Synthesis & Properties of Functional Nanomaterials & Thin Films (SYNFONI)

Advanced Spatial Atomic Layer Deposition (SALD)

Context

- **ALD:** a unique technique offering precise thickness control and conformality
- **SALD:** up to x100 faster ALD approach that can be performed in the open air: appealing for mass production. Yet SALD offers much more than just faster deposition:
  - Close proximity head approach used at LMGP offers easy customization for different substrate applications
  - Spatial CVD can also be performed
  - Exploit atmospheric processing

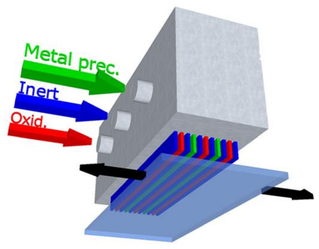
Objectives

- Develop **innovative SALD approaches** for **new materials and applications**
- Deposit materials with **properties comparable to** the ones obtained with **physical methods**
- **Explore original precursors and processing conditions**
- **Develop more sustainable/safe processes**
- **Enlarge the application domains of SALD**

Skills and competences

- Design and fabrication of **custom-made systems**: different substrates/materials/applications
- Optimisation (CFD simulations) & **3D printing** of SALD deposition heads
- Original area-selective deposition methods based on our SALD approach
- N**ew processes** to deposit functional thin films
- **Life Cycle Assessment** (LCA)
- **Alternative processes (plasma, laser) through long-standing collaborations**

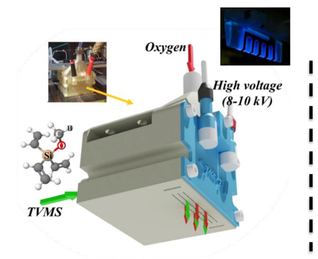
Reactor Design and Customisation



Scheme of a typical close-proximity SALD head.

Circular channels → Area-selective Free-form deposition

C.A. Masse de la Huerta et al. ***Adv. Mater. Tech. (2020)***



Atmospheric plasma activation integrated in the head

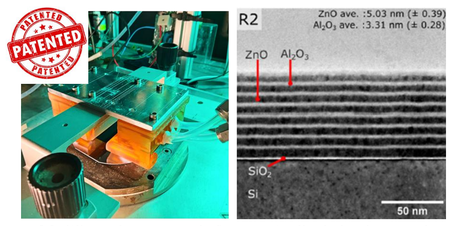
V. H. Nguyen et al. ***Chem. Mater. (2020)***

Cylindrical head for tubular substrates (e.g. membranes)

F. Toldra-Reig et al. ***ACS Sust. Chem & Eng. (2022)***

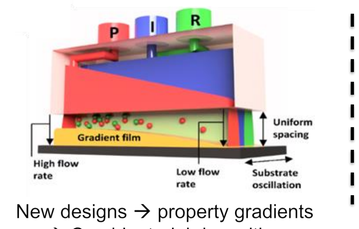
Home made SALD system

D. Muñoz-Rojas et al. ***Mater. Today Chem. (2019)***



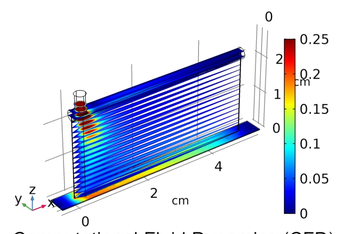
Multihead approach for controlled doping and multilayers

H. Okcu et al. ***Nanoscale (2025)***



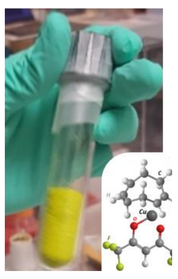
New designs → property gradients → Combinatorial deposition

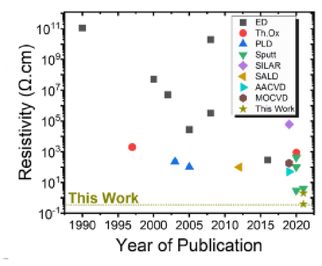
A. H. Alshehri et al. **Adv. Func. Mater (2021)**



Computational Fluid Dynamics (CFD) simulations for head optimisation

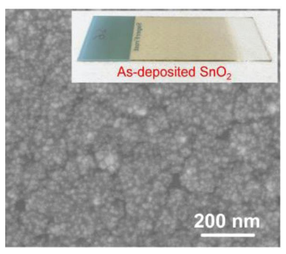
Process Development and Material Optimization



