

Sparsity and Noise Effects on the Reconstruction of Subsampled Scanning Transmission Electron Microscopy Data

Eduardo Ortega¹ and Niels de Jonge^{1,2}

¹INM - Leibniz Institute for New Materials, Saarbrücken, Germany.

²Department of Physics, Saarland University, Saarbrücken, Germany.

The implementation of compressive sensing (CS) methods into electron microscopy has opened an avenue to increase not only acquisition times but also reduce the total electron dose (eD). A direct approach to CS relies in the acquisition of sparse scanning transmission electron microscopy (STEM) data where time and eD become proportional to the number of pixels acquired [1]. Sparsity can be introduced forcing the probe to follow a predefined random walk, where the beam is allowed to jump between adjacent lanes [2]. While most recent research efforts have focused on the implementation of inpainting algorithms in synthetic or post-processed images [3], in this work we will discuss the effect of experimental parameters on the reconstruction quality of the inpainted images.

To this end we have acquired annular dark-field (ADF) sparse STEM data using a JEM-ARM 200F (JEOL; Japan) coupled with a programable scanning unit generator (DE-Freescan, Direct Electron; USA). The reconstructions were compiled using a Beta-Process Factor Analysis via Expectation Maximization algorithm loaded into the Nuxutra Image-Inpainting software (Sivananthan Laboratories; USA) [4]. This algorithm was chosen as neither training data nor sample-dependent parameters are needed to converge on a solution. In this way, each reconstruction was self-contained, and the quality of the final product depended on the raw data itself. Two sample types, namely atomic resolution images of Si (110) and gold nanoparticles (AuNPs; EM2000229/7, JEOL), were compared at different sparsity levels and eD rates.

Fig. 1 presents the application of the inpainting process on atomic resolution STEM images. The Si (100) image shown in Fig. 1a, serves as reference for the relative eD , speed and subsampling experiments. As eD was reduced, i.e., acquiring 20x faster (Fig. 1b), the fine details from the Si lattice were resolved poorly. The same information can be retrieved recording only a fraction of the data, with better signal-to-noise ratio (SNR), owing the fact the periodicity of Si allows to record all relevant features within a few pixels. As an example, in Fig. 1c, a full inpainted frame was recovered using only 16 of the 512 lines available (6.25%). Notwithstanding, as highlighted in Fig. 1d, poorly scanned areas were prone to contrast variations while retaining the proper crystal lattice. The reconstruction quality was comparable to the original data as demonstrated either by inspecting its resultant Fourier Transform (Fig. 1e) or by measuring the signal ratio between the (004) Si dumbbells (Fig. 1f). To test the effect of the operational parameters on a sample with less redundancy but good contrast, we selected a set of AuNPs over a C support as a way to reduce background noise (Fig. 2a). On Fig. 2b-e, we tested different imaging conditions while maintaining the same total eD to find the most critical parameters to optimize the inpainting reconstructions. For these datasets, the quality of the reconstruction was tracked relating the size distribution of the AuNPs (Fig. 2f), and how well they related to the over sampled, high dose, and full-size original data. As a result of these comparisons, the combination of low sparsity levels ($< s4$) at moderate scanning speeds ($\times 2$ to $\times 4$) yielded the best reconstructions outputs in clear contrast with what can be achieved by T_D , $pxsz$, and sparsity alone.

The understanding of the upper and lower resolution limits of experimental sparse STEM data will allow for an improved experimental design in STEM research where both under- and oversampling can be avoided while maintaining a good signal representation at faster and lower dose setups [5].

