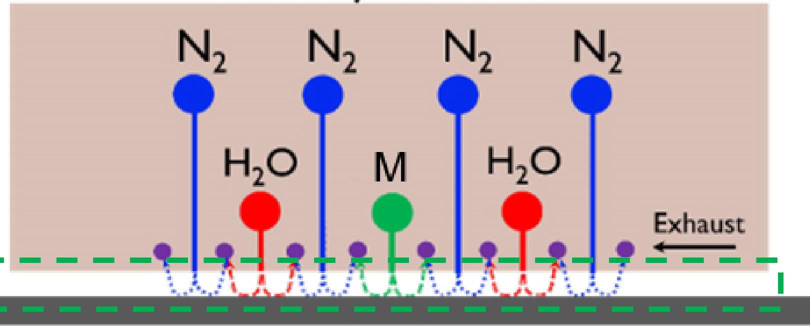
Atmospheric Pressure

Up to two orders of magnitude faster than ALD

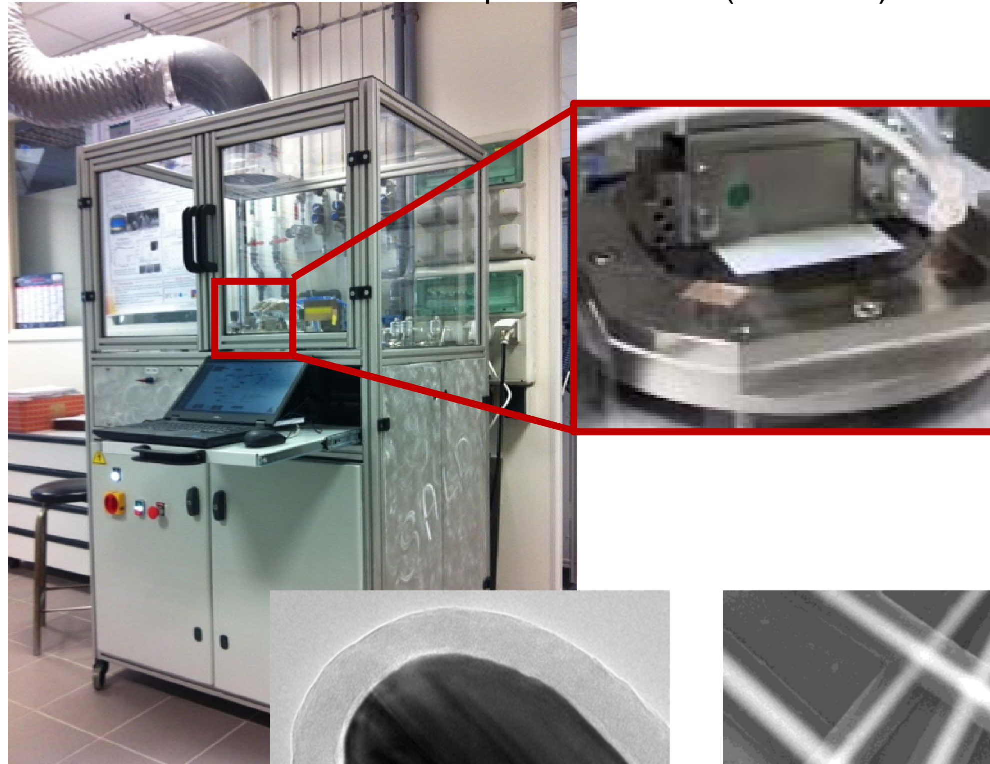
P. Poodt, *et al.*, J. Vac. Sci. Technol., A, 2012, 30, 010802

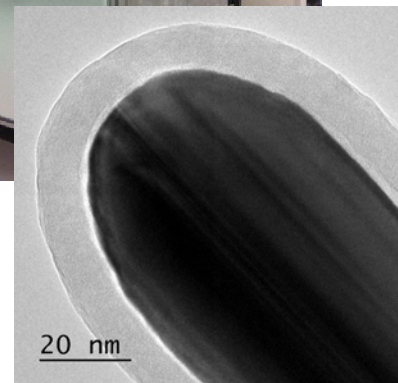
SALD System at LMGP

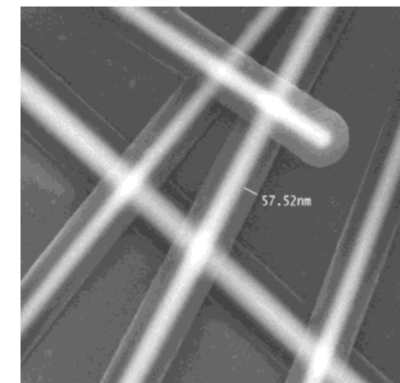




In colaboration with Dominique De Barros (STIGMA)

