

## Advances in STEM-CELL. A Free Software for TEM and STEM Analysis and Simulations: Probe Deconvolution in STEM-HAADF

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Analytical studies with an TEM and STEM are going in the direction of a stronger involvement of computing in the image interpretation.

Geometric Phase Analysis [1] for example has proved to be a useful tool to evaluate the strain in different structures. TEM Image simulation is also a very important tool to compare with complicated structures and to obtain quantitative comparison of the contrast. Moreover the simulation of STEM images is a fundamental step to perform quantitative HAADF measurements [2]. Finally exit wave reconstruction in TEM and probe deconvolution in STEM are useful tools to improve the image information [3].

Many simulation software are already available in literature and on the web however it is difficult to find a free and graphical tool that permits to perform both simulation and analysis on the same platform. For this reason I created the STEM CELL project [4].

The propose of STEM CELL is

- 1) to facilitate multislice simulations by creating, manipulating complicated cells, facilitating the selection of the simulation parameters and interface with simulation routines (the work was based on Kirkland routines [5])
- 2) to implement analysis methods on both simulated and experimental images so that simulation can be more directly used as a benchmark for experiments.
- 3) To implement new simulation methods.

In this contribution we would like to show the implementation of an algorithms for the deconvolution of the probe in HAADF images.

The classical problem of probe deconvolution is based on the assumption that the intensity of an HAADF image can be written as

$$I = O \otimes P^2$$

Where  $P^2$  is the probe intensity distribution , O is the object function related to atom scattering.

The typical naïve deconvolution strategy is to revert to Fourier space where this convolution transform to a multiplication of the transformed quantities. However this typically produces problems and noise enhancement where the Fourier transform of the probe (from now H ) is close to 0. Maximum entropy method(MEM) fills in the missing information with a reasonable guess based on the maximization of the data entropy. The classical Richardson-Lucy[6] algorithm is the most known implementation of this algorithm but in this paper a different iterative approach is proposed. In fact the iterative algorithm of Hollis et al [7] has been implemented instead that should reach for a relatively fast result within few iteration. The actually minimized function in the algorithm is a potential F that is an upper bound to the entropy. The solution tends to the MEM solution after a sufficient number of iteration.

The algorithm is especially suited for highly peaked object functions such as isolated stars or in the present cases atoms but does not have a quality control parameter to decide when stop iteration. Therefore a manual merit factor of the reconstruction by inspection was used. This typically meant 80 iterations.

Fig 1 is the comparison of the experiments and its reconstruction for a Si-Ge interface. The b image shows much more clearly the Si dumbbell. Fig c is a detail of fig b

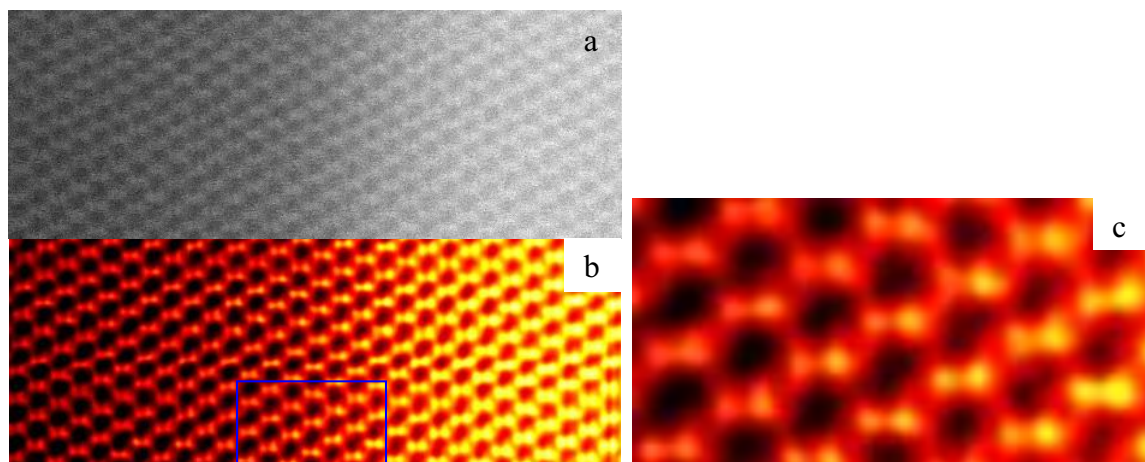


Fig 1 a) Row STEM image of Si in the [110] direction obtained with a JEOL 2200 FS with  $C_s=0.5\text{mm}$  and operated at 200 KeV, b) STEM image after deconvolution c) zoom of image b.

- [1] M.Hytc h et al. *Ultramicroscopy* 74 (1998) 131- 146
- [2] V. Grillo et al. *Phys. Rev. B* 77 (2008) 054103.
- [3] S.J. Pennycook, et al. Proc. 10th Pfefferkorn Conf., Cambridge, 1992, 233-243.
- [4] V.Grillo <http://tem-s3.nano.cnr.it/stemcell.htm>
- [5] E. J. Kirkland, *Advanced Computing in Electron Microscopy* (Plenum,New York, 1998)
- [6]W.H. Richardson, *J Opt Soc Am* 62 (1972) 55; L.B. Lucy, *Astrophysical Journal* 79 (1974) 745.
- [7] J.M. Hollis et al *Astrophysical Journal* 386 (1992) 293