Machine vision for high throughput analysis of nanoparticles

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INTRODUCTION

Analyzing Transmission Electron Microscopy (TEM) images can be a **time-consuming** and sometimes **non-trivial task**. The ability to identify individual nanostructures is crucial, because it allows for the **efficient processing of large datasets**, often containing tens or hundreds nanocrystals per sample, and for the extraction of valuable information concerning **material composition**. Furthermore, high-throughput methods enable us to gather **statistically significant data**, which are essential for **assessing a methodology**. Machine learning (ML) allows us to perform this type of analysis because it can learn from data and automate the entire workflow.
In this study, my focus was on distinguishing nanostructures (referred to as NCs) from the background using ML and basing on greyscale analysis.

ANALYZED MATERIALS

All-inorganic lead halide perovskite nanocrystals (LHP NCs) exhibit **high photoluminescence quantum yield** (PLQY) and possess a **narrow emission bandwidth** that covers the entire visible spectral range. Moreover, LHP NCs display **exceptional tolerance to surface defects.**

In the work of Manna et al.[1], they aimed to shed light on the CsPbCl3 to CsPbI3 halide **exchange process within nanocrystals (NCs)** by investigating its underlying mechanism and intermediate stages.
However, TEM images captured at various stages of the exchange process, demonstrate that **the reaction has minimal influence on the morphology of the NCs** (figure 1).

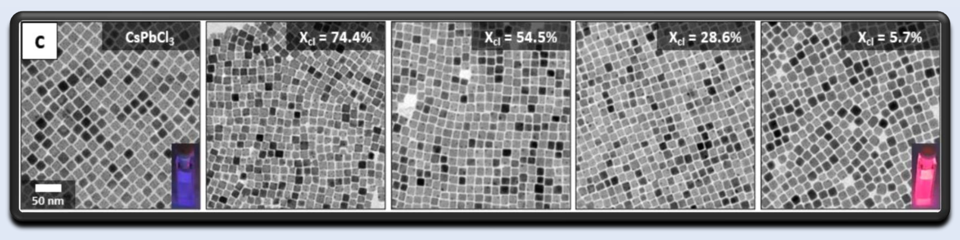


Figure 1. Bright field TEM images collected on NCs

TECHNIQUE USED TO COLLECT DATA

In **scanning transmission electron microscopy (STEM)**, a multitude of signals is available, each providing unique insights into the specimen. A powerful technique known as **high-angle annular dark-field (HAADF)** imaging leverages the high-angle Rutherford-scattered electrons (typically >5°) to reveal compositional contrasts with far greater sensitivity than X-ray imaging[2].

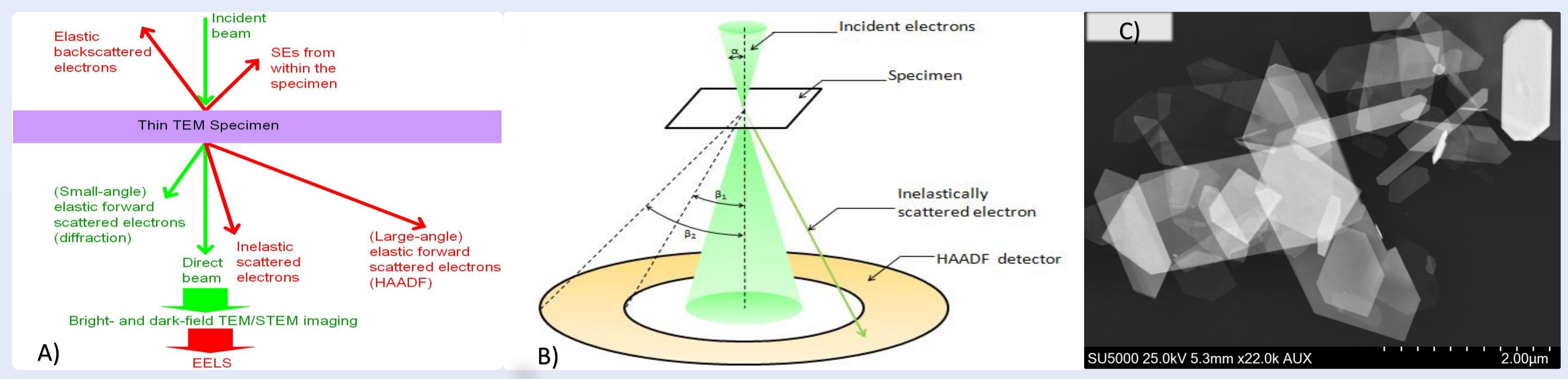


Figure 2.
A) Different types of scattered electrons.
B) HAADF Detector in TEM.
C) Molybdenum Oxide HAADF

