Use of Computational Fluid Dynamics Simulations to Predict the Deposition Regime in Close-Proximity Spatial Atomic Layer Deposition (SALD)

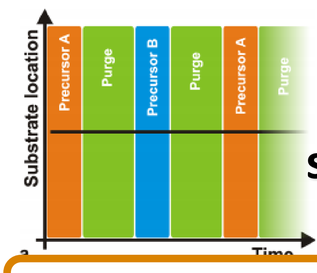
C. Masse de la Huerta [(1)], H. Viet-Nguyen [(1,2)], J.M. Dedulle [(1)], D. Bellet [(1)], C. Jiménez [(1)], D. Muñoz-Rojas [(1)]

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

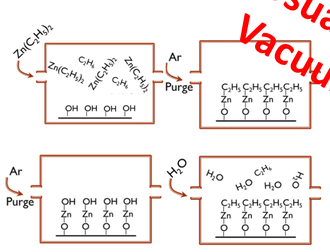
[2)] *Institut National de l'Energie Solaire, Le Bourget-du-Lac, France*

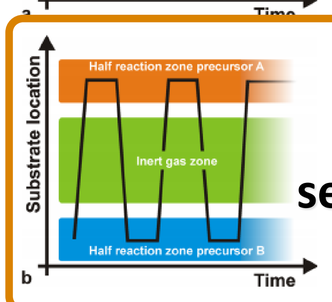
Atomic Layer Deposition (ALD): state-of-the-art materials deposition

ALD: sequential exposure to chemical reactants

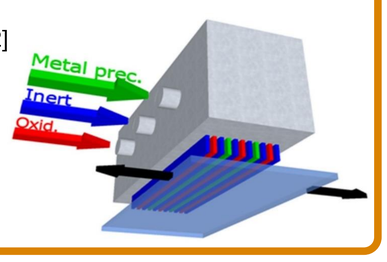


Temporal separation





Spatial separation Ref[1-2]



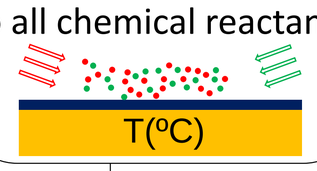
Nanometer Thickness

Conformality

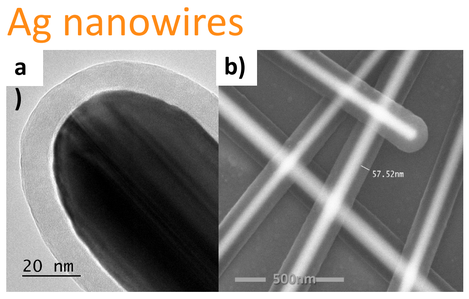
Soft Process

SALD ⇨ Scalable (NO VACUUM), Faster than ALD, Low-Cost

≠ Chemical Vapor Deposition (**CVD**): **simultaneous** exposure to all chemical reactants



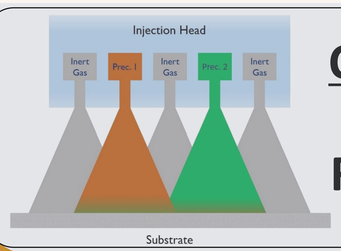
SALD Coating of Al_2O_3 on Ag nanowires



(a) TEM image of Al_2O_3 coated AgNWs.
(b) SEM view of Al_2O_3 coated AgNWs

Spatial gas separation is achieved by a **CLOSE PROXIMITY** between the scanning substrate and the deposition head: **THE GAP IS CRUCIAL**

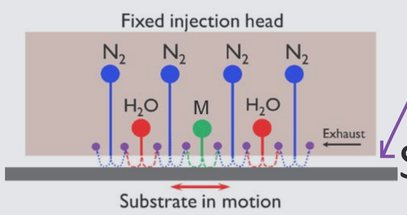
Distance between substrate and injection head: **GAP**



CVD mode

Fast but less controlled growth

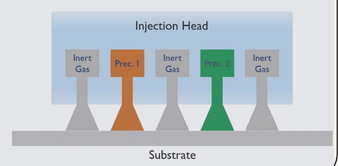
⇦ **Big GAP**



⇨ **Small GAP**

ALD mode

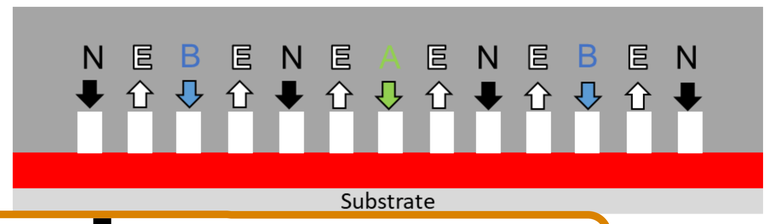
Slow but **nanometric** growth



Computational Methods

2D model to study the **GAP** influence on **INTERMIXING** of volatile precursors