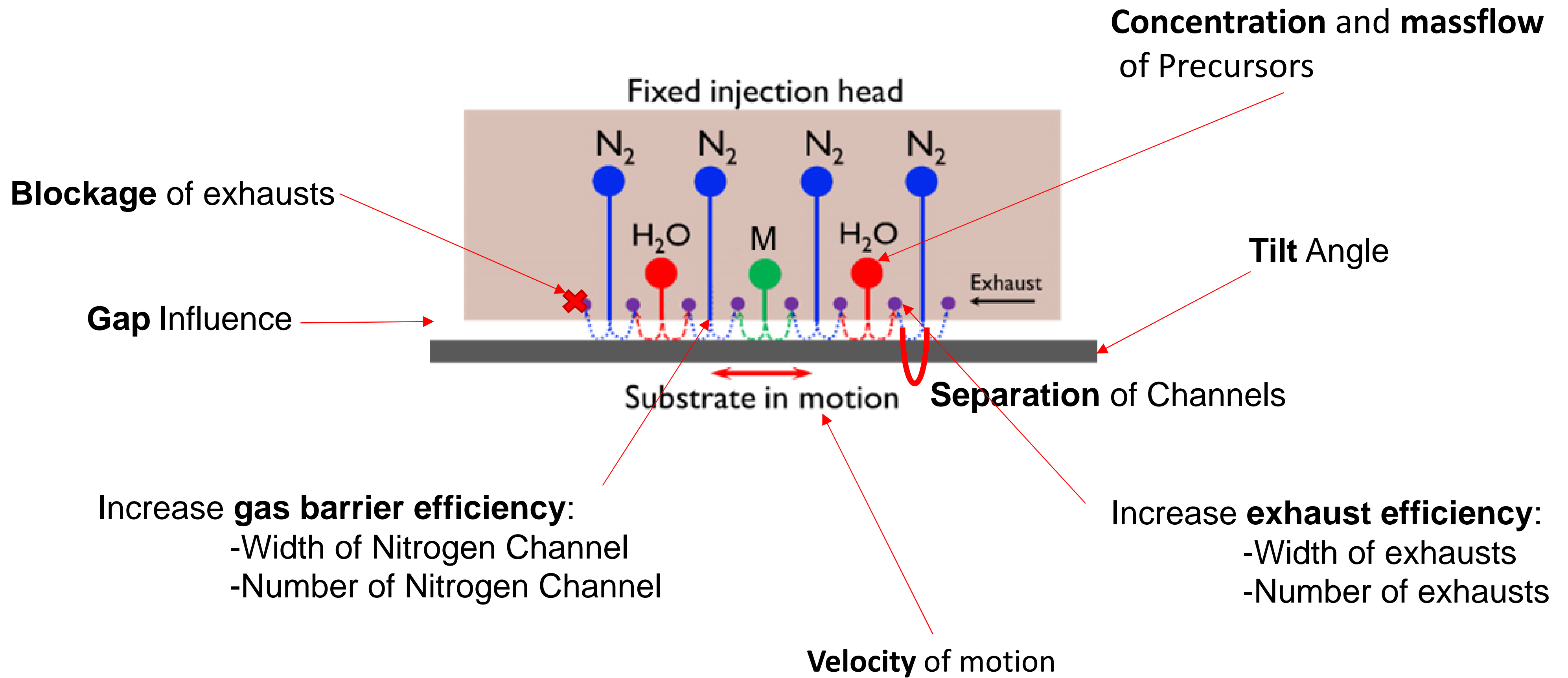






D. Muñoz-Rojas. ***Mater. Horiz.***, 2014,**1**, 314-320

How to control the growth regime?