MACHINE LEARNING ARCHITECTURE

Convolutional networks (CNN) are typically used for classification tasks, where a single class label is assigned to an entire image.
In this work, I used a modified and extended architecture known as the **"fully convolutional network."** It combines contracting and **upsampling layers** to increase output resolution and enhance localization. The architecture includes many feature channels in the upsampling part to propagate context information to higher-resolution layers, resulting in a **u-shaped architecture** (Figure 3). The network doesn't employ fully connected layers and only uses the valid part of each convolution, ensuring that the segmentation map only contains pixels with full context available in the input image.
My architecture is composed by **four encoding blocks**, each with **two convolution layer** and **one of MaxPooling, one layer of dropout**, and other **four decoding blocks**, analogous to the encoding one.
The activation function for each block is the rectified linear unit (ReLu) and the regularizing factor is 0.01.

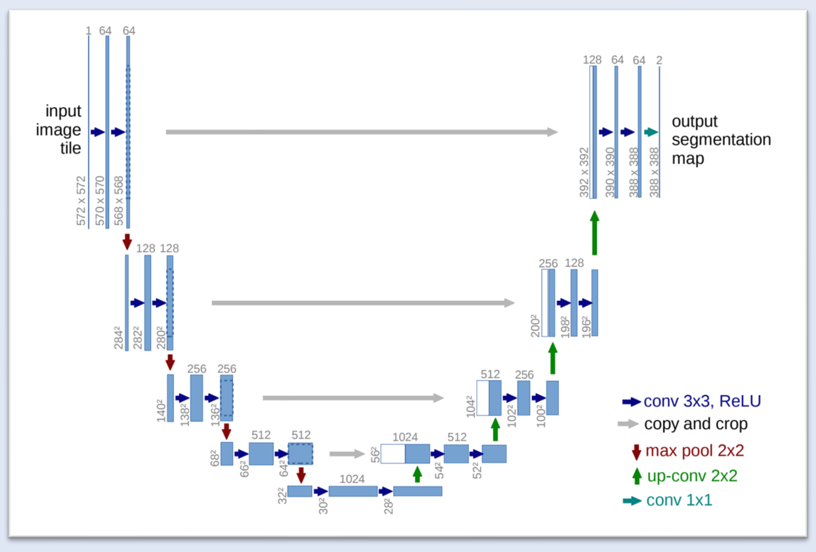


Figure 3. U-Net architecture

WORKFLOW

The initial dataset comprises 1**2 High-angle Annular Dark-field (HAADF) images** of NCs that were previously collected. To increase the number of data available, I rotate some of the picture to obtain a dataset of 22 HAADF images. Since the CNN is space-invariant, this process enhances variability without introducing redundancy. For each image, I generated a **binary mask** using the ImageJ software.

To evaluate the model's performance, I conducted a **K-fold cross-validation** by dividing the dataset into **5 folds** (figure 4).

The model calculates a probability for each pixel in the tested image, indicating the **likelihood that the pixel belongs to a NC** based on its grayscale value. After conducting several experiments, I determined the **optimal threshold** for the probability **within a range of 0.70 to 0.80**, ultimately selecting 0.75 as the threshold. Pixels with a probability exceeding this threshold are classified as belonging to a NC.

Once the model generates the mask, I compared it with the previously generated mask and assessed its performance using the Jaccard Similarity coefficient (figure 5).

