Using Neural Networks to Identify Atoms in HRTEM Images

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We have developed a methodology, where deep convolutional neural networks can be used to identify local structures in high resolution transmission electron microscopy (HRTEM) images. The methods are available as Python modules under an open source license [1, 2].

While conventional image processing and peak finding algorithms can be used to pinpoint the position of the atoms (within the uncertainty due to imaging effects) [3], the fact that contrast varies from image to image, and sometimes even inverts within a single micrograph makes such methods difficult to use. A neural network can act as an advanced filter, giving a clean signal for peak detection.

In most cases, using machine learning (ML) for image analysis is limited by the availability of high-quality pre-analyzed images that can be used for training the ML methods; acquiring the training data can be both time-consuming and expensive. In this case, we are in the fortunate situation that atomic-resolution HRTEM images can be reliably simulated, providing the training data at low cost. We have shown that it is possible to reliably identify the positions of the atoms in experimental micrographs of single sheets of defected graphene, and the atomic columns in micrographs of metallic nanoparticles, even when the signal-to-noise ratio is low due to the desire to limit beam exposure [3].

While a single HRTEM image contains sufficient information for the neural net to identify the positions of the atoms, more information can be extracted from a focal series. We have demonstrated, albeit in simulations only, that a set of three images taken at different defocus is sufficient to identify chemical species and vacancies in single sheets of molybdenum disulfide, and to count the number of atoms in atomic columns in gold nanoparticles [1], which has until now only been possible with STEM.

In conclusion, we find that deep learning is a promising tool within electron microscopy, which may both accelerate analysis of large amounts of microscopy data and enable analyses that would not otherwise be possible, such as counting the height of atomic columns in HRTEM images.

[1] J. Madsen et al., *Adv. Theory Simul.* **1**, 1800037 (2018).
[2] J. Schiøtz et al., *https://gitlab.com/schiotz/NeuralNetwork_HRTEM* - (2019).
[3] J. Madsen et al., *Adv. Struct. Chem. Imag.* **3**, 14 (2017).