Automated defect recognition in two-dimensional materials from low-dose ultrafast HRTEM image series using deep neural networks

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Image processing techniques have significantly advanced in their capability for the analysis of electron microscopic data of various types. However, for the majority of the existing image processing procedures significant human interaction is still required. This not only implies subjectivity, but also puts a hard restriction on the scalability of data processing in some important areas, in particular in areas where the collection of large image series is routine.

In this paper we present two automated solutions, both free from human intervention, for two-dimensional material defect recognition as an exemplar scientific case. The results from this analysis have enabled us to extract local chemical kinetic information from image series of defect formation, migration, transformation recorded at kHz framerates using a direct counting electron detector.

The first method makes use of the geometric properties of the graphene lattice. Each 6 member carbon ring in the graphene lattice has six nearest neighbor rings while defective rings (e.g. 5 and 7 member rings) will have the a number of nearest neighbour rings equal to the number of carbon atoms in the ring. Hence, the identification of defects can be carried out by an automated algorithm that counts the number of nearest neighbour rings at each position.

The second method is based on a deep neural network [1] which performs atomic model abstraction from experimental graphene images. Although the training of such neural networks requires significantly more effort than the classical image processing approach, this method is more general and can readily be extended to studied of other two-dimensional materials.

Figure 1 shows a single image frame extracted from a low dose series of HRTEM images of graphene recorded at kHz framerates (a) before and (b) after defect recognition processing. The defects in the image are accurately identified by the algorithms, even when the signal-to-noise ratio is low due to limited dose and short exposure times. Using this approach large image datasets can be mined for to measure the evolution of defect structures with time giving direct insights into the kinetics of the defect formation processes.

References:
[1] Y LeCun, et. al, *Nature* **2015** (521), 436 - 444

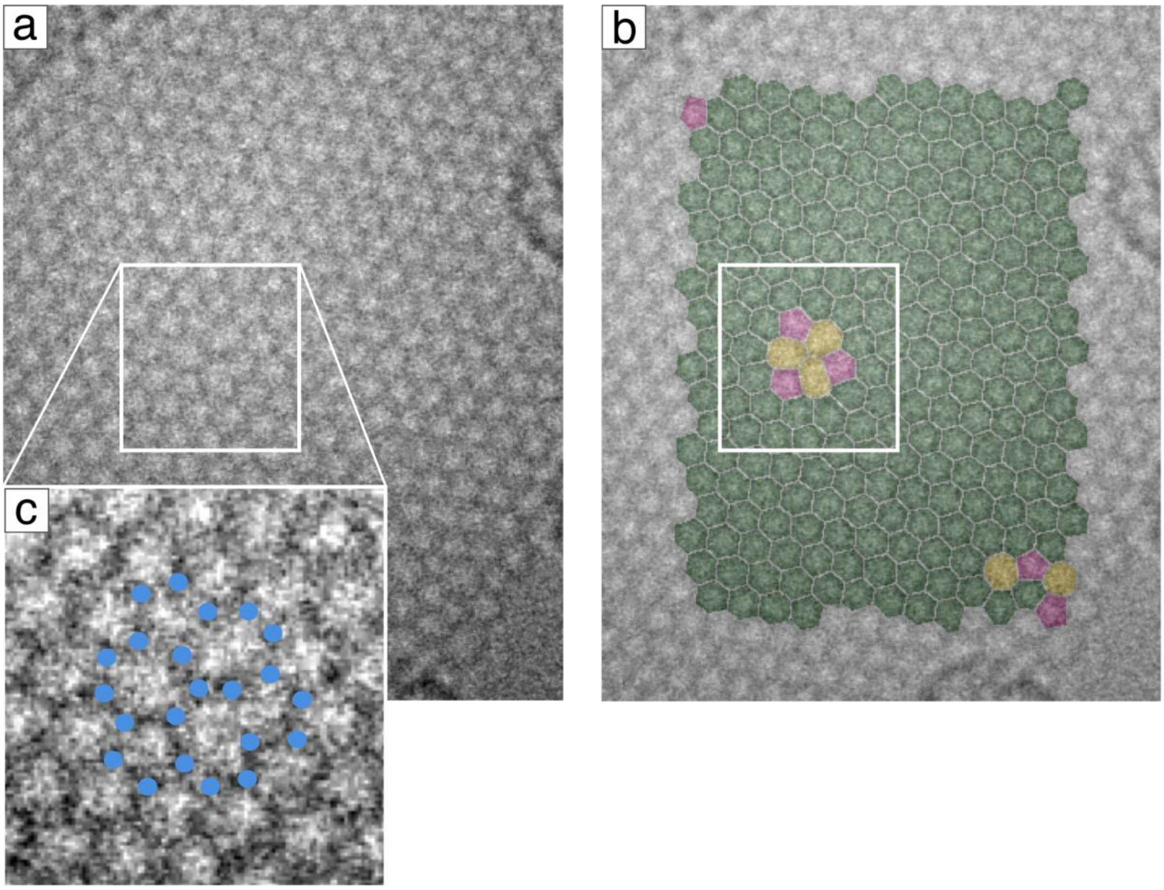

Figure 1. (a) Low-dose image of a graphene sheet recorded with a 50ms exposure at 80KV containing defects; (b) Automatically generated annotation with 5-membered rings (pink), 6-membered rings (green), and 7-membered rings (yellow) overlaid on top of the experimental image; (c) enlarged defect area with carbon atom positions marked by blue circles.