3D atomic resolution tomography from iDPC-STEM images using multiple atom model prior

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3D reconstruction at the atomic scale for specimens consisting of both heavy and light elements is challenging with common scanning transmission electron microscopy (STEM) methods. Integrated differential phase-contrast (iDPC) STEM is a state-of-the-art imaging method with the capability of imaging heavy and light elements simultaneously, which is not possible with annular dark field (ADF) STEM [1, 2]. By acquiring iDPC-STEM projections at different tilt angles, 3D images of compound structures consisting of different elements can be reconstructed using tomographic reconstruction algorithms.

In [3], an atomic resolution reconstruction method for HAADF-STEM tilt series was introduced in which atoms are iteratively detected and replaced by a prior model of the atom potential. In this work, a similar reconstruction method is applied to simulated iDPC-STEM data for the first time by using separate atomic models for different elements. Since no prior knowledge about the structure of the materials is enforced, an unbiased reconstruction of both crystalline and amorphous structures is possible.

iDPC-STEM projections of a platinum nanodecahedron with 4021 atoms [4] on an amorphous carbon substrate with 53598 atoms [5] were simulated using the multislice method [2, 6, 7]. In this work, 181 simulated projections with 1-degree tilt increments were used for the reconstruction. Figure 1 shows a 3D rendering of the sample together with one of the iDPC-STEM and ADF-STEM projection images showing that iDPC-STEM image shows the platinum atoms as well as the carbon atoms which are almost invisible for ADF-STEM.

We aim at 3D reconstruction of both platinum crystal structure and amorphous substrate. Although the detection of the carbon atoms is more challenging due to their amorphous structure and the weaker contrast associated with them, the tomographic reconstruction of the simulated iDPC-STEM projections of the platinum nanodecahedron on the carbon substrate in Figure 2 reveals the heavy element (Pt) of the crystal as well as the light element (C) of the amorphous substrate which can not be done with ADF-STEM. In conclusion, 3D image of both heavy and the light atoms is reconstructed by using a multi atom model prior and iDPC-STEM projection.

Fig 1. a) Model of a Pt (red) nanodecahedron particle on a substrate consisting of amorphous carbon (blue); b) One of the simulated iDPC-STEM projection images; c) A simulated ADF-STEM projection image with the same tilt angle. The field of view is 8x8 nm2. The beam energy used is 80 keV and the beam convergence (semi) angle is 20 mrad.

Fig 2. Reconstruction of simulated platinum nanodecahedron on an amorphous carbon substrate. A slice through the 3D reconstruction is shown for the SIRT reconstruction (a), the final reconstruction consisting of platinum and carbon atoms by using the atom model prior (b)

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Figure 1.

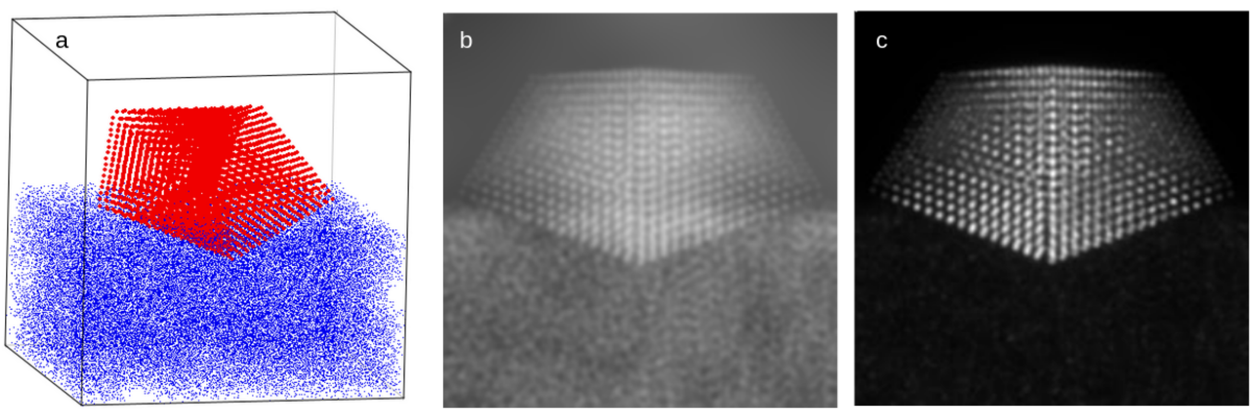
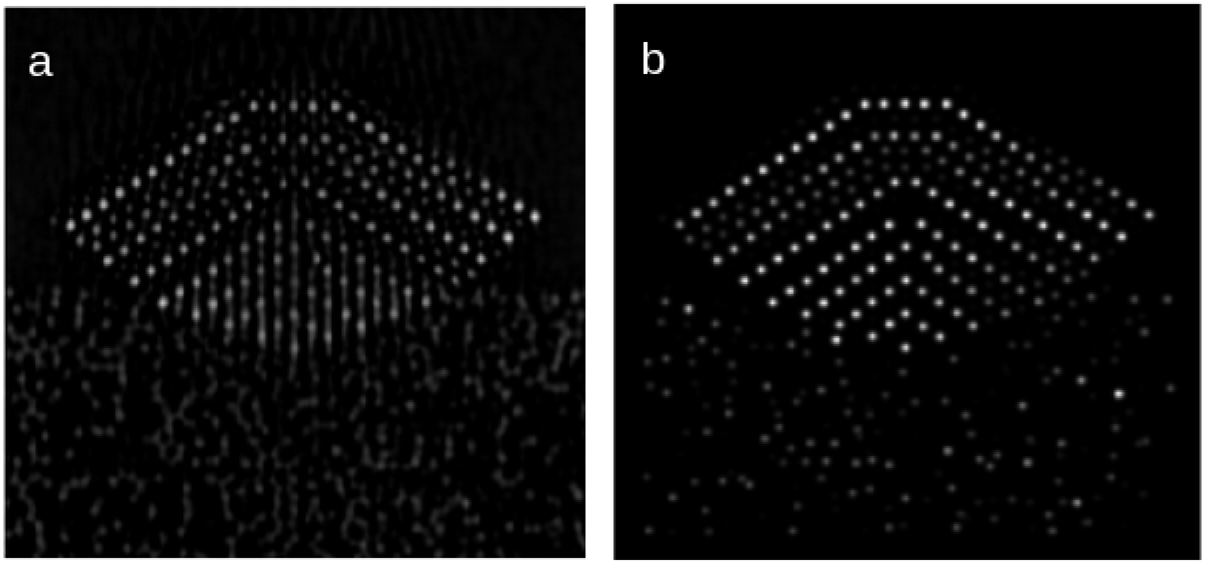


Figure 2.


a
b