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COMSOL Multiphysics

CFD Simulations for the SALD Close Proximity System

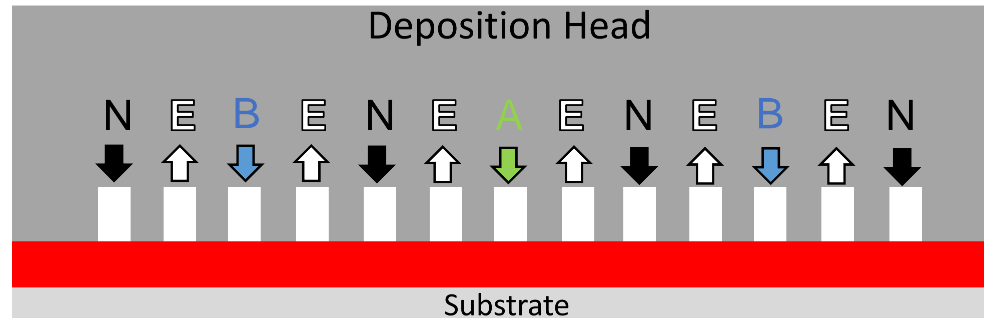
A: ALD Precursor

B: Oxygen Precursor

N: Nitrogen Barrier

E: Exhaust Outlet

$0.15\ mm < Gap < 2\ mm$



Input **Mass Flow**

- 125 SCCM per Inlet

Diffusion coefficients1

$\sim 10^{-3}\ \frac{m^2}{s}$

