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Atomic Resolution Binary Tomography of Gold Nanorod Surface Morphology

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Summary: We describe how to reconstruct 3D gold atom locations from two projections of a gold nanorod collected with a scanning transmission electron microscope (STEM). A binary implementation of the Discrete Algebraic Reconstruction Technique (DART) is employed assuming the object with a maximum indentation of a single atomic layer from convexity.

1. Introduction

Discrete binary tomography has been used to reconstruct lattice structured objects, such as gold nanoparticles [5]. In the last decade or so, it has become possible to grow metal nanoparticles into a number shapes, opening a range of potential applications in plasmonics, photonics and optical communications. It is important to be able to measure the orientation and stability of the crystal surface facets in order to understand what controls the growth of a gold crystal, such as a nanorod [3, 4]. These facets are often just a few atoms in diameter, so measuring orientation and stability can be a significant challenge. An aberration-corrected FEI Titan3 80-300 FEG-S/TEM can be used to image nano-scale samples with atomic resolution [3, 7]. A quantitative analysis of scanning transmission electron microscope (STEM) images of a gold nanorod can enable the image to be converted to a measure of the thickness of the gold nanorod in terms of number of atoms. Such projection measurements are taken along a zone axis so atoms are aligned in a stack parallel to the projection direction [3]. Two zone-axis projection measurements are collected for a 3D tomographic reconstruction [4]. For a horizontal-vertical (HV) convex binary object [2], two orthogonal and noise-free projections are sufficient to reconstruct the exact object using the max rectangle approach [2]. Binary DART's [1] constraints on the object is less strict compared to HV convexity. Therefore binary DART together with suitable indented convex boundary condition is used to reconstruct a suitable 3D tomographic reconstruction.

2. Methods

Binary DART assumes the boundary between the two binary states is well defined [1]. This assumption leads to a reduction in the number of projection angles required for a satisfactory reconstruction compared to the general Mojette discrete reconstruction [6]. Satisfying this assumption, DART requires as few as two projections to obtain a satisfactory reconstruction by iteratively updating the boundary [1]. Here we assume that the surface between gold nanorod and void is generally well defined. Gold nanorods are not strictly HV convex as there may exist surface indentations; it is also difficult to obtain orthogonal projections due to tilt-angle limitations of the microscope.

Gold has a face-centred-cubic structure; we represent a 2D slice of this lattice on a square array as [*x-x-; -x-x; x-x-; -x-x*] (see the projections in Fig (c)), where *x* represents a lattice site, - represents a void location and *;* represent a new line. Our approach is to reconstruct an object that is a *dilation* of the filled lattice sites, i.e., where $x=1$, with suitable boundary conditions on the reconstructed object. *Dilation* is an operator in mathematical morphology that fills the internal lattice voids of the gold nanorod producing well defined boundaries. We apply binary DART with the binary threshold updated in each iteration to preserve the total number of atoms in each lattice plane parallel to the projection angles. We assume a geometric convex object with patches of at most one atom level of indentation. The lattice structure is imposed to determine the exact location of the gold atoms. Up to 200 iterations are employed. The 3D reconstruction (Fig (d)) takes approximately 30 minutes on a single CPU thread. It can be trivially parallelised by separately reconstructing each parallel plane. With ~5% experimental error and only two projection angles, we aim to reconstruct the surface with an error of no more than one atom for both the simulated and real experimental data.

3. Results

The simulation shows the accuracy of the reconstruction process for different shaped objects by reconstructing an octagon and a circle both with a vertical height of 100 atoms. For real data, we present the two projections (Fig (c)) taken using STEM [4] and the reconstruction of the gold nanorod (Fig (d)) using those two projections.

