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Large-scale Automated Analysis of High-Resolution Transmission Electron Microscopy Data Assisted by Deep Learning Neural Networks

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Large-scale analysis of High-Resolution Transmission Electron Microscopy (HR-TEM) data can be a cumbersome task. To minimise irreversible damage to the sample, electron dose-rates are often kept low resulting in images with low signal-to-noise ratios, which can be challenging to interpret. This is an area where machine learning can step in to assist the process.

Here we will report advancements on the tailoring of deep learning neural networks for fast detection of nanoparticles and atomic columns. This concept has previously been demonstrated for tracking gold atoms in HR-TEM image sequences [1] with an industry standard U-net architecture [2]. In this work, a less common network architecture known as the Mixed-Scale Dense (MSD)-net [3] has been trained on large datasets of simulated HR-TEM data, labelled with pixel-level accuracy, to solve various segmentation tasks.

Nanoparticle segmentation involves differentiating regions in images where a nanoparticle of interest is present relative to other features. In Figure 1, this is shown to be possible even at low dose-rates where nanoparticle identification becomes difficult for the human interpreter. The performance of the network in the low dose-rate regime is optimised by carefully fitting the modulation transfer function (MTF) of the microscope's detector using images of vacuum regions and applying the fitted parameters to the MTF of the simulated data.

The network inference can be used to crop the image in real space, from which the Fourier domain of just the nanoparticle can be obtained. This facilitates an automation of nanoparticle information extraction at low dose-rates. Figure 2 illustrates how this can be used to map information from the Fourier domain to a real space image, where multiple nanoparticles are segmented with pixel-level accuracy consistently over many frames. The ratio between the brightest pair of symmetric peaks to the dimmest pair of symmetric peaks in the Fourier domain is used to scale the network inference to identify nanoparticles oriented along a zone axis, where their atomic columns can be resolved.

The concept of using the brightness ratio between symmetric pairs of peaks in the Fourier domain is also applied to filter out uninterpretable frames of nanoparticles in a dataset consisting of several thousands of frames. A frame is deemed uninterpretable by a brightness ratio threshold that highlights a nanoparticle where atomic columns are ill-resolved. The remaining frames with a sufficient nanoparticle alignment are then further analysed using atomic column segmentation to count diffusion events as a function of time. The neural network assists in data selection and atomic column counting in large scale data analysis.

In addition to nanoparticle segmentation, we also present a network capable of distinguishing between atomic species in HR-TEM images of multi-component material samples purely based on phase contrast. This is achieved by feeding the network a focal series of images i.e., three images are simulated at three different defocus settings for each atomic structure in the dataset. As an example, given three images of an MoS₂ sample at three different defocus settings, the neural network can differentiate between atomic columns consisting of either 1 molybdenum, 2 sulphur, or 1 sulphur atom.

This is applied to experimental data of suspended monolayer MoS₂ to count the number of sulphur vacancies present in each frame. Utilising this in HR-TEM allows for a time resolution not achievable with other imaging modes. This makes it especially suited to *in situ* experiments, where it can provide insight into dynamic events such as defect formation, diffusion, and phase transition in real time.

