Quantitative 3D reconstruction of nano-particles based on atom counting in STEM

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1. INTRODUCTION

Mastering the chemical and physical properties of nano-objects in nanomaterials such as nanoparticles is a crucial issue in materials science. These properties are strongly correlated with three dimensional (3D) morphology and composition of nano-objects, which can be accessed by electron tomography. However, although the modern microscopes with aberration correctors allow a spatial resolution below 1 Å, atomic resolution for electron tomography is not obvious. To perform electron tomography and 3D characterization at nanometer scale, high angle annular dark field scanning electron microscopy (HAADF-STEM) is widely used [1–3]. Sandra Van Aert et al.[4,5] proposed a statistical approach to determine the number of atom in each column on HAADF-STEM micrographies in zone axis. Coupling atom counting along different orientations of a same nano-object, these authors demonstrated the possibility to achieve a 3D reconstruction at atomic scale of nano-particles [6,7]. Based on this statistical method, we developed an original algorithm to reconstruct in 3D at atomic scale one nano-object with only three different orientations. Our 3D reconstruction algorithm was tested with three images from simulations of one nanoparticle under different orientations.

2. RESULTS

Image simulations were performed using a parallelized version (provided by Pr. M.D. Robertson, Canadian Centre for Electron Microscopy [8][9]) of the multislice algorithm developed by Kirkland [10]. The simulation includes the contribution of thermal diffuse scattering using the frozen phonon approximation [11]. In this approximation each image corresponds to one particular frozen lattice configuration that is why we must average on several images to obtain realistic result. In order to obtain images in reasonable time, the simulations were performed on the supercomputer CRIHAN and the nanoparticles used for simulation were created by NanoFabric[12].

The atom counting software developed in the GPM is based on the statistical method proposed by Sandra Van Aert *et al.*[4,5]. After a deconvolution of the point spread function of the electron probe, the reliability of the methodology is demonstrated (cf. Figure 1, Figure 2). It is hence possible to determine the number of atoms for each atomic column with accuracy. Using atom counting software, we developed an original algorithm to reconstruct in 3D at atomic scale one nano-object with only three different orientations. Our 3D reconstruction algorithm was tested with three images from simulations of one nanoparticle under different orientations (Figure 1).

Figure 1*:* On the left, nanoparticle made by NanoFabric [8] used for HAADF-STEM simulation, on the right, 3D reconstruction based on three HAADF-STEM image simulations. The 3D reconstruction is very close of the input data.

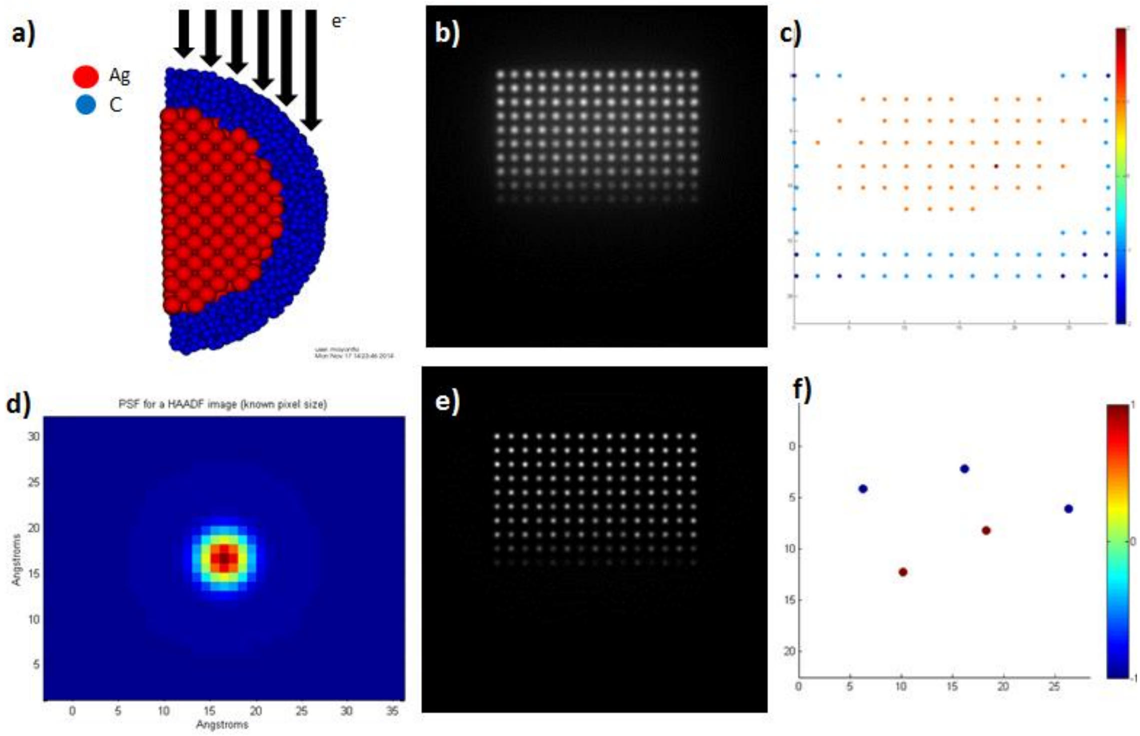

Figure 2 a) Particle created by NanoFabric[12], red dots are silver and blue dots are carbon. b) Result of the STEM-HAADF simulation image. Picture size is 5nm*5nm. c) Difference in atom count on each column between the reality and result of atom counting program. d) Point spread function of the electron probe for this simulation. e) Image simulation after the deconvolution by the point spread function. A more sharply peaked image is obtained. f) Difference in atom count on each column between the reality and result of atom counting of the deconvolved image,. The agreement is almost perfect.

3. CONCLUSION

Thanks to its accuracy this method can be applied for different applications as reconstruction at atomic scale of very small nano-objects or correlative microscopy with atom probe tomography [13].

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