Low Re-nµmber turbulence model

Mass Fraction of each Species

Intermixing of species

ALD ⇔ CVD

1. J. van Deelen et al. / Surface & Coatings Technology 230 (2013) 239–244

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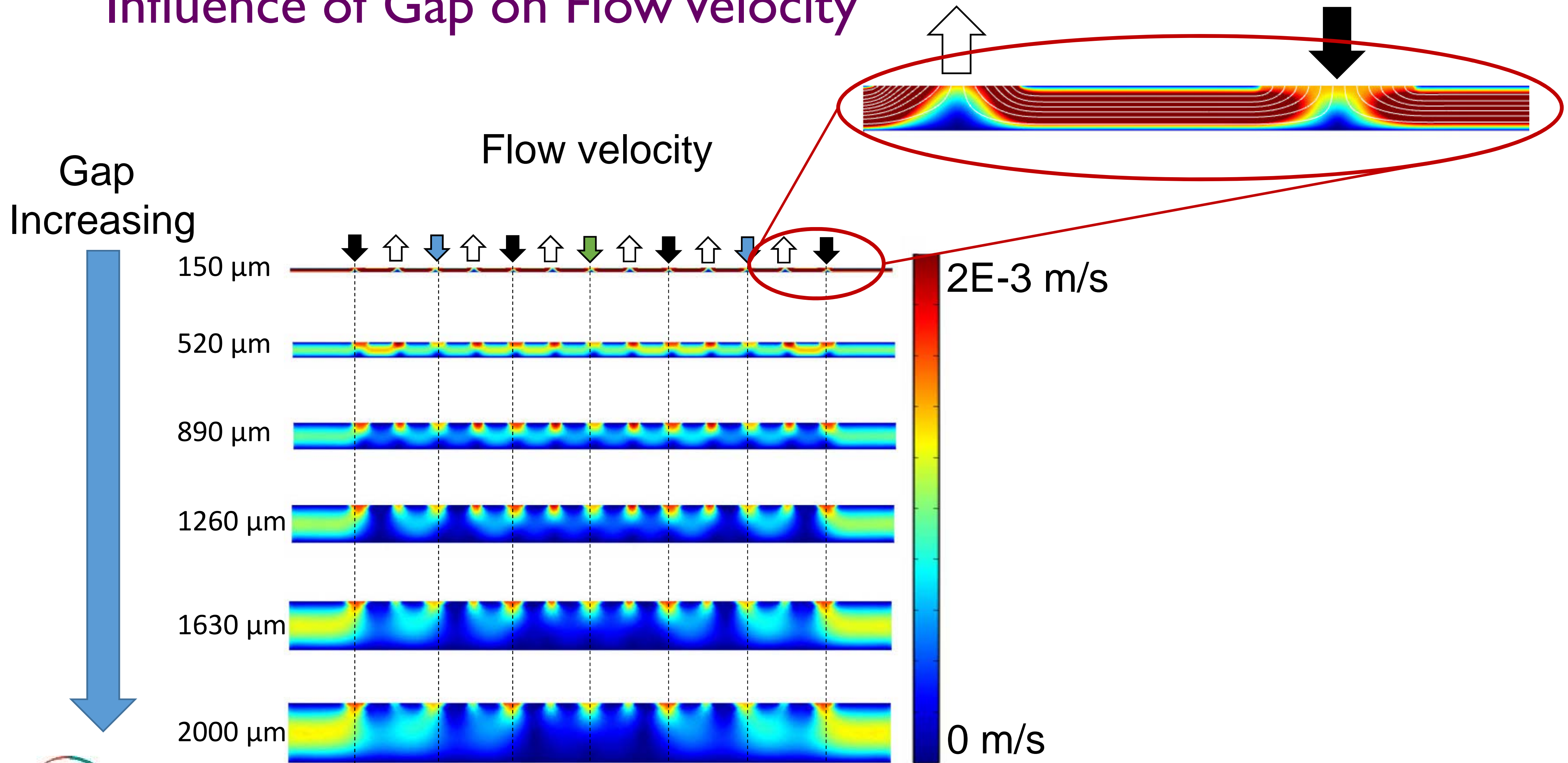
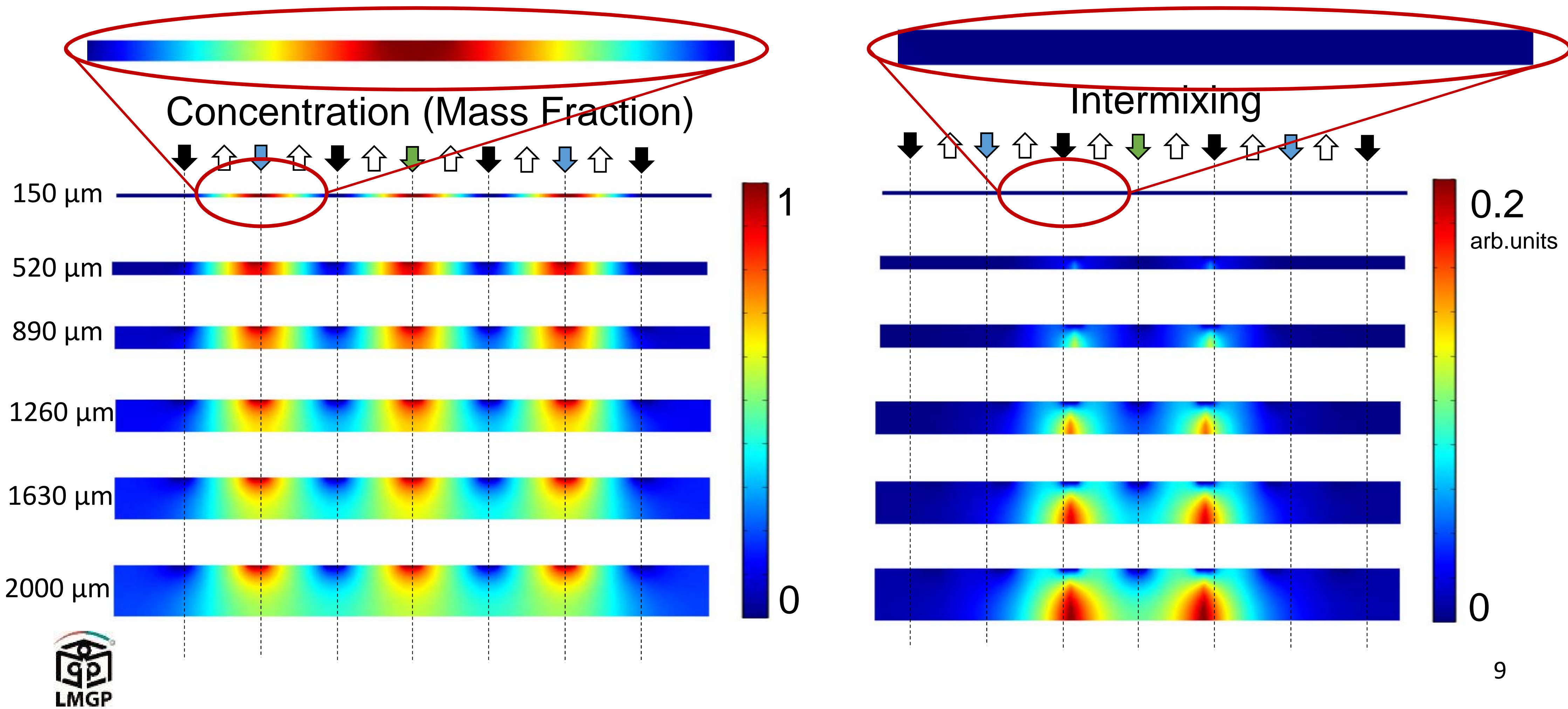
Influence of Gap on Flow Velocity



