

## 3D Imaging of Nanomaterials by Discrete Tomography

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Electron tomography is a powerful imaging technique in electron microscopy that can be used to investigate the 3D structure of nanomaterials. At present, most reconstruction algorithms are based on either backprojection or algebraic reconstruction techniques (see, e.g. [1]). A drawback of these methods is that they require a large number of images (> 50-100) to obtain sufficient accuracy in the reconstructions. Even then, artifacts are often visible in the reconstructed volume, e.g. due to the limited tilt-range and tilt-step during data acquisition.

Recently, new reconstruction algorithms have been developed in the context of Discrete tomography [2,3,4]. Discrete tomography focuses on the reconstruction of images that contain only a small, discrete set of gray values. In the context of electron tomography this corresponds directly to samples that consist only of a few different materials. If these materials are known in advance, this knowledge can be used by the reconstruction algorithm in addition to the tomographic projection data, which may yield a vast reduction in the number of projections that is required to compute an accurate reconstruction.

Many challenges in materials science involve complex structured samples, which nevertheless consist only of a limited number of separated, well-defined materials. Using discrete tomography for such samples may have several advantages. Besides a reduction of the required number of projections and suppression of certain types of artifacts, a main advantage of discrete tomography is that the reconstruction is already segmented into the different materials. In contrast, if a conventional reconstruction algorithm is used, such as filtered backprojection or SIRT, the segmentation is often difficult and time consuming.

As an example, we consider the 3D reconstruction of nanoparticles formed by doping of SiC with Er followed by high-temperature annealing [5,6]. Previous analysis showed that the sample mainly consists of ErSi<sub>2</sub> nanocrystals in a SiC matrix. The reconstructed image should be a binary image, consisting of only two gray values for the interior of the ErSi<sub>2</sub> nanocrystals and the surrounding SiC matrix (see Fig. 1, 2). Investigating the distribution and shape of such particles in 3D is of great interest to understand the formation and growth mechanism as well as the electronic properties of the nanocrystals.

Preliminary results will be presented on the application of discrete tomography to the ErSi<sub>2</sub>/SiC example, in order to investigate the number of required projections, the segmentation capabilities and the ability to reduce the artifacts present with conventional reconstruction methods.

## References

- [1] A.C. Kak, M. Slaney, Principles of Computerized Tomographic Imaging, SIAM, 2001.
- [2] G.T. Herman, A. Kuba, eds., Discrete Tomography: Foundations, Algorithms and Applications, Birkhäuser, Boston, 1999.
- [3] K.J. Batenburg, Electronic Notes in Discrete Mathematics, 20 (2005) 247-261
- [4] K.J. Batenburg, J. Sijbers, Proc. of SPIE Medical Imaging 2006, (to appear)
- [5] U. Kaiser, D.A. Muller, J.L. Grazul, A. Chuvilin, M. Kawasaki, Nature Materials, 1-2 (2002), 102-105
- [6] U. Kaiser, A. Chuvilin, Microsc. Microanal., 9 (2003), 36-41
- [7] One author (K.J.B.) acknowledges support of the Netherlands Organization for Scientific Research (NWO) under contract 613.000.112.

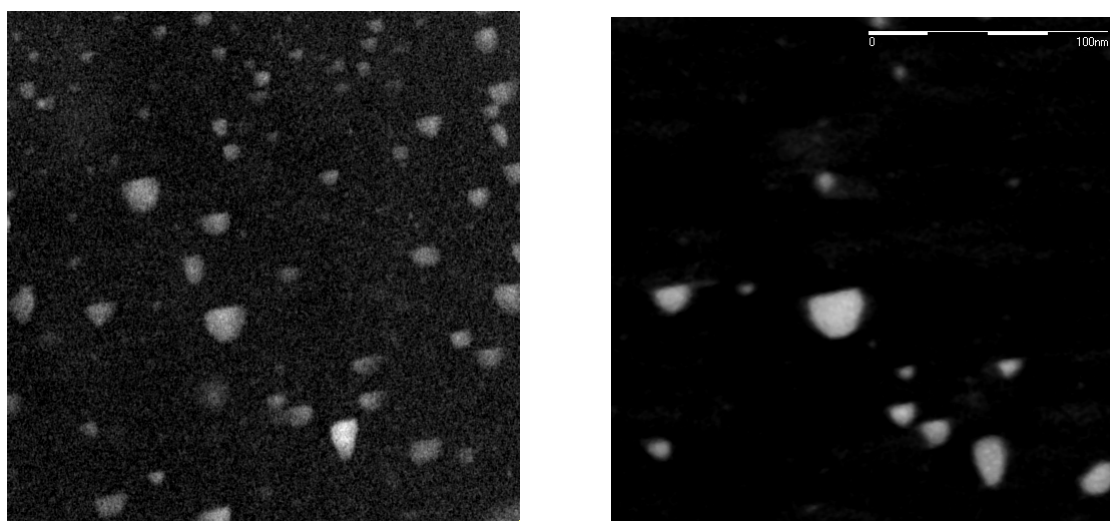


Fig. 1. Left: Projection image from a HAADF-STEM tilt-series (177 images) of SiC, highly doped with Erbium. Right: Cross-section in the xy-plane of a 3D reconstruction, computed from the tilt-series using the SIRT algorithm. The particles can be considered as homogeneous objects on a constant background, so the sample seems to be suitable for discrete tomography.



Fig. 2. Left: Two cross-sections in the xz-plane of a 3D reconstruction (see Fig. 1), computed from the tilt-series using the SIRT algorithm. Streak artifacts are visible around the particles, which make it difficult to segment the image. Right: 3D visualization of the reconstructed volume.