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On the Representation of Beam/Specimen Interactions

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The Monte Carlo technique was first applied to SEM in the early 1960s. Initially, its usefulness was limited due to lengthy simulation times and the poor availability of computers. Modern personal computers can obtain the same results in a fraction of the time, making simulations a viable research and teaching tool for understanding beam/specimen interactions. Here we examine the representation of such interactions using data from a single scattering Monte Carlo model [1].

A traditional representation of the interaction volume from a Monte Carlo simulation is shown in figure 1 for a 20 keV beam interacting with a gold specimen. The Y and Z axes are shown, and the X axis points into the page, with the origin at the beam entry point. This representation was obtained from the simulation data by a "connect-the-dots" construction, where each elastic scattering event is projected onto the image plane and connected to its sequential neighbors by straight lines. Variations of this representation include color-coding the connecting lines by energy. Unfortunately, this concept of the interaction volume can be misleading. For example, compare figure 1a to figure 1b. At first glance, the interaction volume appears to be larger in figure 1a. However, this is not true: simply more electrons have been simulated. Additionally, since the data is projected, it is tempting to conclude that the interaction volume has radial symmetry. This is certainly incorrect if the beam is at near-grazing incidence, as is the case for figure 1 (70 degrees from normal incidence).

Here we suggest alternative methods of representation that we feel provide more insight into beam/specimen interactions. Figures 2 and 3 show 2 nm thin slices in the YZ plane of the specimen at X = 0 nm. The simulation parameters are identical to those in figure 1. In figure 2, the density of scattering events per 2x2x2 nm voxel of the slice, D_V, is presented. The number of simulated electrons divided by 10^6 is a normalizing factor, so the representation is independent of the number of electrons in the simulation. It is clear from this representation that the density of scattering events is highly asymmetric close to the surface. Moreover, the log scale shows both the extent of the interaction and the importance of the region near the impact point. Figure 3 shows the average energy of electrons in each voxel, which is again independent of the number of simulated electrons. The asymmetry is clearly displayed. Finally, figure 4 is a surface plot of the normalized secondary electron density, D_A, per 0.4x0.4 nm discrete area. Figure 5 is the same plot but for a beam of normal incidence to the surface. These figures show only the peak in the secondary emission (SE I); there is a large, weak skirt surrounding this peak. A direct comparison of these two figures shows that the spatial distribution of the SE I signal does not vary much with the incidence of the beam. Collectively, the scattering density, average electron energy, and secondary electron density representations provide a lot more information than conventional figures [2].

References

[1] D.C. Joy, *Monte Carlo Modeling for Electron Microscopy and Microanalysis*, Oxford University Press, New York, 1995.

[2] Support from DOE, under grant DE-FG02-00ER45819, is gratefully acknowledged.

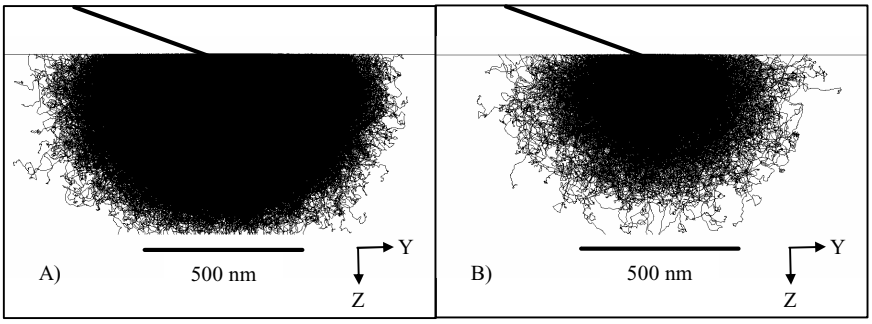

FIG. 1. Conventional display of the interaction volume: 20 keV, 3nm FWHM beam on gold tilted 70°. A) 100000 simulated trajectories B) 5000 simulated trajectories (identical simulation parameters)

