doi:10.1017/S1431927614012409
Microsc. Microanal. 20 (Suppl 3), 2014
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A Brief Tutorial for the STEM-CELL Software

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TEM and STEM analytical studies are going in toward a stronger involvement of computing for 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 simulations are another very important tool to be compared with complicated structures to obtain quantitative interpretation of the contrast. Moreover the simulation of STEM images is a fundamental step to perform quantitative HAADF measurements [2]. Finally phase retrieval methods in TEM and probe deconvolution in STEM are useful tools to improve the image information [3]. Many simulation software are already available in the 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 we created the STEM CELL project [3][4]. The proposal 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/analysis methods.

Among the most recent new features it is worth mentioning the probe deconvolution in STEM HAADF images, the phase reconstruction by means of the transport of intensity equation, the simulation of diffraction patterns for any unit cells and the column by column quantitative analysis of the HAADF contrast.

For sake of example we show in fig. 1 a simulation of two GaAs tetrapods and a Ni particle. A layer of amorphous carbon has been also added to provide a more realistic effect. The sample has been constructed within STEM-CELL and simulated using the embedded Kirkland's software. Fig. 2 is an example of experimental analysis of the contrast of a CeO_2 nanoparticle. The reported experimental image has been obtained by deconvolution of the original image (not shown). The contrast of each column is interpreted approximately in terms of thickness (i.e. number of Ce atoms per column) using a "quick" calibration based on the analysis of the intensity histogram and of the minimal intensity step. Fig. 3 is an example of the transport of intensity equation application on magnetic particles [6]. The group of magnetism at IMEM-CNR is thanked for providing the samples shown in fig 3.

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https://doi.org/10.1017/S1431927614012409 Published online by Cambridge University Press

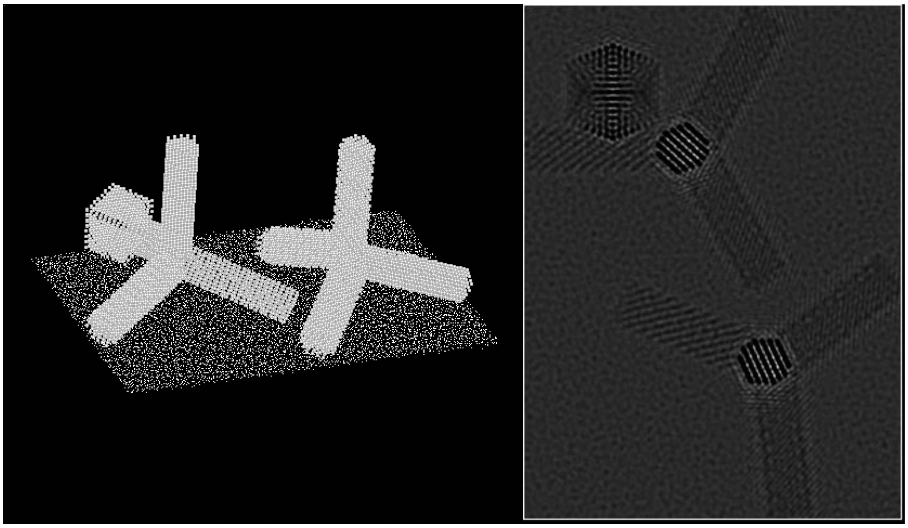

Figure 1. Model and HREM Simulation for 2 GaAs tetrapods and a Ni particle

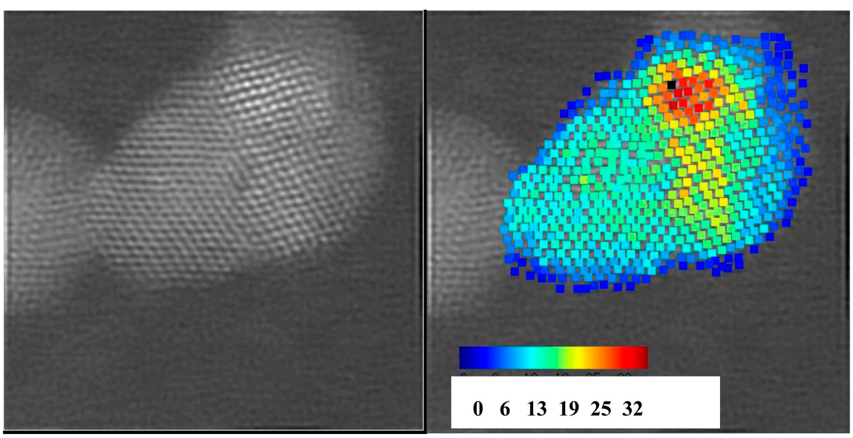

Figure 2. a) Deconvoluted STEM image of a CeO2 nanoparticles and quantitative column by column analysis of intensity

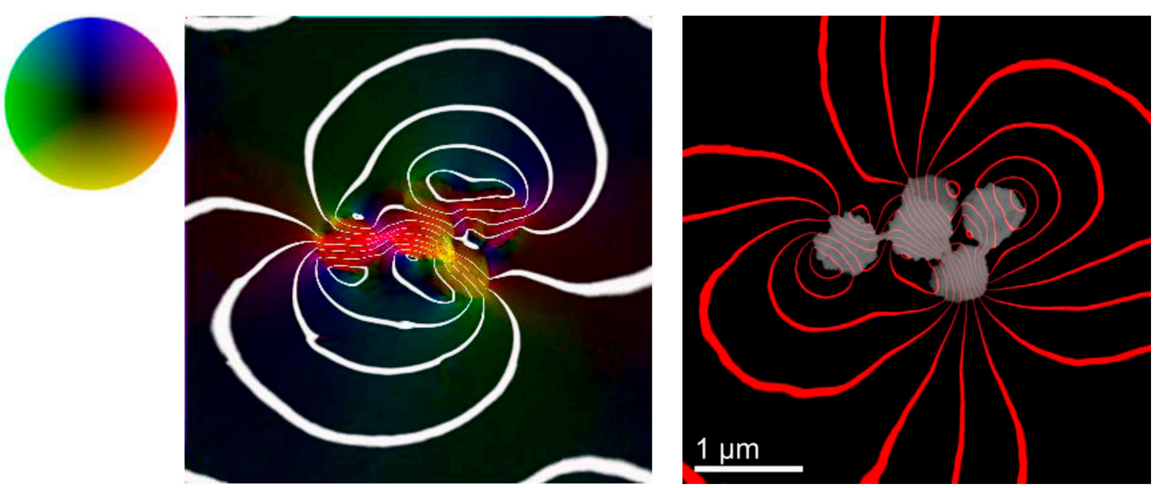

Figure 3. Example of TIE (transport of intensity equation) analysis and graphical representation of magnetic field of two different groups of magnetic nanoparticles. The hue and brightness refer to different B direction/modulus. The line of the field are also shown.

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