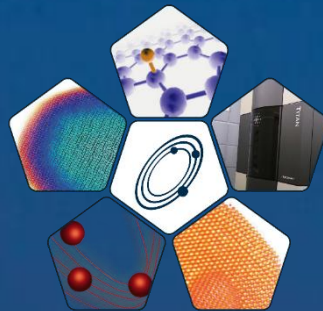


Advanced structural characterization and multiscale simulation of nanomaterials



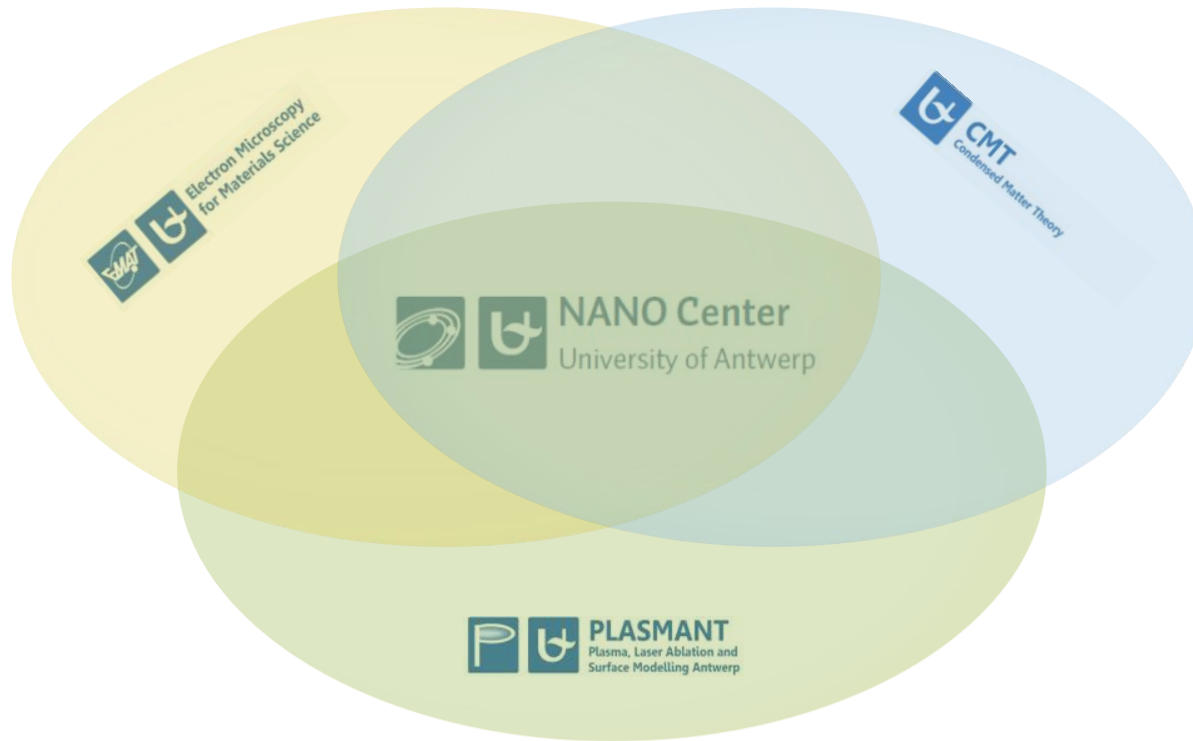
Alexander Neirinckx

Contact: alexander.neirinckx@uantwerpen.be



NANOcenter consortium

1 of 7 spearhead domains at the University of Antwerp



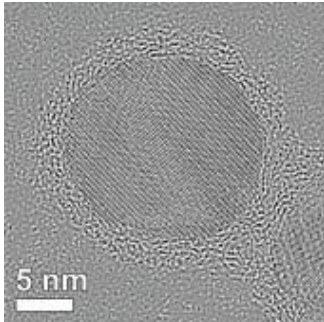
10 professors + approx. 110 researchers at PhD and Post-doc level
3 active ERC grants, 1 ERC-POC, 1 ITN, 1 Flag-Era, 2 INFRA projects



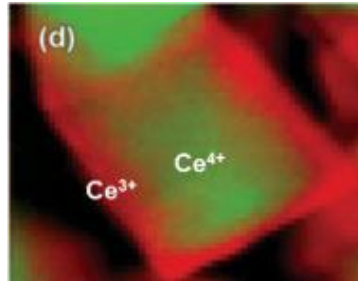
Goal: Advancing insight in and improving design of (nano)materials by advanced characterization and computer simulations

