Measuring the Interpretability of High-Resolution Transmission Electron Microscopy Images

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Background

Nanoparticles find uses in a plethora of applications ranging from food preservation and pharmacology to industrial catalysts. Obviously, the first question which is asked when it comes to nanoparticles is the size. However, several aspects of nanoparticles dictate their shape and function. This includes morphology, chemistry, crystallography, oxidation state and environment.

When it comes to providing answers on these topics, transmission electron microscopy (TEM) has been the go-to tool. Modern microscopes easily provide answers on all these topics. However, there are three main challenges. 1) the structure of nanoparticles is not always unaffected by the exposure to high-energy electron beams; 2) to provide statistically relevant information, a large number of nanoparticles should be analyzed; 3) the environment inside the TEM is most often not the same as that where the nanoparticles are used. To accommodate the beam sensitivity, we can lower the electron dose rate to levels where the effect is negligible or otherwise easy to accommodate for. To improve the statistical significance, we can count large numbers of particles and use automated data analysis approaches. Lastly, to image the particles under realistic conditions, we can control the environment in which we image them.

Methods

Here we use environmental transmission electron microscopy to monitor the size, shape and dynamics of nanoparticles relevant for catalytic applications. We focus particularly on gold nanoparticles on cerium dioxide which catalyzes the oxidation of carbon monoxide. Using a CMOS based OneView camera from Gatan, we have acquired data series at varying electron dose rate and under different environments. Using these datasets, we evaluate the signal to noise ratio (SNR) based on different models. Furthermore, we estimate the usability of the structure similarity index measure (SSIM) to detect structural changes of the gold nanoparticles and how prefiltering and adjusting can help our data analysis. We compare these results to measurements performed using data analysis by convolutional neural networks trained on simulated data [1, 2].

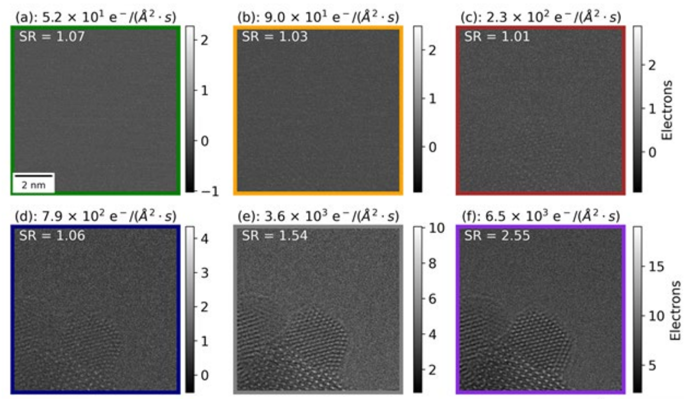
Results

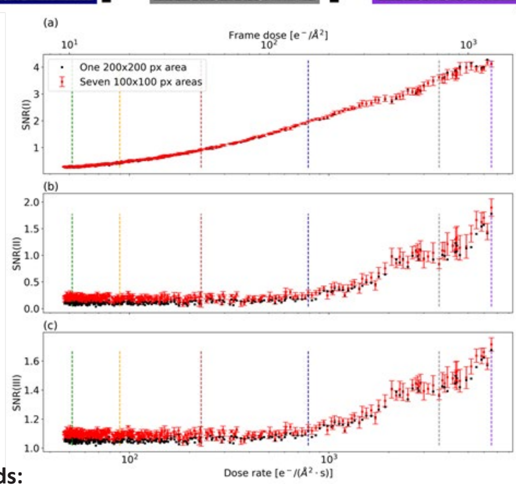
Using three models of the signal-to-noise ratio we estimate the interpretability of HRTEM images and rate the measured SNR against the output of data analysis based on convolutional neural networks. SNR(I) is the traditional method of calculating SNR. SNR(II) uses the standard deviation of the nanoparticle and background region separately. SNR(III) takes the high intensity variation of phase contrast images into account. Figure 1 top pane shows images extracted from sequence acquired at increasing dose rate. The bottom pane shows the SNR calculated based on different models showing data from the entire image series. We have further pursued the analysis of Au nanoparticle structure as a function of the environment.

Conclusion

Determining the SNR of an image can tell us something about the interpretability and if it makes statistical sense to continue a more thorough analysis. Here we have attempted alternatives to the traditional method of determining SNR which may not be well-suited to estimate the interpretability of HRTEM images. We have correlated this with data analysis based on convolutional neural networks.

Graphic:





Keywords:

Nanopareticles, TEM, Interpretability, Low-dose

Reference:

1. Madsen, J., et al., A Deep Learning Approach to Identify Local Structures in Atomic-Resolution Transmission Electron Microscopy Images. Advanced Theory and Simulations, 2018. 1(8): p. 12.

2. Leth Larsen, M.H., et al., Quantifying noise limitations of neural network segmentations in high-resolution transmission electron microscopy. Ultramicroscopy, 2023. 253: p. 113803.