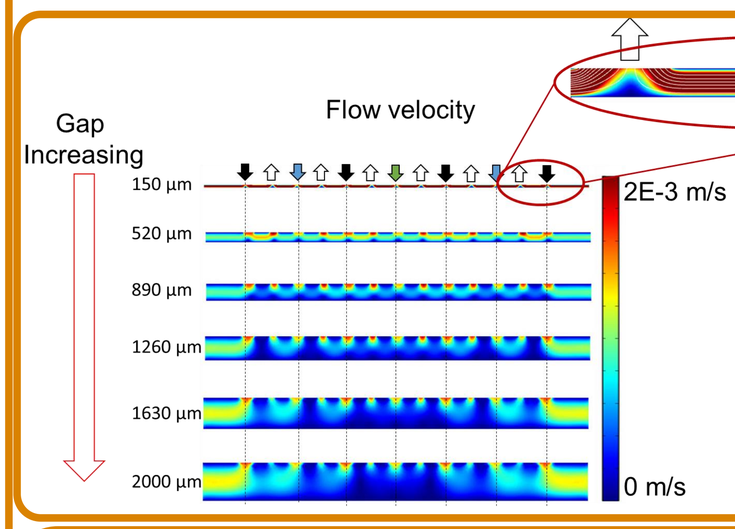
Navier-Stokes (Flow) + Fick's Law (Diffusion)



Low Re Turbulence model ⇨ Transport of concentrated Species

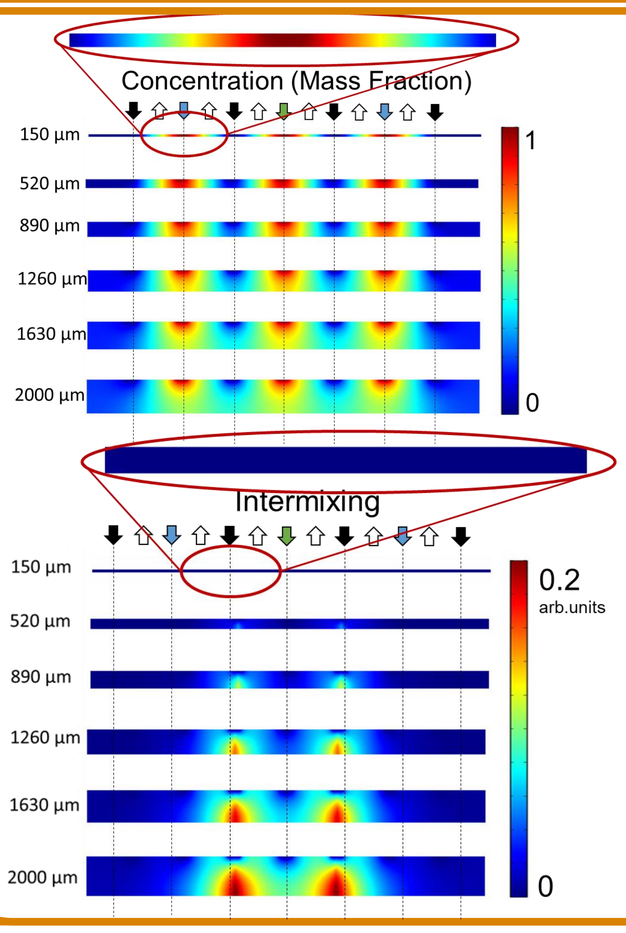
Diffusion Coefficient	~10^{-1}	cm^2/s	Ref[3]
Inlet Velocity	125	SCCM	Ref[4]
Mean Molar Mass	~100	g/mol	Ref[5]
GAP dimension	150-2000	µm	
Gas Carrier (solvent)	Nitrogen		

Flow



Flow velocity is well confined when **GAP** is small (**close proximity**). At *larger gap values*, velocity is **not confined on top of the substrate.**

Intermixing

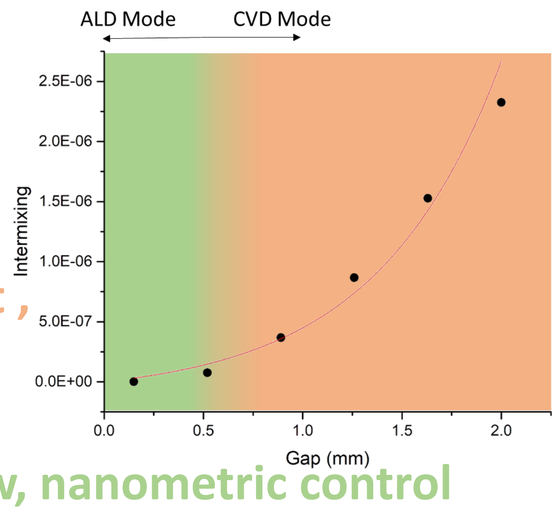


At smaller **GAPs**, the two precursors are **well separated**, allowing to *emulate* ALD conditions for the growth of the material.

At larger **GAPs**, the two precursors are **not separated**, hence, CVD conditions appear during deposition of materials.

Conclusions

SALD relies on spatial separation of gaseous precursors, hence, it relies also on the physical geometries which are crucial to control the deposition. **The deposition GAP** was studied to differentiate depositions regimes:



MIND THE GAP

Big GAP:
CVD Regime- Fast , not controlled

Small GAP:
ALD Regime- Slow, nanometric control

[1] P. Poodt, *et al.*, J. Vac. Sci. Technol., A, 2012, 30, 010802
[2] Muñoz-Rojas, D., *et. al., Mater. Horiz.,* 2014,1, 314-320
[3] Edward B. Winn, Phys. Rev. 80, 1024
[4] Muñoz-Rojas, D., *et. al., Comptes Rendus Physique*18 (7): 391–400.
[5] National Center for Biotechnology Information. CID=11185

Excerpt from the Proceedings of the 2018 COMSOL Conference in Lausanne