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Autonomous Detection and Identification of Defects in Nanoscale Devices using Electron Diffraction Imaging

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Transmission electron microscopy (TEM) offers a unique combination of superior spatial resolution and highly sensitive elemental analysis capabilities that has seen increasing demands in the advancement of materials for technologies. The need for the analysis of individual dopants and defects especially stands out in quantum materials where controlling defects and strain plays an important role in realizing the quantum entanglement. For example, control of local lattice perturbations near optically-active defects in semiconductors is a key step to harnessing the potential of solid-state qubits for quantum information science and nanoscale sensing [1]. While traditional defect analysis was carried out using various contrast mechanisms at nm and sub-nm spatial resolution, advances in aberration corrected (scanning) transmission electron microscopy ((S)TEM) has made possible for imaging individual atoms in a broad range of two-dimensional (2D) quantum materials and has renewed the interest in the defect analysis in semiconductors using high resolution electron microscopy [2]. Determining atomistic structure from a projection electron image, however, requires image interpretation. This can be relatively simple in the case of Z-contrast STEM of 2D materials or highly involved in the study of three-dimensional (3D) defects. Considerable efforts have been taken recently in developing machine-learning (ML) based strategies for image segmentation and classification aiming at autonomous defect analysis [3]. The success of these atomic resolution imaging-based approaches, however, is fundamentally limited by the very-thin sample requirement and the type of defects that can be imaged.

An emergent solution is electron diffraction imaging [4]. By collecting a large diffraction pattern (DP) dataset in a STEM for every probe position using scanning electron nanodiffraction (SEND) or four-dimensional STEM (4D-STEM) techniques, the structure of materials can be interrogated at multiple levels. For example, at Å scale, ptychography achieves the spatial resolution near the diffraction information limit. At nm scale, orientation and strain mapping provides critical information about lattice rotation and deformation in the presence of defects and interfaces. A much less explored part of electron diffraction is diffuse scattering, which can provide information about local disorder, from short-range order (SRO) to the presence of dislocations and stacking faults. However, electron diffuse scattering presents weak signals and complex patterns; the combination of these two factors has prevented the broad use of electron diffuse scattering for materials characterization.

Manually identifying defects from the collected large DP datasets is impractical for multiple reasons. Chief among them is the size of the DP dataset can easily reach 10^5 for a scan over several minutes using the latest fast electron detectors. Even in the case of a small scan, manual identification and analysis of DPs are still problematic. Thus, automated DP analysis is essential to unlock the potential of SEND or 4D-STEM analysis. Automation could significantly reduce the analysis time as well. Along this direction, the abilities of ML, including deep learning, using artificial neural networks (ANNs) present exciting opportunities for the analysis automation and augmentation of DPs. In computer vision, deep learning has been used to solve difficult problems, such as image classification, segmentation and

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detection [5]. In electron microscopy, deep learning has been proposed and demonstrated for an arrange of applications related to image and DP analysis, for example, see Ref. [3].

Here, we report on a deep learning framework to locate and differentiate different types of defects in a SEND experiment automatically (Fig. 1). The main idea of this heuristic approach is that different types of defects create different diffuse scattering patterns, which can be captured by electron diffraction and used to locate and identify defects with the specificity of the electron probe size, which is about 1 nm or smaller. To test this idea, we built a convolutional neural network (CNN) and applied to a FinFET devices to local and identify defects, including hidden defects, based on the detected diffuse scattering in electron DPs (Fig. 2). The capability of this approach will be further demonstrated in this talk [6].

Figure 1. Training of CNN for defect identification. Labelled diffraction patterns are used as input.

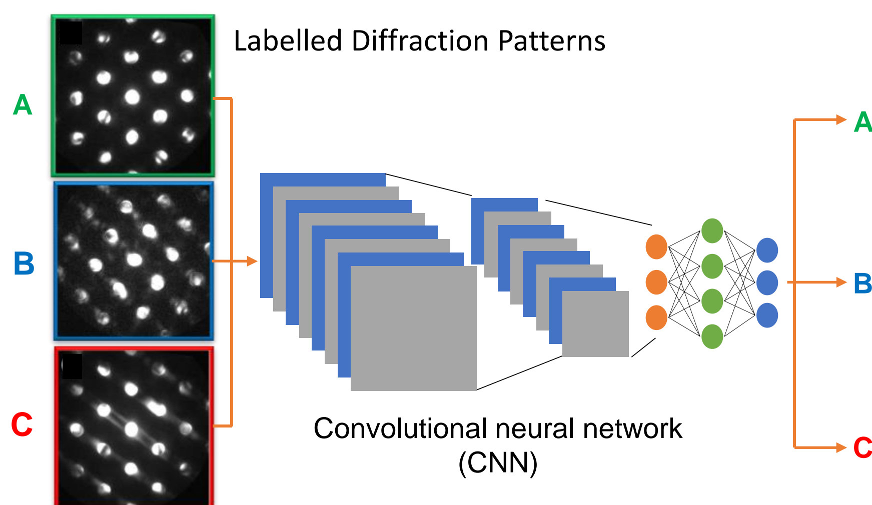
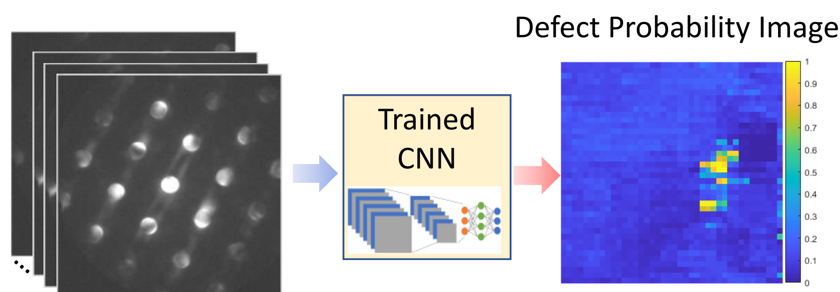


Figure 2. Application of trained CNN to a SEND data set produce the defect probabilty image. The ouput is a defect probability map.



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