FIRST YEAR REPORT

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Aim of the project

The aim of the PhD is the characterisation of nanostructures using advanced electron microscopy techniques. Accordingly, the first year of the PhD has focused on developing a pipeline for the analysis of data obtained from transmission electron microscopy (TEM) and scanning transmission electron microscopy (STEM) techniques to obtain morpho-structural information and optoelectronic properties.

Research activity

In situ TEM movies are widely used because they provide a direct information about the evolution of a sample over time and under an external stimulus. In this context, movies of the thermal evolution of nanostructured thin films mad of gold contains a plethora of information, such as porosity, fractal dimension, interconnectivity, fragmentation of the system, etc. Accessing this information is essential for understanding the processes occurring at the nanoscale in such complex systems. To achieve this, we developed a python script to analyse the movies obtained from *in situ* experiments. More specifically, the script enables us to evaluate the evolution of all the properties as a function of the time, with a resolution on the order of tenths of a second (Fig. 1).

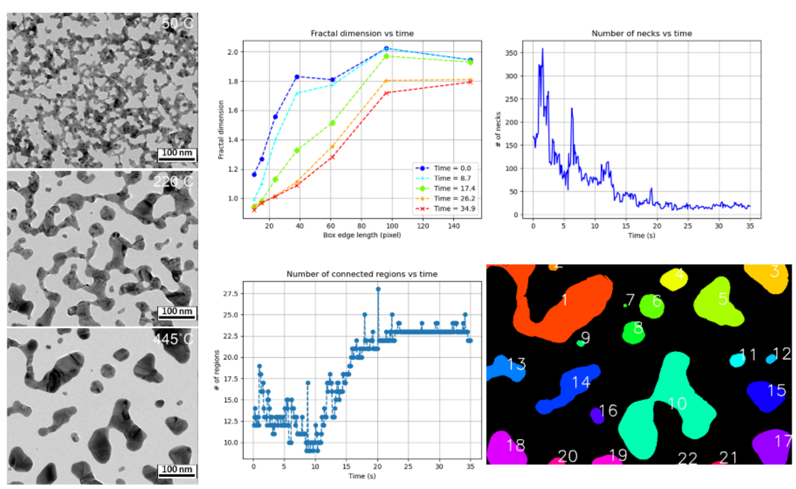

Fig. 1: Evolution of a gold network under thermal stimulation (left) and calculation of selected morphological properties, such as fractal dimension, interconnectivity, and fragmentation (right).

In more detail, the script takes as input an mp4 video showing the entire evolution of the sample under an external stimulus—whether thermal, electrical, or otherwise—and splits it into individual frames. Each frame is then binarised, assigning a value of 1 to the sample (signal) and 0 to the SiN substrate (background). For each frame, the selected morphological properties are computed and stored in an array. Once all frames have been analysed, the results are displayed in a graph.

The development and application of this analysis tool laid the groundwork for a collaboration with the University of Milan, aimed at calculating how the average distance between gold clusters varies in a gold/zirconia network under heating. Specifically, the addition of zirconia to the gold nanoparticle network enables the tuning of the thermal response of the film, which we aimed to study quantitatively. By employing two different approaches—one based on the calculation of Euclidean distance (ED) and the other on nearest-neighbour (NN) distance—it was possible to measure the variation in distance distribution at different temperatures and at varying Au/Zr ratios. The results are shown in Fig. 2. In this case, the script binarises the input image and first computes the Euclidean distance map, followed by the ridge map to obtain the local minimum distance at each point along the skeleton. Distance values are then extracted from this map.