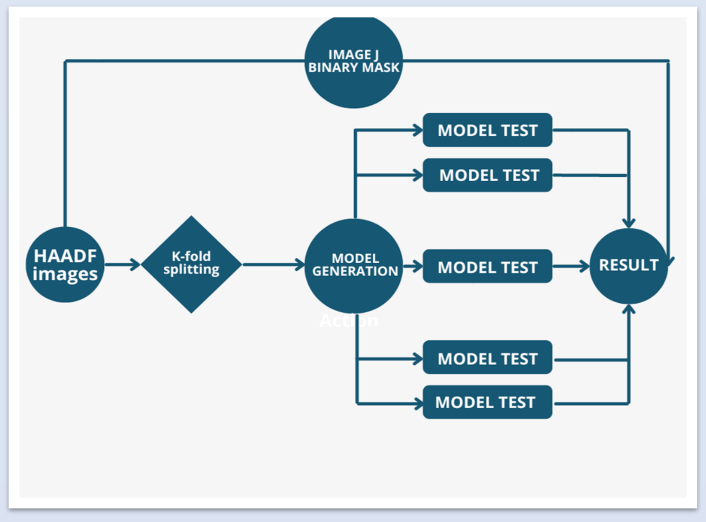


Figure 4. Workflow of the project

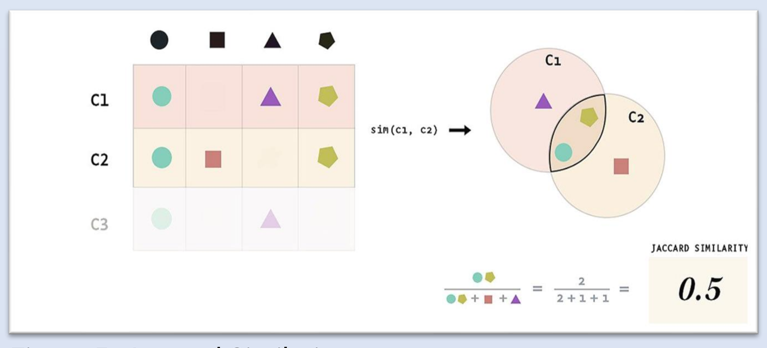
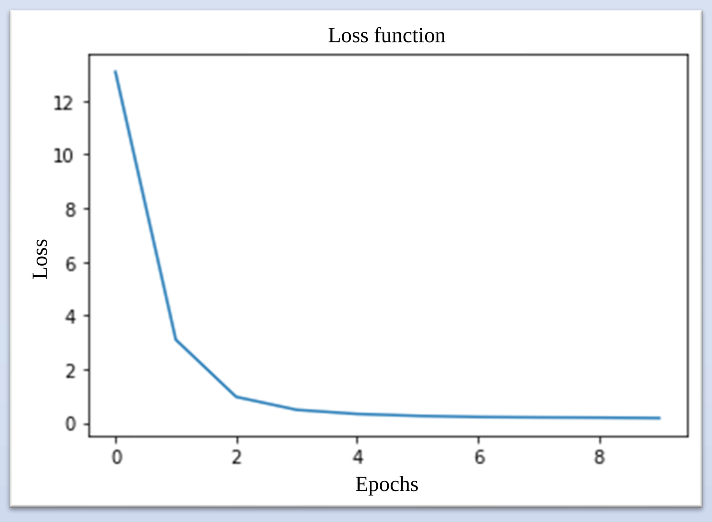
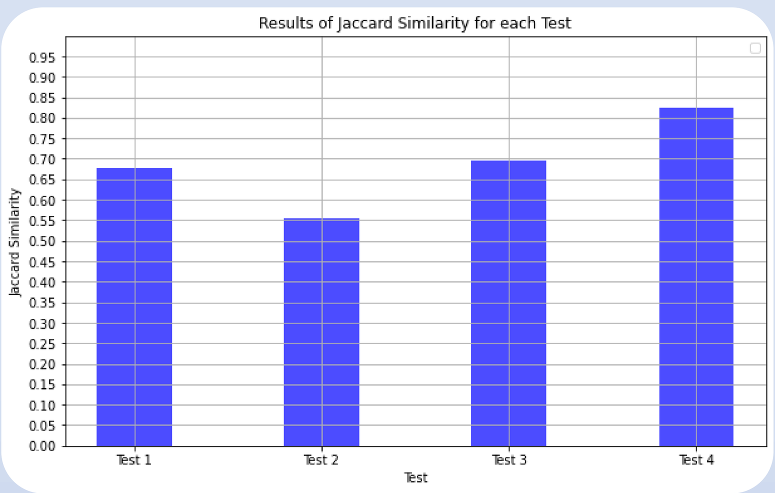
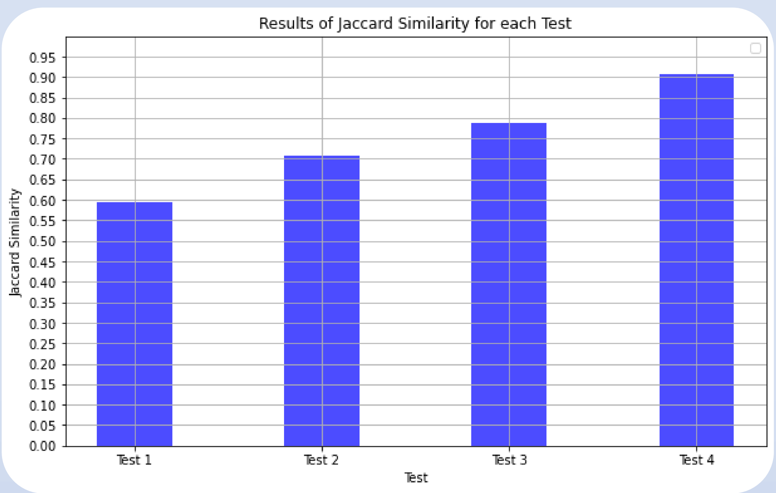


