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3D atomic-resolution imaging of nanomaterials based on exit wave reconstruction

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Breakthroughs in transmission electron microscopy (TEM) have opened for visualizing nanomaterials with atomic resolution and uncovering the surface terminations that are governing e.g. catalytic properties. In a TEM experiment, the most informative outcome is the recovery of the electron wave function exiting the nanomaterial. While different experimental and mathematical reconstruction schemes exist to recover the underlying exit wave, the transformation of exit waves into a three-dimensional (3D) structural model is still being debated. Recently, our group presented an analytical model to describe the 3D atomic-scale arrangement in an excited 2-dimensional Co-Mo-S nanocrystal [1]. The model was based on channeling theory and made for the first time use of the full shapes of the atomic columns in the exit wave. Extending this model to an arbitrary 3D nanomaterial is challenged by the role of extinction distance in relation to the sample thickness as well as the irregular surface both at entrance and exit of the nanomaterial. Here, we will outline the development of this analytical approach to investigate arbitrary nanomaterials at 3D atomic-resolution.

We examine nanometer-sized metal nanoparticles with a focus on their terminating surface structure. The exit waves are reconstructed from experimental focal series of bright-field TEM images, which carries most signal pr. electron. This is vital for investigating surfaces of nanomaterials since under coordinated atoms at the surface are particularly prone to beam-induced alteration compared to the bulk. Imaging is therefore done with low electron dose rates using direct electron detectors (DED) to establish sufficient SNR for the reconstruction while maintaining the pristine structure of the material.

With the complex exit wave, we use the channeling approaches in [1,2] to determine the 3D atomic position and stoichiometry of atomic columns of a carbon supported Pt nanoparticle with a diameter of 5 nm. We present a strategy to counteract the influence of extinction and show how this drastically reduces the elongation of the 3D tomogram along the beam direction. Furthermore, we also present a strategy for the non-uniform entrance and exit surface of the nanoparticles.

In this work, we present an approach to reconstruct 3D structural information about nanoparticles from electron wave functions exiting the sample. Based on channeling theory, an analytical model is outlined to establish the location and stoichiometry of the atomic columns and approaches to counterbalance the role of extinction and irregular entrance and exit plane surfaces are demonstrated. The present work therefore build a foundation to recover a 3D atomic model of a nanoparticle and thereby uncover its exposed surface structure. The present approach should be generally applicable to any nanomaterial even under exposure to reactive environments and should thus aid the understanding of gas-surface interaction is diverse fields such as crystal growth, corrosion, and catalysis.

Keywords:

Holography, exit waves, 3D atomic-resolution

Reference:

[1] Chen, F. R., Van Dyck, D., Kisielowski, C., Hansen, L. P., Barton, B., & Helveg, S. (2021). Probing atom dynamics of excited Co-Mo-S nanocrystals in 3D. Nature communications, 12(1), 5007.
[2] Chen, F. R., Van Dyck, D., & Kisielowski, C. (2016). In-line three-dimensional holography of nanocrystalline objects at atomic resolution. Nature communications, 7(1), 10603.
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