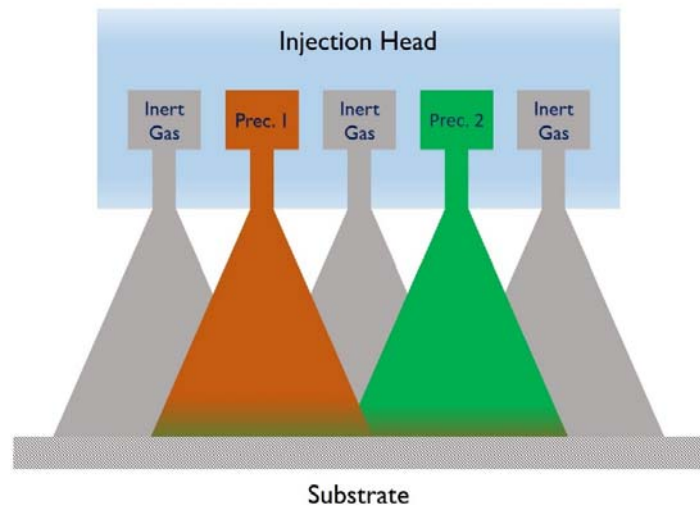
Gap influence on Concentration and Mixing



SALD can work on CVD Regime and ALD Regime

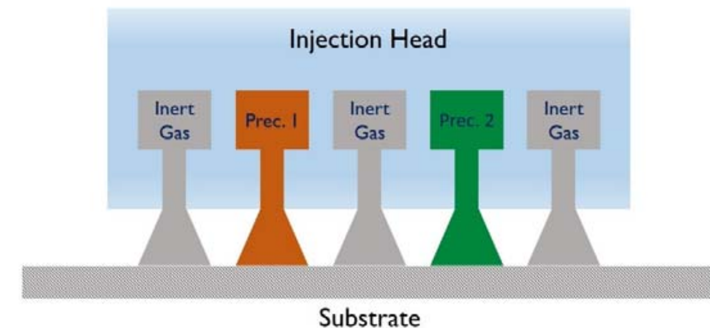
CVD Regime

- Fast non-self-limited reactions on surface.
- Faster but non-conformal deposition on high aspect ratio
- More difficult to control thickness and homogeneity of film
- Lower film density



ALD Regime

- Reactions are self-limited.
- Slower deposition but highly homogeneous and conformal.
- Thickness is controlled by the cycles
- Higher film density



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Muñoz-Rojas, D., *et. al., Comptes Rendus Physique*, Demain l'énergie, 18 (7): 391–400.

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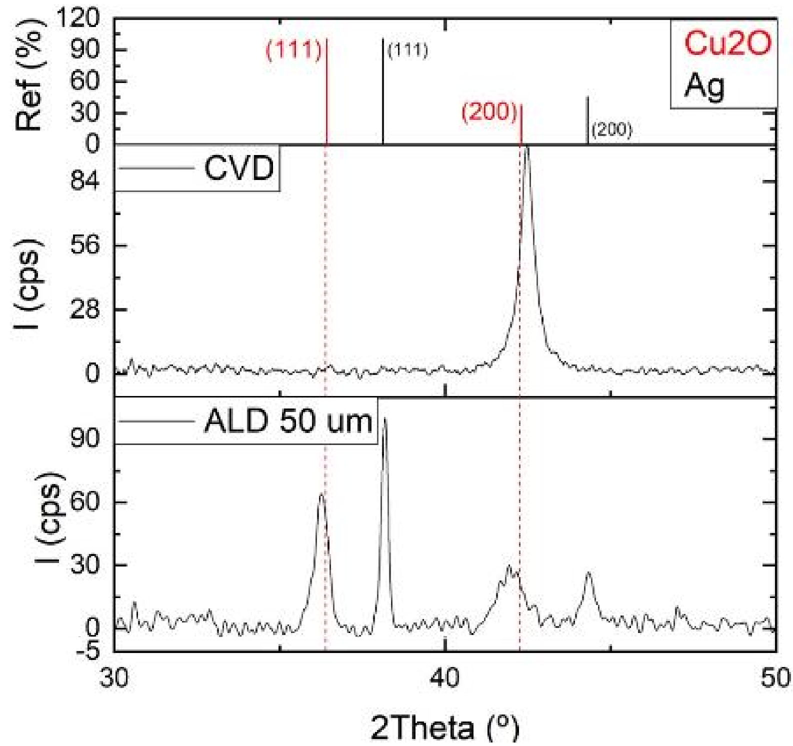
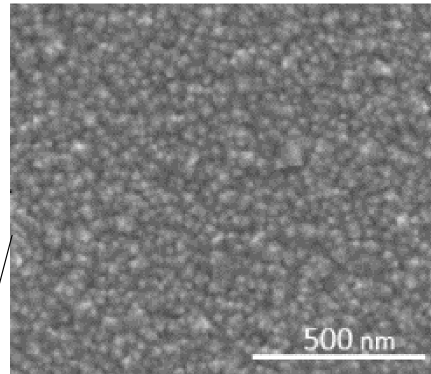
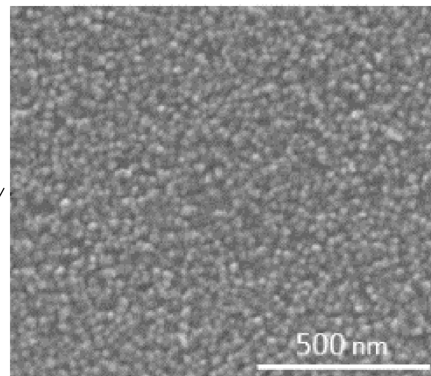
Comparison with Experimental Results

