doi:10.1017/S1431927611005770
Microsc. Microanal. 17 (Suppl 2), 2011

Simulating STEM Imaging of Nanoparticles in Micrometers-Thick Substrates

N. Poirier-Demers,* H. Demers,* D. Drouin* and N. de Jonge**

* Electrical and Computer Engineering department, Universite de Sherbrooke, Sherbrooke, Quebec, J1k 2R1, Canada
** Department of Molecular Physiology and Biophysics, Vanderbilt University School of Medicine, Nashville, 37232-0615

The scanning transmission electron microscopy (STEM) can be used to image biological and other soft materials with nanometer resolution on nanoparticles in micrometers-thick specimens [1]. For the imaging of thick samples, the spatial resolution is not limited by the optics of STEM, as is the case for ultrathin amorphous substrates, but the interaction of the electron beam with the specimen plays a major role, and the resolution is limited by noise or by beam broadening. It is crucial to have knowledge of the electron beam-specimen interactions, so that the imaging settings can be optimized for maximal resolution, especially when imaging radiation-sensitive samples. Knowledge of the beam broadening can potentially be used to enhance the resolution of 3D datasets by using deconvolution procedures. A precise way to study the interaction between an electron beam and a specific specimen geometry and composition is via the use of Monte Carlo simulations. We present a STEM version of the CASINO Monte Carlo software [2].

The CASINO Monte Carlo software has been modified to include the simulation of STEM with the annular dark-field (ADF) detector [3], exhibiting atomic number (Z) contrast. The electron trajectory calculation is based on to the previous version of CASINO [4]. The electron beam model included the Poisson noise and a conical shape of the electron source, such that realistic STEM images were obtained with these simulations. By using the 3D geometry of the sample and the 3D programming of the electron beam shape and focal point position, various STEM imaging sequences were simulated, including focal series. The electron scattering physical models used in the previous version of CASINO were extended from the energy range of the SEM to energies of up to 300 keV as needed for STEM imaging.

For the imaging of radiation sensitive samples, such as biological materials or polymers, it is important to optimize the achievable resolution in terms of the maximal electron dose. This optimization requires the calculation of the resolution and signal-to-noise level obtained for a specific sample and STEM imaging settings. The Monte Carlo simulation of STEM imaging presents a precise method to conduct such calculations. As an example, we have simulated line scans (one-dimensional images) for a sample consisting of gold nanoparticles placed on the top surface—with respect to the electron beam propagation direction—of a 1 mm thick carbon support substrate (see Fig. 1A). Fig. 1C shows an increased noise level compared to Fig. 1B as expected, as the number of electrons has been reduced by a factor of 50. Nanoparticles were assumed to be visible in the noise of the background when the Rose criterion [5] was satisfied, i.e., when SNR $\geq$ 5. In Fig. 1B,C, the dashed horizontal line indicates the signal level for SNR = 5. The smallest nanoparticle (d = 1 nm) is just visible in Fig. 1B, while it vanished in the noise in Fig. 1C. These results demonstrate that the CASINO software can be used to simulate the achievable SNR for specific sample and microscope settings. Monte Carlo simulations can be used to optimize microscope settings, e.g., for high resolution, in imaging sessions where a low electron dose is crucial. The simulations can also be used to analyze the image features in a particular experiment for the analysis of the composition of a certain specimen. [6]

References
[1] N. de Jonge et al., *Proc. Natl. Acad. Sci.* 106 (2009) 2159.
[2] http://www.gel.usherbrooke.ca/casino/index.html.
[3] H. Demers et al., *Microsc. Microanal.* 16 (2010) 795.
[4] D. Drouin et al., *Scanning*, 29 (2007) 92.
[5] A. Rose, Advances in Electronics and Electron Physics, 1 (1948) 131.
[6] This work was supported by NIH grant R01-GM081801 (to N.P.D., H.D., and N.J.).

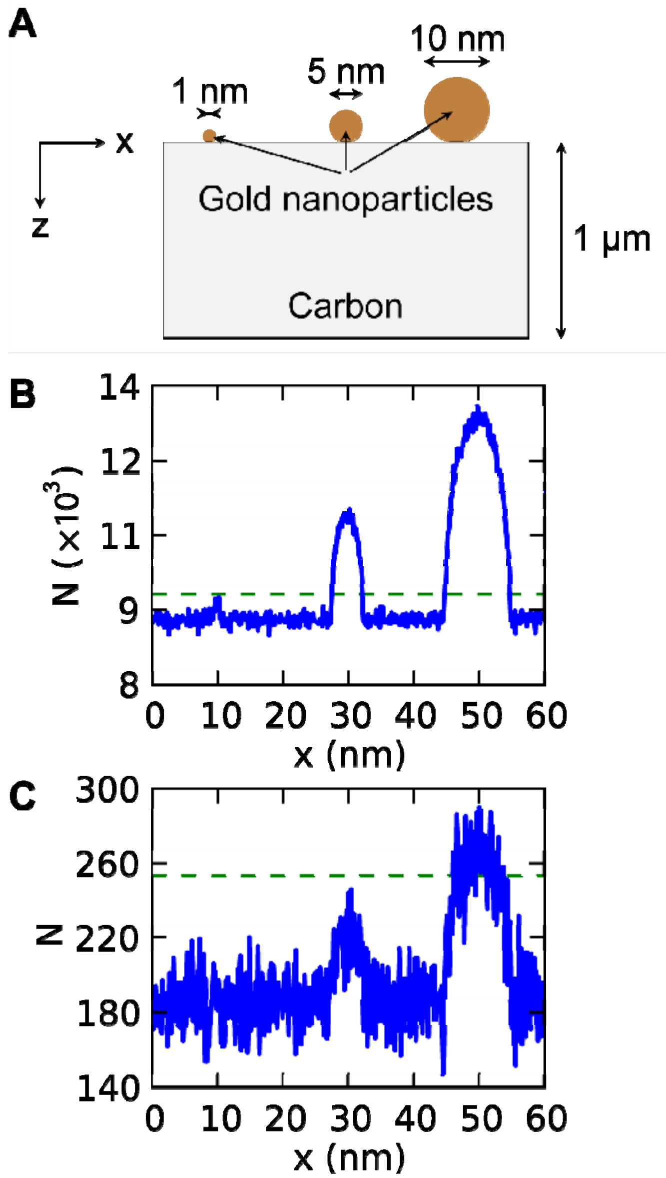

FIG. 1. Monte Carlo simulation of line scans recorded with the ADF detector of a STEM. **A:** Schematic of the sample geometry (not to scale) used for the simulation. The sample consisted of 1, 5, and 10 nm diameter gold nanoparticles located on the top surface of a 1 µm thick carbon substrate. **B**, **C:** Line scans showing the number of detected electrons N versus horizontal position x, simulated for 62,415 and 1,248 electrons per pixel, respectively. The dashed line indicates the Rose criterion (SNR = 5) for nanoparticle visibility.

https://doi.org/10.1017/S1431927611005770 Published online by Cambridge University Press