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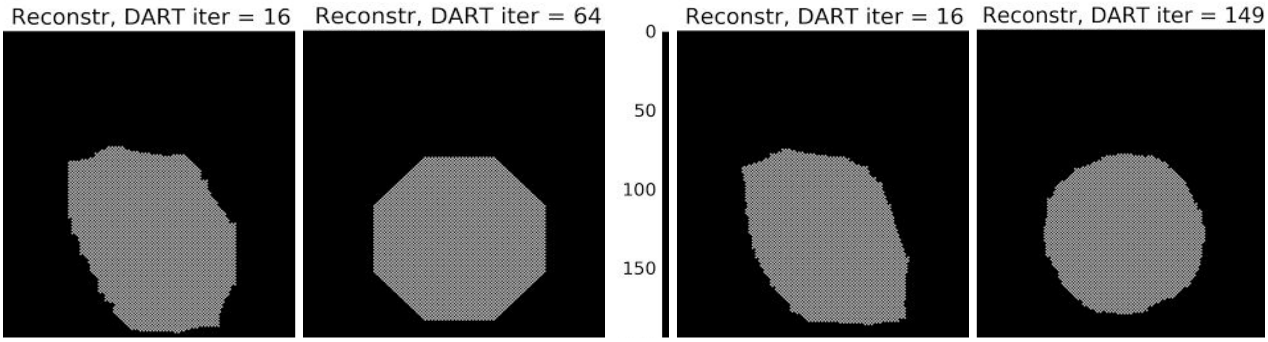
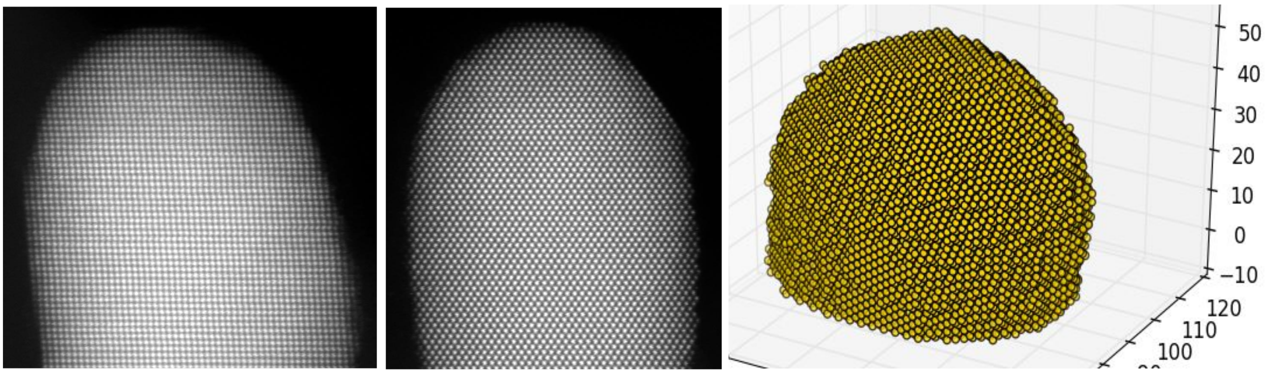


(a) (b)



(c) (d)

Fig: (a) DART of an Octagon: an exact reconstruction; (b) DART of a circle: 26 mislocated atoms. (c) Real projection data (<001> and <011> axis respectively); (d) 3D reconstruction of a gold nanorod tip.

4. Conclusion

Using only two projections, 45 degrees apart, we demonstrated the binary DART can reconstruct an octagon, but has difficulty reconstructing a circle (see Fig (a, b)) given error-free simulated projection data. The gold nanorod being reconstructed has 16 facets [4], so we expect a reconstruction error level between the octagon and circle case. Applying our algorithm to real experimental data, preliminary results provide some insight as to the complex morphology of the gold nanorod tip (see Fig (c, d)) close to the atomic scale. The effect of experimental uncertainty was explored by adding noise to the projection data; we found that inconsistencies would aggregate on the object surface perpendicular to the projection direction. As expected, obtaining two orthogonal projections (as opposed to 45 degree separation) would improve reconstruction quality but this is challenging experimentally.

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