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4D-STEM Optical Sectioning of Dopants in Diamond

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Due to improvements of aberration correctors in scanning transmission electron microscopes (STEM), larger convergent semi-angles can be used as more of the probe can be collected without introducing aberrations to the image. These larger convergent semi-angles lead to two notable improvements in the reconstructed image; an improved lateral resolution and a reduced depth of field [1]. The benefits of a better lateral resolution are immediately obvious, but by reducing the depth of field, new methods of imaging can be obtained, namely optical sectioning [2]. Optical sectioning involves collecting many micrographs of a sample with varying defocus which allows for investigation into the third dimension of the material instead of the two lateral dimensions as in conventional STEM. Four dimensional scanning transmission electron microscopy (4D-STEM) builds on conventional STEM by using superfast pixelated detectors to collect the entire diffraction pattern which allows us to reconstruct the sample using different methods such as conventional reconstructions like high angle annular dark field (HAADF) as well as more advanced methods, only available to 4D-STEM such as centre-of-mass (COM) imaging and ptychography. Here we present a body simulation work to investigate the efficacy of optical sectioning through a range of 4D-STEM data reconstruction techniques and a range of dopants within the sample.

Simulations are done using the ab initio simulation software plugin abTEM which utilizes the multislice algorithm [3]. Using this software we generate 4D-STEM datasets with a 200kV accelerating voltage and a convergence angle of 30mrad. For this work, the probe aberrations are set to zero to match ideal imaging conditions. The samples used were diamond crystal of 15nm thickness with different substitutional and interstitial dopants of masses ranging from 14Si to 82Pb. The location in the z direction of these dopants was also varied to investigate efficacy of the techniques dependent on the depth of the dopant within the sample.

The reconstruction techniques used here consist of HAADF which has been the standard for imaging heavy elements within materials since the contrast of HAADF reconstructions follows a power law of z^n where 1≤n≤2 [4]. Common 4D-STEM techniques are also implemented. COM which works by finding the average deflection of the probe by the sample in the diffraction plane, as well as its subsidiaries, integrated centre of mass (iCOM) and differentiated centre of mass (dCOM). Furthermore, the recently proposed

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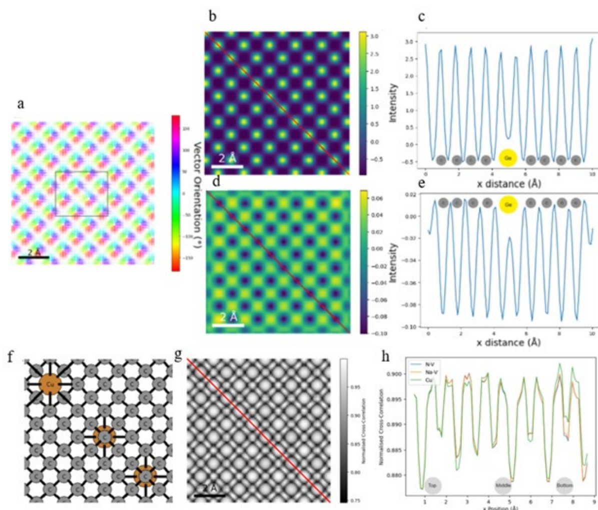
technique of symmetry STEM (S-STEM) which involves investigating the symmetry of the diffraction pattern by rotating or reflecting the diffraction pattern and cross correlating it with the original diffraction pattern to reconstruct [5].

Using the techniques described we find that different imaging methods excel depending on the relative weight of the dopant compared to the bulk crystal. As expected, HAADF provides a simple and effective method for imaging heavier atoms regardless of position in the crystal. The comparison is less clear when investigating lighter atoms such as silicon. In these regimes methods such as iCOM and dCOM prove themselves to be powerful tools for finding the location of the atom within the structure. We find that S-STEM is less of an effective tool than the others described, but this may be a poor representation of the true case, since relaxation of the crystal lattice may lead to strain in the sample for which S-STEM has been suggested to be a useful tool for identifying point defects [5]. It still may be an unreliable tool for optical sectioning though since S-STEM is robust at reconstructing atomic resolution images regardless of defocus as we have demonstrated with our results, as symmetry is independent of defocus.

The methods here result in a detailed analysis of how utilizing all the variables and tools available when imaging these materials using 4D-STEM can be leveraged to obtain the best results for optical sectioning. This work focuses on diamond as a bulk crystal within which dopants are placed so could be used as an effective framework for investigating the composition of colour centres such as nitrogen and silicon vacancy centres.

Figure 1: (a), (b) and (c) shows COM, dCOM and iCOM reconstructions of diamond respectively with germanium dopant within box drawn on (a). (c) and (e) show line profiles of (b) and (c) along the line drawn. (f) Schematic of diamond view down <100> zone axis with Cu dopant place on the top surface, middle and bottom surface of the crystal, respectively. (g) S-STEM reconstruction of the lattice shown in (f) with 180o rotation of the diffraction pattern, red line shows path of line profile shown in (h). (h) Intensity line profile of S-STEM reconstruction with different dopants/vacancies in the crystal.

Graphic:



Keywords:

4D-STEM, iCOM-STEM, Optical Sectioning, 3D-Imaging

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