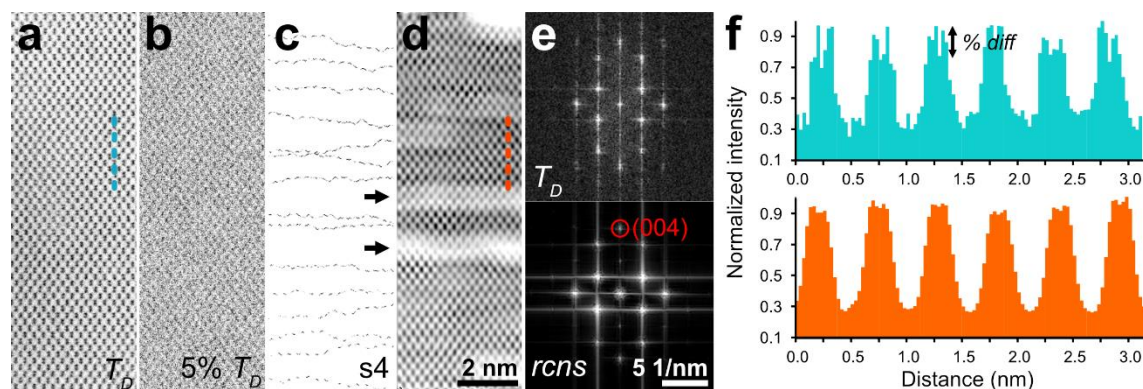


Figure 1. Subsampled reconstruction of atomic resolution Scanning Transmission Electron Microscopy (STEM) images. The contrast was inverted to improve visualization. Reference Si (110) image acquired with a dwell time $T_D = 40 \mu\text{s}$. (b) Same image but with $T_D = 2 \mu\text{s}$. (c) Subsampled STEM image and its corresponding (d) reconstruction where linescans zigzag a width of 32 pixels (s32). (e) Fourier transform (FT) of the reference (top) and reconstruction (bottom). (f) Corresponding intensity profiles along Si $\langle 002 \rangle$ to highlight the presence of the (004) Si dumbbells and their respective signal contrast.

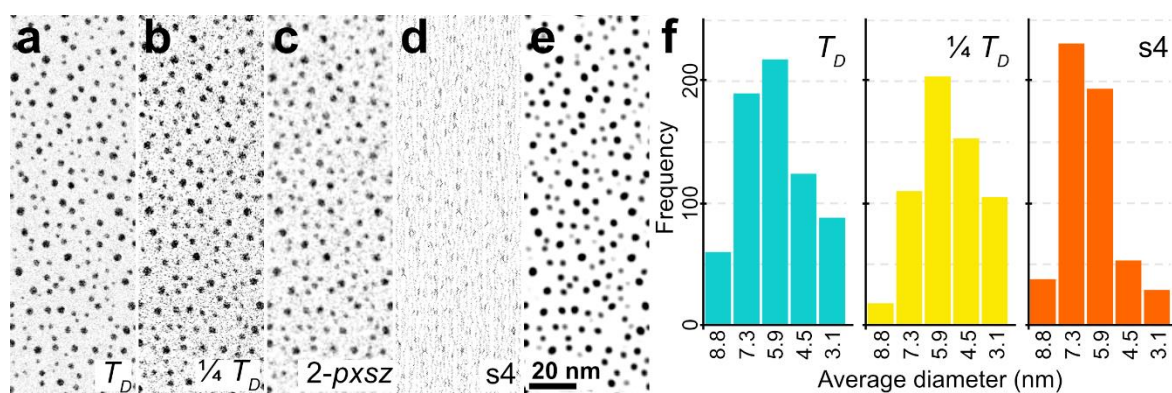


Figure 2. Comparison of the influence of T_D , sparsity, and pixel size ($pxsz$) on the size distribution of a set of gold nanoparticles (AuNPs). (a) Reference AuNPs acquired at $T_D = 16 \mu\text{s}$. STEM images acquired: (b) 4x faster, (c) with double the $pxsz$, and (d) recording 25% of the pixels for (e) reconstruction. (f) Size histogram of the AuNPs from (a), (b) and (e).

References:

- [1] B.L. Mehdi *et al.*, Appl. Phys. Lett. **115** (2019), p. 063102. doi: 10.1063/1.5096595
- [2] E. Ortega *et al.*, Sci. Rep. **11** (2021), p. 22722. doi: 10.1038/s41598-021-02052-1
- [3] J Schwartz *et al.*, Microsc. Microanal. **25** (2019), p. 705. doi:10.1017/S1431927619000254
- [4] D Nicholls *et al.*, Ultramicroscopy **233** (2022), p. 113451. doi: 10.1016/j.ultramicro.2021.113451
- [5] The authors thank E. Arzt for his support through INM. The research was supported by the German Research Foundation.