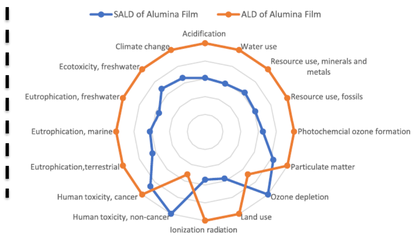


Record moblity and conductivity for chemical, non-epitaxyal Cu_2O film. Tuning of properties with precursor, temperature and O_2 partial pressure. Selective deposition of $Cu/Cu_2O/CuO$

A. Sekkat et al. ***Commun Mater (2021)***
A. Sekkat et al. ***Nature Commun. (2022)***
A. Sekkat et al. ***Mater. Today Chem. (2023)***

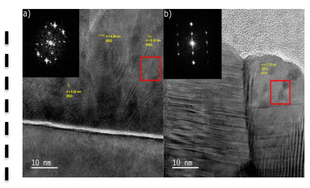


Other New processes: ZrO_2, Y_2O_3, CeO_2, NiO, Ga_2O_3, ZnO, MgO…



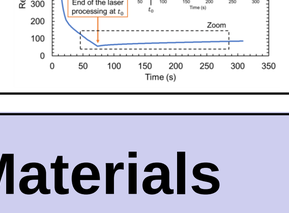
LCA studies of SALD processes and precursors

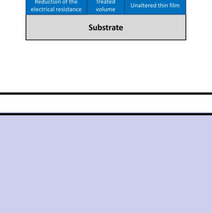
M. Farooq et al. ***ACS Sust. Chem & Eng. (2023)***
L. Johnston et al. ***RSC App. Interf. (2024)***



Control of texture of ZnO films for piezoelectric applications

H. Okcu et al. ***App. Surf. Sci. (2025)***





Post deposition laser annealing: Phase and property control

Transparent Conductive Materials

Context

Transparent conductive materials (TCMs) constitute a research topic that has been extensively studied in recent decades since they are of great interest for applications or devices such as transparent electrodes for solar cells or for OLEDs, gas sensors, transparent heaters or for transparent electronics.

Objectives

- Design, understand and optimize two different types of TCMs and their combination in composites:
  - Metallic nanowire networks (AgNW, CuNW…)
  - Transparent conductive oxides (TCOs) both n and p-type
- Particular focus on In-free compounds such as Cu(I)-based oxides & electron correlated material
- Combine experimental studies with modelling for comprehensive understanding

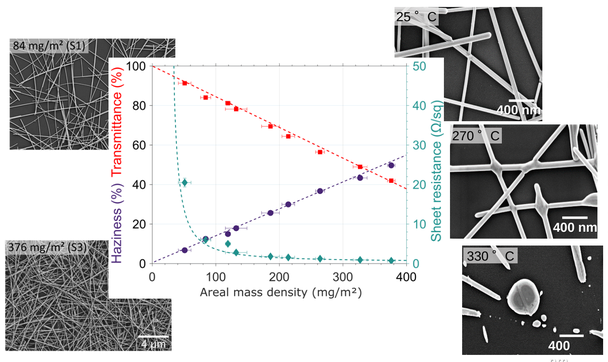
Skills and competences

- Understand and control key parameters to tune physical properties of MNW networks and composites
- Combine physical modelling and Monte Carlo simulations for understanding of MNW network behaviour
- Enhance film properties by optimizing microstructure, composition, and doping
- Integrate p-type and n-type layers into devices as transparent p–n junctions in sensors and hole transport layers (solar cells)
- Deposition methods: SALD, Aerosol Assisted CVD, Pulsed-injection MOCVD, Sol-gel
- Applications, Electronic & optoelectronic devices, flexible electronics

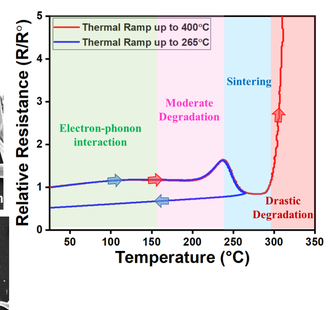
Silver Nanowire (AgNW) Networks

Properties of AgNW networks

AgNW dimensions (diameter & length), network density and thermal annealing influence drastically the physical properties of AgNW networks.