Micro- & nanoscale characterization of materials

Polymer coated Ag particle



Ceria catalyst



Heating a nanostar
25°C



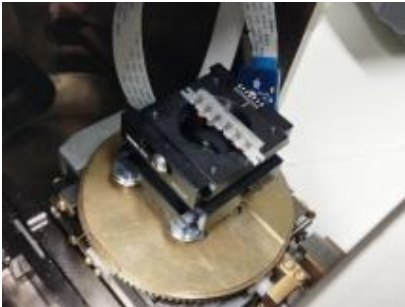
900°C



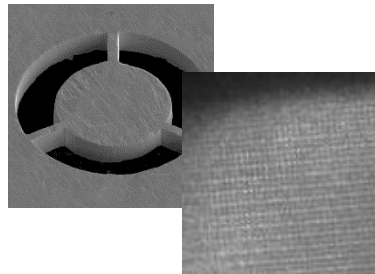
Structural ⇔ **Elemental** ⇔ **in situ**

Development of EM instrumentation and image/data processing software

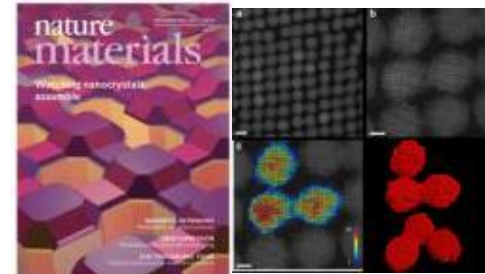
Lowtech SEM diffractometer



Specialized TEM apertures

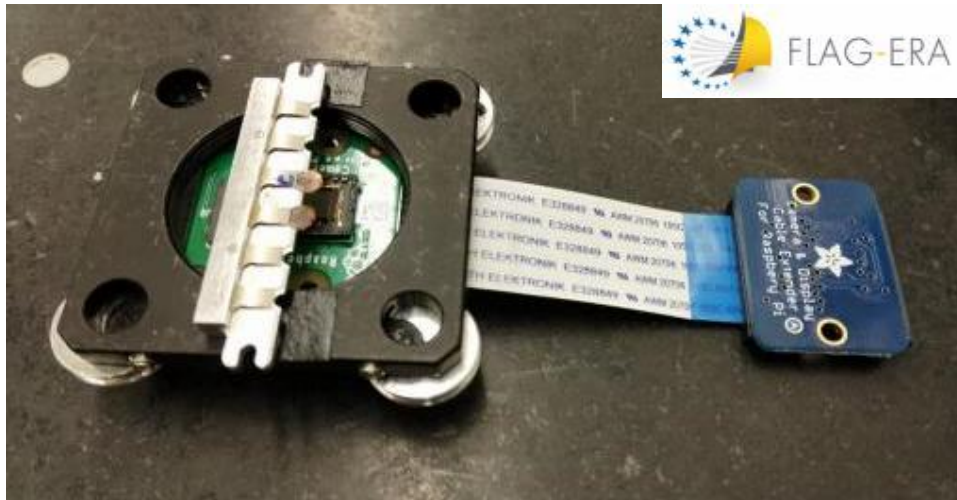


Atom counting & 3D reconstruction



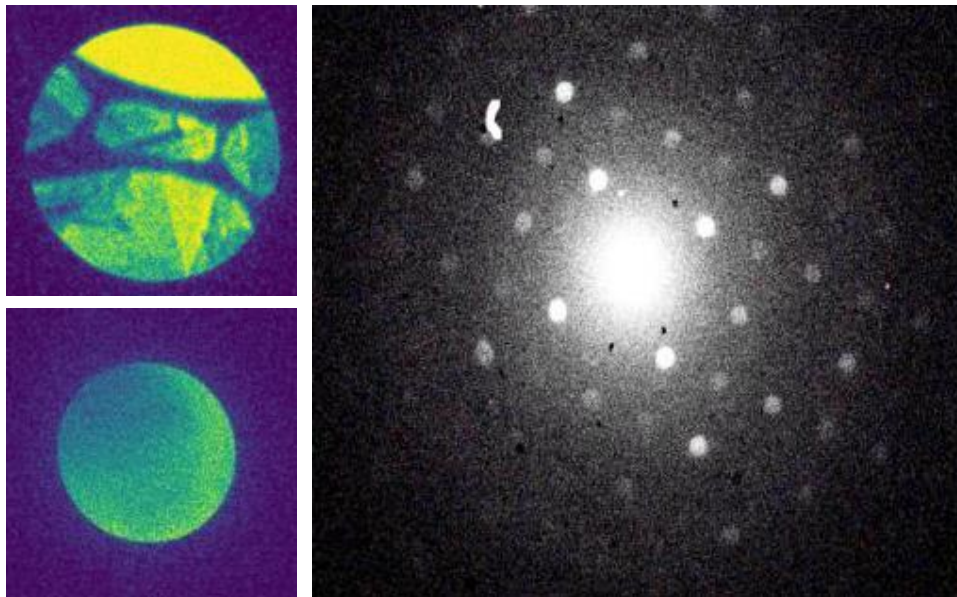
⇒ Materials: catalysts, semiconductors, (3D printed) steels & alloys, polymers, battery materials,...

