Unlocking 3D Nanoparticle Shapes from 2D HRTEM images: A Deep Learning Breakthrough

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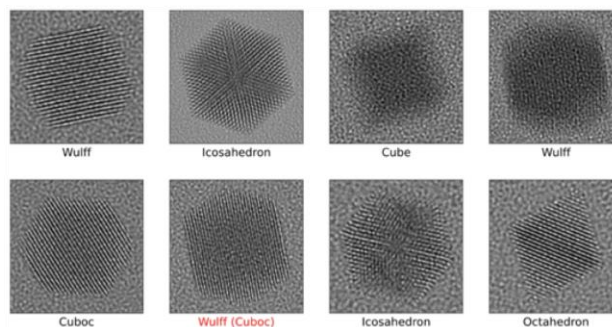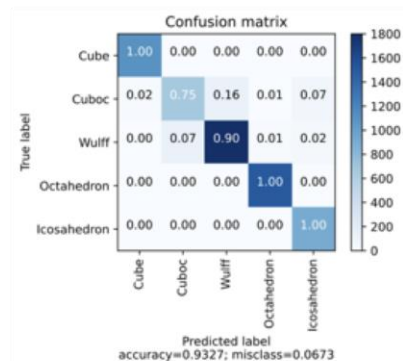
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Nanoparticles (NPs) are typically observed and analysed using High Resolution Transmission Electron Microscopy (HRTEM) for highly precise structural studies at the atomic scale. However, determining their 3D shapes from 2D HRTEM images is a tedious 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.

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.

Figure 1. (Top) Performance of the model (confusion matrix) trained with around 45 000 images for classifying five different shapes of NP. (Bottom) Examples of 3D shape predictions on simulated TEM images.

References

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