FFT denoising methodology through CNN for the study of WS2 vacancies

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2D materials as WS2 have become increasingly relevant and widely studied in recent years due to their electronic and optical applications [1]. One of the most effective techniques for characterizing these materials and studying their physical properties is High-Angle Annular Dark-Field (HAADF) imaging in a Scanning Transmission Electron Microscope (STEM). On the other hand, to study lighter atoms it is common to use Integrated Differential Phase Contrast (iDPC) STEM. These techniques allow researchers to study the crystallography of the material to determine the presence of defects.

These images often contain noise that poses a challenge when studying vacancies. Consequently, we developed an FFT denoising technique employing a Convolutional Neural Network (CNN) with a U-NET architecture [2, 3]. The CNN was trained using more than 5000 simulated spectra from diverse materials and various orientations. After FFT denoising, we could perform an inverse FFT (IFFT) to return to real space. This results in a significantly cleaner image, rendering crystallographic analysis more accessible, as atomic positions become much more discernible. Conversely, the FFT denoising method leads to the emergence of ‘fake atoms' in locations where vacancies should exist. While this outcome may initially appear counterproductive, it was, in fact, the crucial element that enabled the execution of this study. In this way, by subtracting the original experimental HAADF-STEM image from the filtered one, we obtain a new images where the bright spots correspond to the atomic vacancies

(Figure 1).
In conclusion, the methodology employed in this study has enabled a statistically significant analysis of vacancies across multiple images. Each image has been subjected to a detailed examination of more than 3000 atomic positions, yielding robust and reliable results. This approach not only provides a profound understanding of vacancy distribution but also gives the way for automating the statistical analysis of vast amounts of images within short timeframes. This potential for automation not only enhances process efficiency but also holds promise for accelerating the pace of discovery and understanding in research fields reliant on atomic-scale image analysis.

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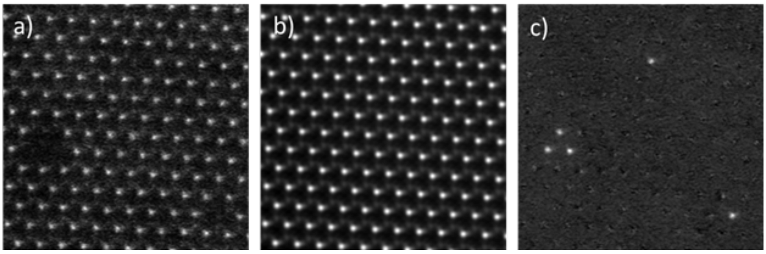
Graphic:



Keywords:

CNN, FFT, iDPC, HAADF-STEM, vacancies

Reference:

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