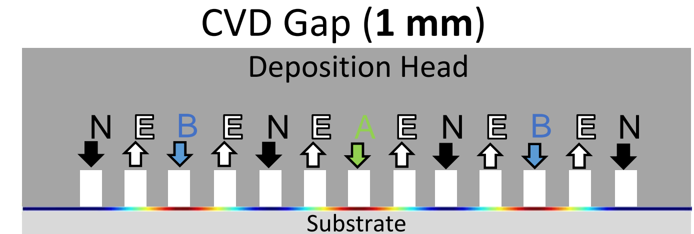
Gap Influence – ALD vs CVD mode







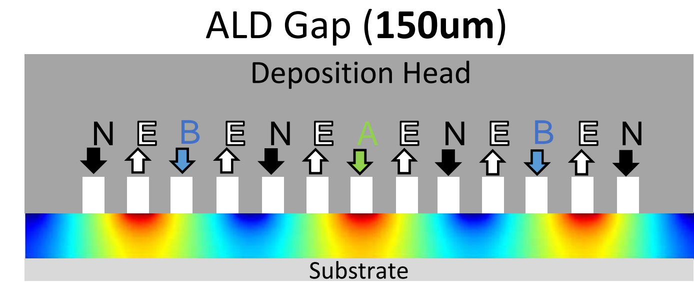
CVD Gap (**1 mm**)



Thickness ~ 90 nm

33.1 Ohm·cm

ALD Gap (**150um**)

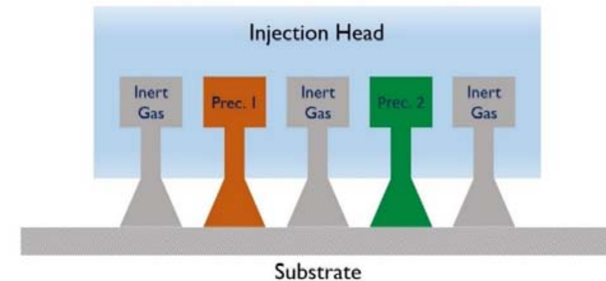


Thickness ~ 50 nm

ρ = ~9 Ohm·cm

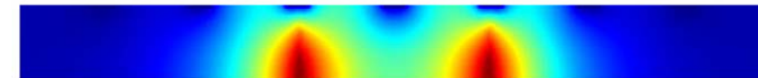
Cu_2O on glass

Conclusions and future work



- Close proximity SALDprovides flexibility to switch growth mode: ALD vs CVD

Couple many other parameters of SALD into a general **topography optimization**



- Computational Fluid Dynamics is a powerful tool to simulate and control the many different parameters of SALD.

3D simulation and chemical coupling of film growth and **Growth per Cycle** determination

- Correlate gap values and intermixing to physical properties of the deposited film.

Correlation between chemistry kinetics and experimental film depositions

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Thanks you for your attention

César MASSE

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