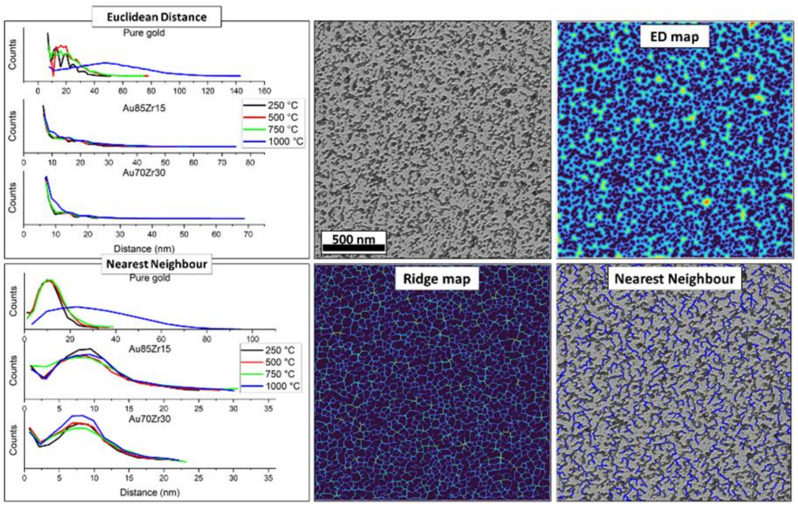

Fig. 2: Distribution of distances at different temperatures and for samples with varying compositions (left). Reference image showing the Euclidean distance map and the ridge map, with an overlay of the distances calculated between nearest neighbours (right).

The nearest-neighbour method, on the other hand, calculates the minimum distance between each pixel on the boundary of a cluster and the boundary of the nearest neighbouring cluster.

Building upon the experience gained from 2D analyses, we analysed multidimensional datasets, with the aim of investigating the optoelectronic properties of nanostructures. This study was carried out using STEM-EELS (Electron Energy Loss Spectroscopy), a technique that provides, for each individual pixel in the scan, a spectrum containing the energy losses of the electrons. The resulting dataset can be represented as a three-dimensional array (X, Y, Energy), containing all the necessary information for characterising the sample. In this specific case, the analysis focuses on the low-loss region, particularly on identifying the band gap value in each spectrum using the first derivative method. All extracted values are then compiled into a map to visually represent the spatial distribution of the band gap (Fig. 3). This method proved especially effective in the presence of interfaces between different materials, as it allows for immediate visualisation of spatial variations in the band gap across the interface.

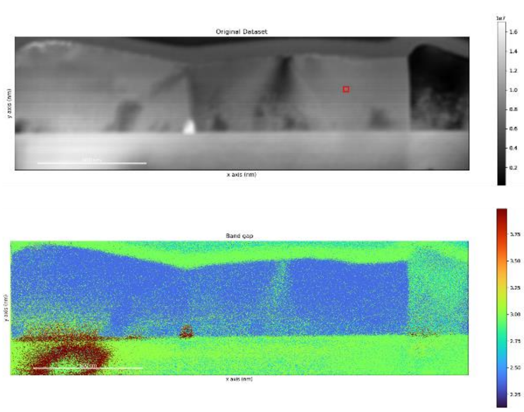

Fig. 3: FIB-lamella of a perovskite (top). Band gap map (bottom).

Towards the end of the first year, the research activity further expanded to include the development of another Python script, this time for the analysis of 4D-STEM datasets. These datasets were acquired with a new experimental setup, these datasets were acquired using a new experimental setup, and the goal of this work was to optimise the analysis pipeline to enable a more detailed study of the crystal structure. This analysis has the potential to reveal strain distributions, particularly in regions involving interfaces between dissimilar materials.

In conclusion, over the course of the year, a comprehensive pipeline has been developed to study nanostructures using electron microscopy techniques. The tools and methods introduced form a strong foundation for advanced analysis. The future goal is to optimise all the processes presented and to implement additional analyses in the fields of optoelectronics and morpho-structural characterisation.

List of publications:

- Casu, A., Melis, C., Divitini, G., Profumo, F., **Lizzano, M**., Borghi, F., ... & Falqui, A. (2025). An In Situ TEM Study of the Diffusivity of Gold Atoms in Nanocomposite Thin Films by Zirconia Co-Deposition: Implication for Neuromorphic Devices. *ACS Applied Nano Materials*, *8*(4), 1762-1772.

List of conferences and summer school:

- QEM 2025 – Quantitative Electron Microscopy 2025, Port Bacares, Francia (poster presentation)
- 17MCM – 17th Multinational Congress on Microscopy, Portoroz, Slovenia (poster presentation)