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DOI: 10.1017/S1431927606063720
Microsc Microanal 12(Supp 2), 2006

Atomic Resolution Electron Tomography Based on Discrete Mathematics

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Electron tomography has become a valuable technique in materials science to investigate the three-dimensional (3-D) structure of nanomaterials [1, 2]. Efficient reconstruction algorithms are available, capable of making accurate tomographic reconstructions from around 100 projections of samples that are rotated in steps of 1-2 degrees to create a tomography series. By now, the spatial resolution of such methods, that commonly utilize back projection schemes for the reconstruction, reaches towards 1 nm^3 [1, 2]. Preferred imaging modes involve Z-contrast methods. These approaches usually avoid zone axis sample orientations in order to minimize non-linear intensity contributions caused by dynamic electron scattering. On the other hand it is desirable to exploit the atomic resolution capability of TEM or STEM, which benefits from dynamic scattering. However, it is impossible to record zone axis images every 1-2 degrees, because suitable zones do not occur that frequently.

We apply a novel reconstruction procedure to achieve atomic resolution in electron tomography [3, 4]. This method utilizes zone axis crystal orientations. We make use of high spatial resolution of electron microscopes and an improved signal-to-noise ratio (S/N) for the detection of single atoms [5] in order to reconstruct the 3-D location of all atoms in test structures with atomic resolution (see example in Fig. 1). Our reconstruction algorithm exploits the fact that crystals are discrete assemblies of atoms (atomicity) and was developed in the context of Discrete Tomography (DT), which is concerned with reconstructing binary (black-and white) images from a small number of projections [6].

Simulation experiments have been performed for a variety of test structures. Exit-plane wave images (phase contrast) and Z-contrast images have been simulated in different zone axis orientations. The discrete number of atoms in every column has been determined by application of the channeling theory to reconstructed electron exit waves and by local intensity measurements from Z-contrast images. The procedure is experimentally validated by experiments with gold samples ([5] and ref. therein). One finding is that the phase contrast of an aberration correction of the microscope as proposed in DOE's TEAM-project dramatically improves the S/N ratio. Thereby, the phase image of an atomic column gets more localized and, in our case, a ~ two times larger phase change per contributing atom in a column occurs (see Fig. 2) [5]. The high S/N and the atomicity constraint enable us to obtain a 3-D reconstruction of test structures from less than 10 projections even in the presence of noise (Fig. 3) [4].

An important property that is utilized by our approach is the fact that the atoms in a crystal are positioned in a discrete lattice. Using this property makes the search space of all possible reconstructions that have to be considered by the algorithm much smaller, which makes the reconstruction procedure computationally more feasible. Although the discrete lattice property is computationally convenient, it is not always satisfied perfectly in real crystals. We will present

the next steps to extend our approach to more complex crystalline samples containing a second atomic species or vacancies. The compositional difference will be arranged in a given order or randomly distributed (one example in Fig. 1c). For certain defects, such as vacancies, incorporation into our model is straightforward. Defects that strongly distort the column structure through their strain field and result in larger displacements in the projection data require more elaborate extensions.

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[7] This work was supported by the US Department of Energy (Director of the Office of Science, contract DE-AC03-76SF00098). The authors acknowledge support of the staff and the facilities at NCEM. K.J.B. wishes to thank the Netherlands Organization for Scientific Research (NWO, contract 613.000.112). H.A.C. acknowledges support from IPN and CONACYT.

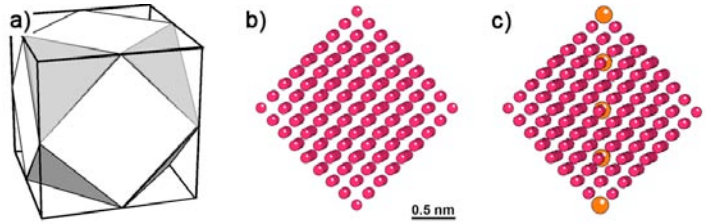

Fig. 1. (a) Cube octahedron (b), (c) Size, shape and atomic distribution of the nanocrystal used for image simulation. Two different species of atoms are represented by the smaller and larger spheres.

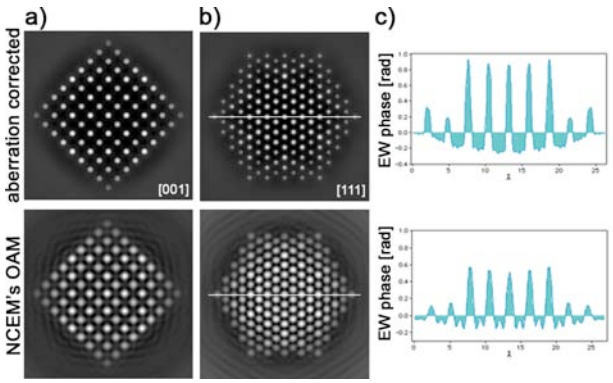

Fig. 2. (a),(b) Exit-wave phase images of the nanocrystal simulated for the TEAM microscope (upper part) and Berkeley's OAM (lower part) in two different projections: (a) in [001] and (b) in [111]; The improved S/N in the TEAM microscope due to aberration correction leads to a larger signal (phase change) per contributing atom in a column (~2x) - see line scans in (c).

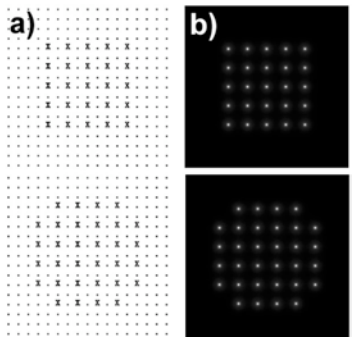

Fig. 3. Atomic resolution tomogram: (a) Two of the final nine slices obtained from the reconstructed nanocrystal of FIG. 1 using a DT algorithm. Filled positions representing atoms are marked by "X." (b) Two of the nine atomic layers of the cube-octahedron nanocrystal in a [001].

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