SEM for structure solution



Proof of concept:

- Texture mapping of graphene
- Simple camera with scintillator & cheap hardware used at 1-30 kV
- Field of view up to 3 mm
- Alternative for single crystal XRD



Application:

API / thin films / polymers / binders
(cement) / embedded nanoparticles

Partner search:

1. RTO/industry partners
 - a) detector development
 - b) automation & engineering
2. Use cases

PLASMANT: modelling plasma interaction

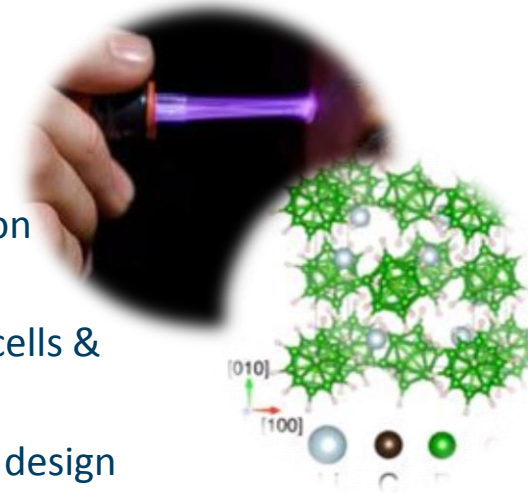
CMT: modelling of functional materials

Materials/micro-electronics/nanotechnology

- ⇒ How to control plasma etch/deposition/growth process? (atomic scale)
- ⇒ High throughput computational screening of materials & (opto-electronic) properties

Energy/environment

- ⇒ Underlying mechanisms of efficient CO_2 conversion & N_2 fixation & formation value added chemicals?
- ⇒ Influence of material choice in solar cells & battery materials
- ⇒ Plasma/catalyst interaction + reactor design



Analytical chemistry

- ⇒ Most important pathways for analytes + optimization?
- ⇒ Effect of source design on performance?

Plasma medicine

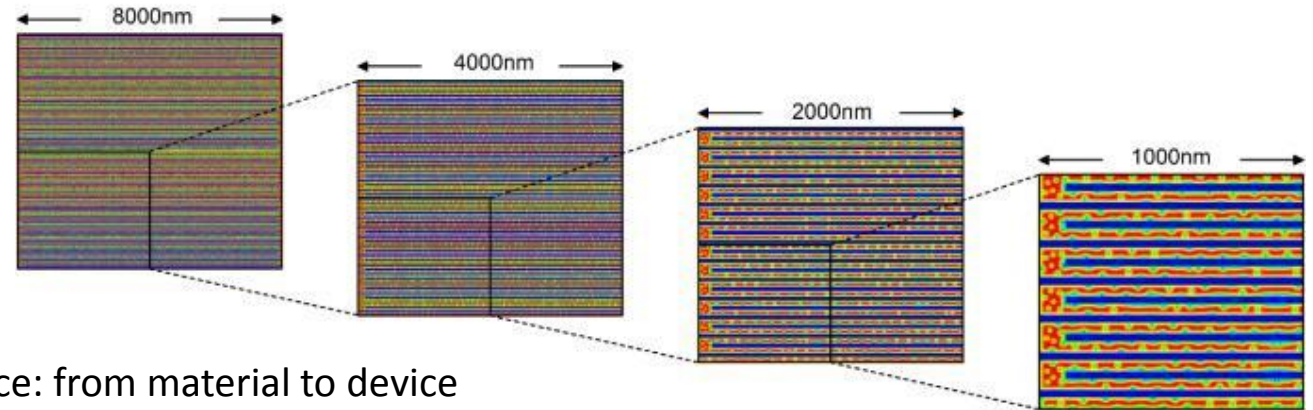
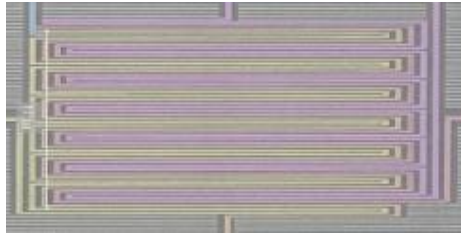
- ⇒ Anti-cancer mechanisms of direct plasma treatment and plasma activated media
- ⇒ How to increase effectiveness AND selectivity cancer cells?

Methodology:

Computational fluid dynamics / Monte Carlo & fluid models / Molecular dynamics / Density Functional Theory / Chemical kinetics / Experimental reactor design for CO_2 & N_2 conversion

Modelling of functional materials

Project: Software for predictive performance simulations of Superconducting Single-Photon Detectors (SSPDs)



Proof of concept:

- Simulating SSPD performance: from material to device
- Validated for lab scale prototypes of other RTOs
- Goal to limit need for costly fabrication and testing phases

Application:

quantum encryption/ quantum computing / laser
communication / satellite technology

Partner search:

1. electronic device for validation of technology
2. R&D partners to synthesize novel materials
3. End users for application of novel SSPDs