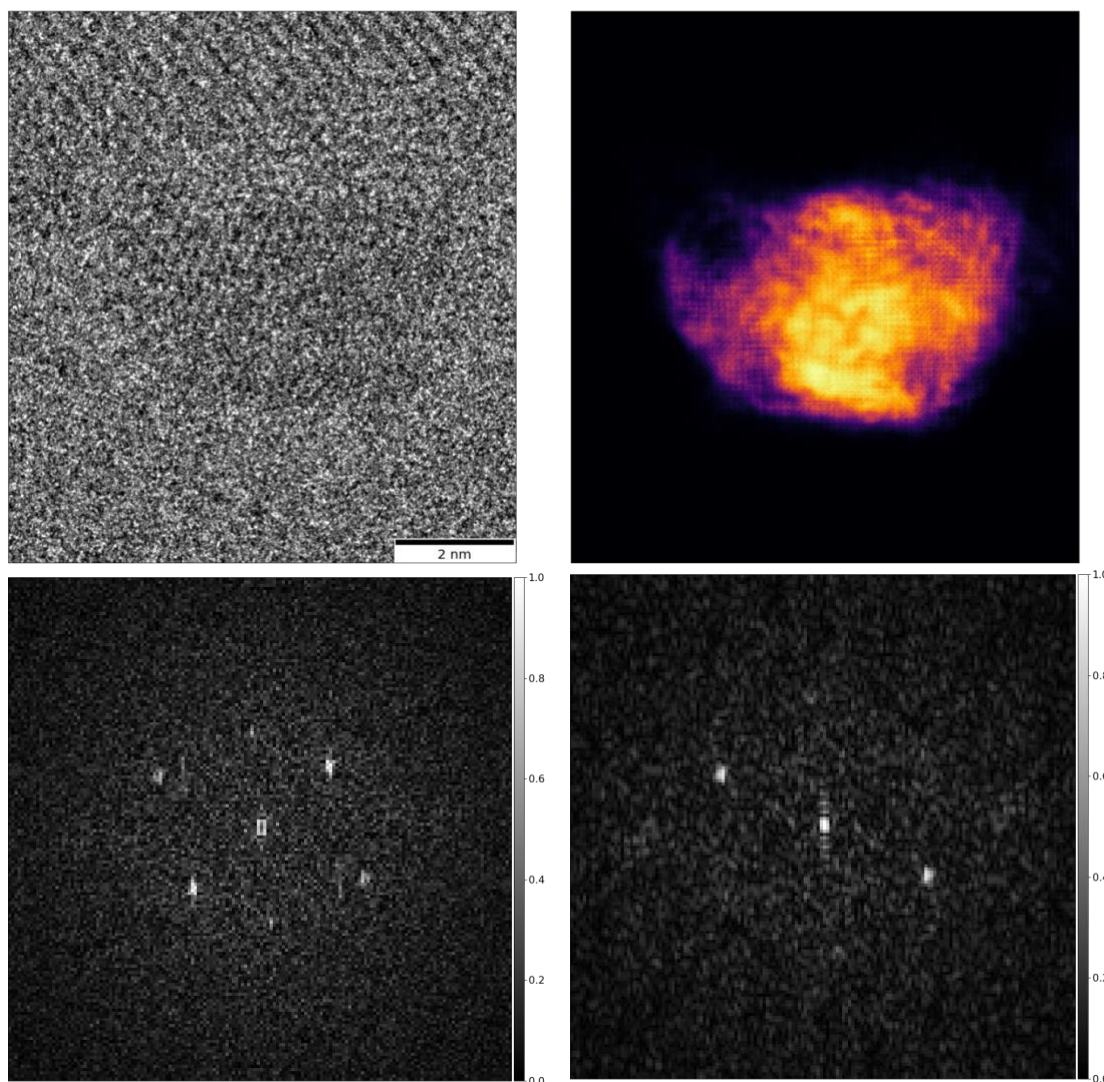


Figure 1. Upper left: HR-TEM image. Upper right: Network Inference of image (upper left). Lower left: Fourier domain of image (upper left). Lower right: The network inference (upper right) is used as a mask to crop out the nanoparticle in the HR-TEM image (upper left). This is the Fourier domain of the cropped-out region, which highlights peaks corresponding to the nanoparticle and filters out peaks related to the substrate and other features in the image.

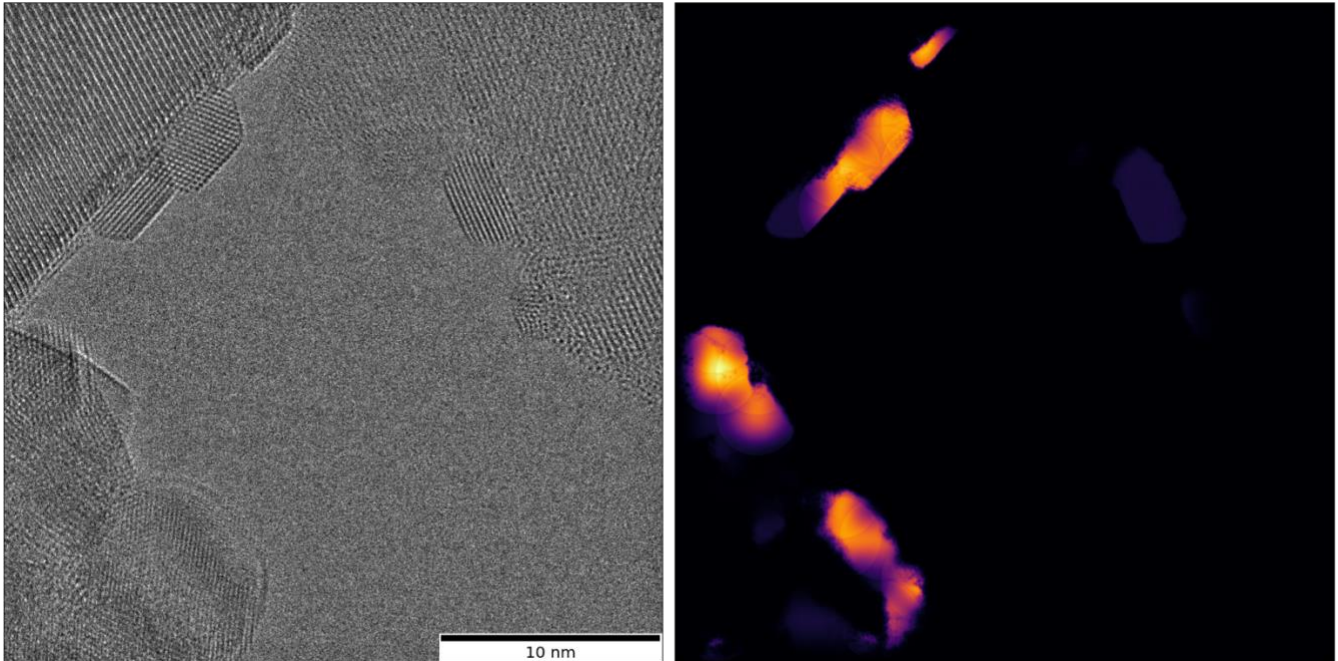


Figure 2. Left: Large HR-TEM image with multiple nanoparticles. Right: Network inference scaled by the ratio between the brightest and dimmest Fourier peaks corresponding to the nanoparticle. The image consists of 4096x4096 pixels and thus the segmentation is carried out in windows across the image to have spatial information and avoid memory limitations. Hamming filters are applied to each window to smoothen out borders. This does not alter the shape of the network inference, only the value.

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