Unlocking 3D nanoparticle shapes from 2D HRTEM images: a Deep Learning breakthrough

Romain Moreau[1], Dr. Hakim Amara[1], Dr. Maxime Moreaud[2], Dr. Jaysen Nelayah[3], Mr. Adrien Moncomble[3], Dr. Damien Alloyeau[3], Pr. Christian Ricolleau[3], Dr. Riccardo Gatti[1]
[1]Université Paris-Saclay, ONERA, CNRS, Laboratoire d'Études des Microstructures, Châtillon, France, [2]IFP Énergies Nouvelles, Solaize, France, [3]Université Paris Cité, CNRS, Laboratoire Matériaux et Phénomènes Quantiques (MPQ), Paris, France

Background incl. aims

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 or human bias performed at post-experimental stage. In this context, the integration of artificial intelligence (AI) methodologies into data acquisition and analysis protocols is a very promising approach [1]. To tackle the problem of identifying the 3D shape of NPs, we developed a Deep Learning (DL) model to automate this task ensuring reliable statistical analysis of a large number of NPs many of which cannot be identified by conventional methods.

Methods

For this purpose, we extend an approach we had developed to identify the structure of carbon nanotubes from their Moiré patterns obtained from HRTEM images [2]. 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 derived from a tight-binding framework and noise models, to mimic experimental conditions [3]. Finally, HRTEM images were simulated using the Dr Probe code [4] based on the multi-slice method with parameters consistent with aberration-corrected transmission electron microscopes.

Results
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.
Conclusion
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 (see figure).

Graphic:

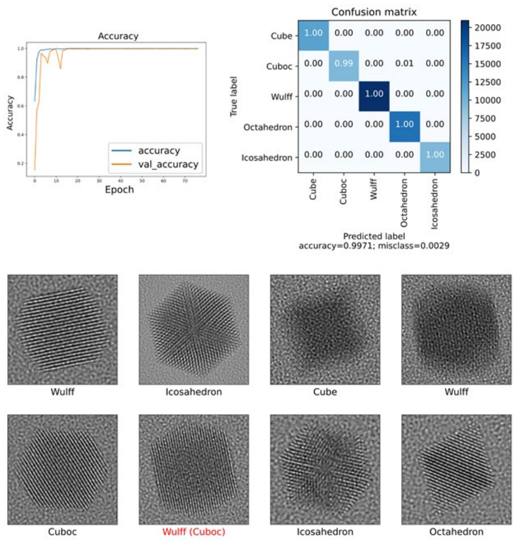

Figure. (Top) Performance of the model (confusion matrix) trained with around 45 000 images for classifying five different shapes of NP. (Bottom) Examples of 3D shape predictions on simulated TEM images with one error (in red).

Keywords:

DL; nanoparticle; TEM; atomistic simulation

Reference:

[1] S. R. Spurgeon et al., Nat. Mater. 20, 274 (2021)
[2] G. D. Förster et al., Carbon 169, 465 (2020)
[3] C. Ricolleau et al., J. Appl. Phys. 114, 213504 (2013)
[4] J. Barthel, Ultramicroscopy 193, 1 (2018)