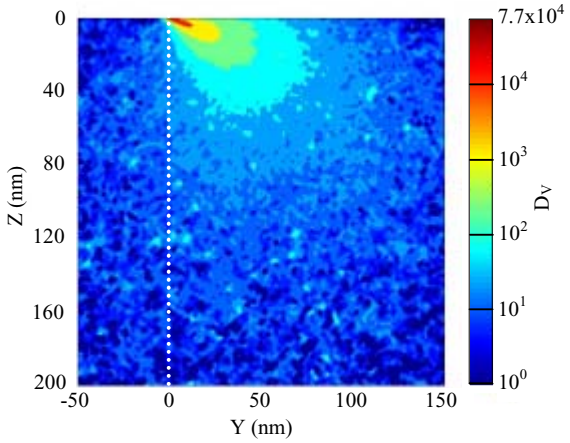

FIG. 2. Density of scattering events in a 2 nm YZ slice, centered at X = 0 nm. Density shown with log scale.

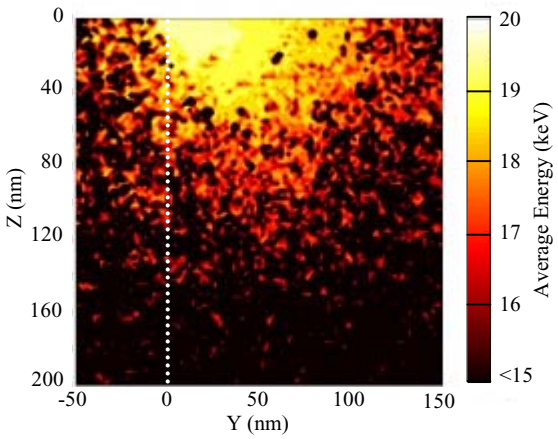

FIG. 3. Average energy of electrons in a 2 nm YZ slice, centered at X = 0 nm.

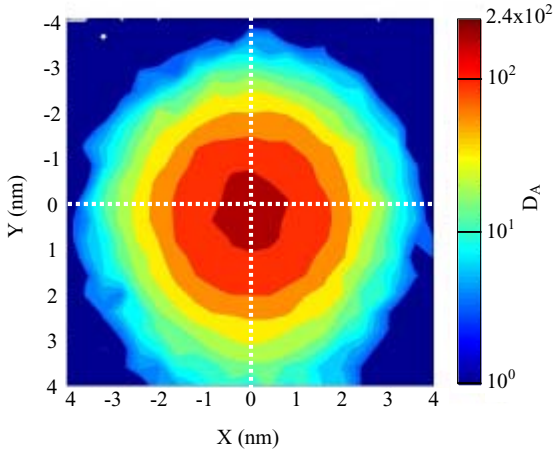

FIG. 4. Density of secondary electrons per unit area in the surface (XY) plane. Beam at 70^0 to normal. Log scale.

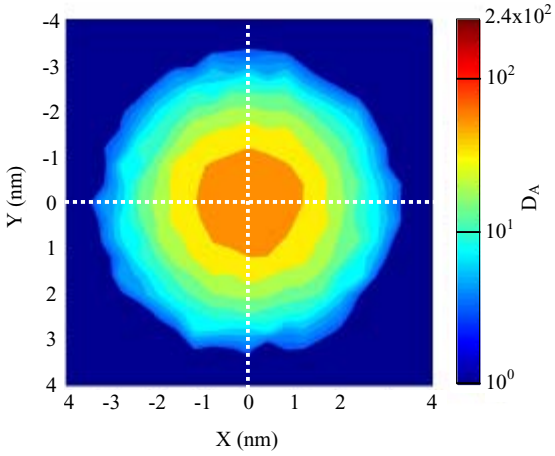

FIG. 5. Density of secondary electrons per unit area in the surface (XY) plane. Beam at normal incidence. Log scale.

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