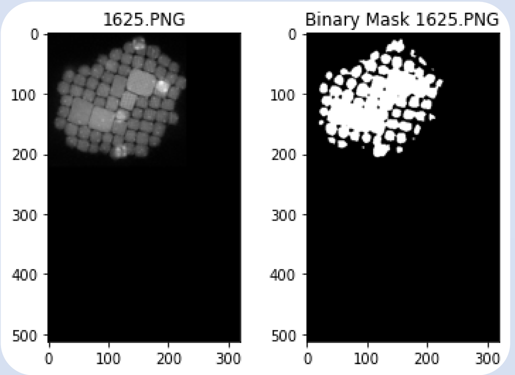
Figure 5. Jaccard Similarity

RESULTS









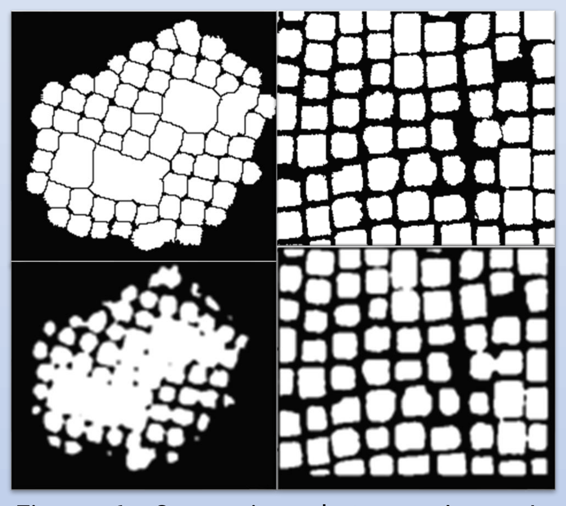
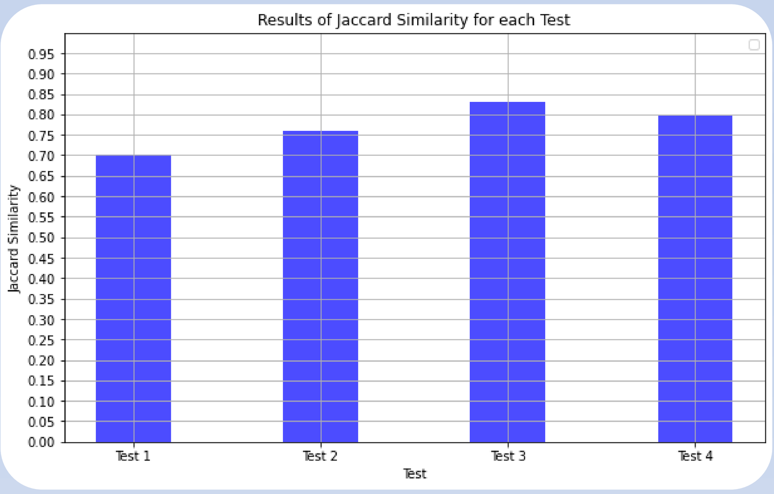
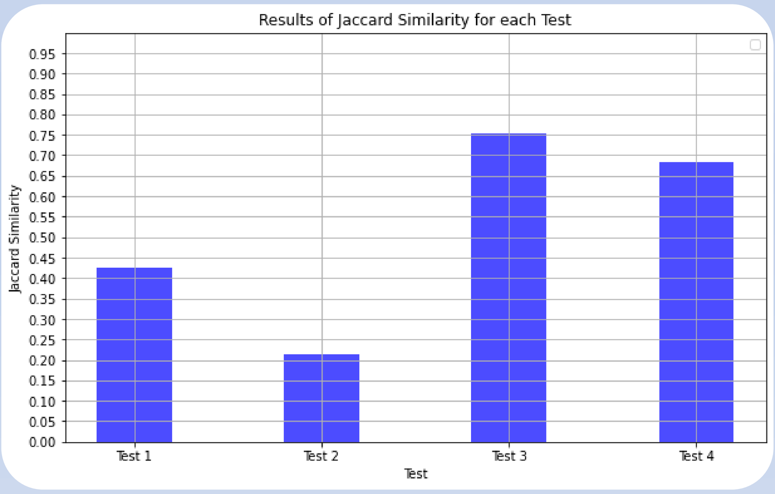
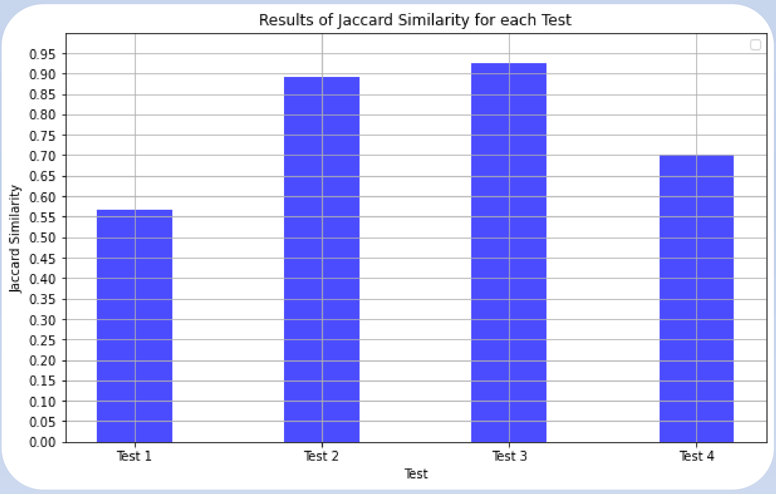
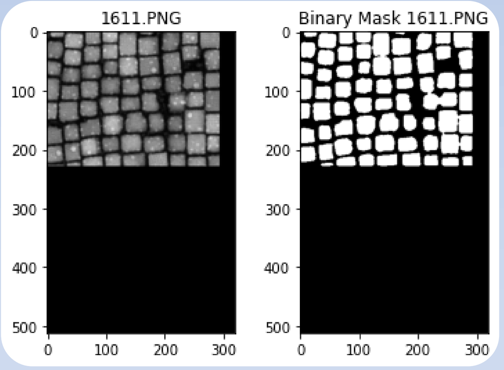


Figure 6. Comparison between ImageJ mask (up) and U-net mask (down)









REFERENCES

1) **Nikolaos Livakasa, b, Stefano Tosoa , Yurii P. Ivanovc , Tisita Dasd , Sudip Chakrabortyd , Giorgio Divitini , Liberato Manna.** $CsPbCl_3 \rightarrow CsPbI_3$ Exchange in Perovskite Nanocrystals Proceeds Through a Jump-the-Gap Reaction Mechanism. *Journal of the American Chemical Society,* 2023
2) **Otten, M.T.**, High-Angle annular dark-field imaging on a tem/stem system. *J. Elec. Microsc. Tech., 17: 221-230.* 1991. https://doi.org/10.1002/jemt.1060170209
3) **Olaf Ronneberger, Philipp Fischer, Thomas Brox.** U-Net: Convolutional Networks for Biomedical Image Segmentation. *MICCAI 2015*
4) **Rasband, W.S.**, ImageJ, *U. S. National Institutes of Health, Bethesda, Maryland, USA, https://imagej.nih.gov/ij/, 1997-2018.*
5) **Jaccard, Paul.** "The Distribution of the Flora in the Alpine Zone.1". *New Phytologist.* 11 (2): 37–50. February 1912.
6) **DEBEN website**, HAADF Annular SEM STEM detector, https://deben.co.uk/sem-detector/haadf-annular-sem-stem-detector/