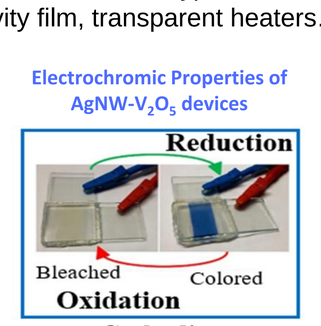
L. Bardet et al. ***Nanoscale (2024)*** *&* ***ACS Appl. Nano Mat. (2023)***



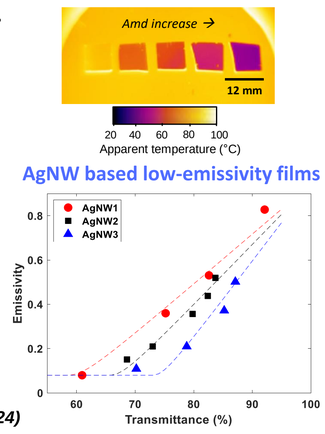
S. Maurya et al. ***Adv. Physics X (2025)***

AgNW networks integration

AgNW networks can be a good candidate as transparent electrodes for several types of devices such as solar cells, low emissivity film, transparent heaters…

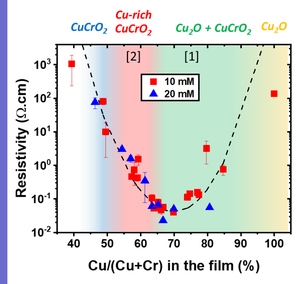


A. Khan et al. ***ACS Appl. Mater. Interf. (2024)***



p-type TCO

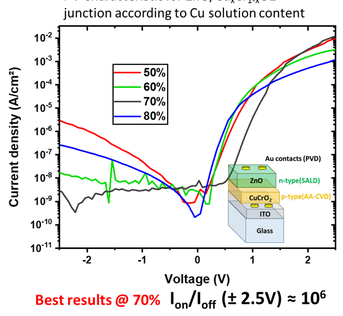
Development of new compounds through a coupled approach between Elaboration and first principle DFT calculation (collaborations)



Optimization of composition and microstructure: $CuCrO_2$ out of stoichiometry , Cu_2O, NiO

L. Bottiglieri et al. ***Mater. Adv. (2021)***

- Transparent p-n junction



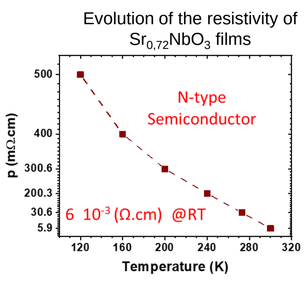
Best results @ 70% I_{on}/I_{off} (± 2.5V) ≈ 10^6

L Bottiglieri et al. ***ACS Appl. Elect. Mat. (2022)***

n-type TCO

Development of In free TCO with strongly correlated electron oxides, mainly as Perovskite compound such as $SrNbO_3$, $CaNbO_3$, $SrVO_3$, …

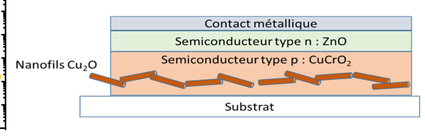
Optimisation of other standard n-type TCO (SnO_2, AZO, etc)

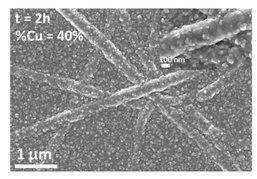


Nano-Composite TCM

p-type TCO

Development of a new controlled nancomposite material, based on a **Cu_2O nanonet** (NaBioS collab) and a **$CuCrO_2$ thin film**:

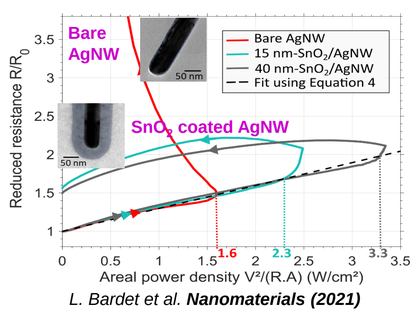




➢ Encapsulation upon t_{dep} = 2h

AgNW and metal oxide coating

SALD coating leads to highly conformal coating for many metal oxide coating on AgNW networks. Such coating drastically enhances AgNW network stability.



L. Bardet et al. ***Nanomaterials (2021)***

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More information: