Unlocking 3D Nanoparticle Shapes from 2D HRTEM images: classification and denoising at atomic resolution

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Nanoparticles (NPs) are typically observed and analysed using High Resolution Transmission Electron Microscopy (HRTEM) for highly precise structural studies at the atomic scale. However, determining their 3D shapes from 2D HRTEM images is a tedious process. Indeed, this type of analysis is based on manual post-processing which suffers, among other issues, from experimental noise. To tackle this issue, we develop a Deep Learning (DL) model to automate this task ensuring reliable statistical analysis of a large number of NPs.

In this context, we extend an approach we had developed to identify the structure of carbon nanotubes from their Moiré patterns obtained from HRTEM images [1]. More precisely, the DL model, leveraging Convolutional Neural Networks (CNNs), is trained on datasets of simulated HRTEM images of NPs, labelled according to their shapes, ranging from 4 to 8 nm. A critical point of this study was generating a representative and optimised dataset. To accomplish this, we constructed atomistic 3D models of NPs deposited on an amorphous carbon substrate, subjecting NPs to random rotations to encompass all potential observed orientations. Furthermore, we simulated the amorphous substrate using realistic carbon membrane and noise models, to mimic experimental conditions [2]. Finally, HRTEM images were simulated using the Dr Probe code [3] based on the multi-slice method with parameters consistent with aberration-corrected transmission electron microscopes. The objective of generating an optimal training dataset was attained through comprehensive studies evaluating the impact of various parameters, including amorphous carbon, resolution, focusing conditions, NPs' size, and NPs' orientations, on DL model predictive accuracy (see Figure 1).

However, when the contrast between the investigated nanoparticles and the substrate is highly degraded, performances may drop. Hence, we are training a Deep Learning (DL) model to automatically restore best nanoparticle-substrate contrast on acquired images. To this end a UNet-like model [4] has been trained on our simulated dataset with patches procedure [5]. By applying our DL model, we have exhibited promising outcomes: across various regions of simulated HRTEM images under different defocusing conditions, the model demonstrates an ability to generate contrast close to the best achievable (ground truth) as seen in Figure 1.

This approach has resulted in the development of an efficient and accurate DL framework for predicting 3D NP shapes from 2D HRTEM images, validated across both simulated and experimental datasets.

References

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Figures

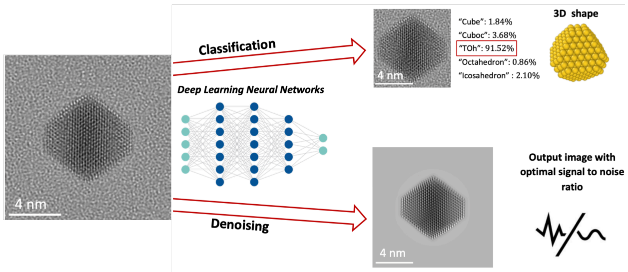

Figure 1. Performance of our classification and denoising models to predict 3D shapes of Au nanoparticles on amorphous carbon substrate.