Visualizing Monte Carlo Data in Microscopy

Andrew Deal, Xiaodong Tao, and Alwyn Eades (jae5@lehigh.edu)

Department of Materials Science and Engineering
Lehigh University, 5 East Packer Avenue, Bethlehem, PA 18015

Monte Carlo simulations are widely used by microscopists to investigate and understand beam/specimen interactions. When first applied to the SEM in the 1960s, use was restricted by availability and the speed of computers, but today this is no longer the case. A variety of commercial packages, such as Electron Flight Simulator [1] and Metrologia [2], and freely available programs, such as CASINO [3] and Joy's Single Scattering Model [4], exist. Additionally, modern computers can complete a reasonably detailed simulation in minutes. One issue, however, not receiving much attention is the representation of the Monte Carlo data that is now so easily generated. Here we address some of the shortcomings of conventional representations and suggest a more insightful alternative.

A conventional representation of Monte Carlo data from an SEM simulation is shown in figure 1A. An interaction volume is generated for a normal incidence 20 keV beam on a nickel specimen. This representation was constructed using the typical "connect-the-dots" method, where each elastic scattering event is projected onto the image plane and connected to its sequential neighbors by straight lines. The connecting lines are color-coded so that lower energies are darker. It is tempting to infer the size and shape of the interaction volume from figure 1A, but this conventional representation is very misleading. Compared to figure 1B, the interaction volume of figure 1A appears smaller; however, both figures represent the exact same beam/specimen conditions. Simply fewer electrons are simulated for figure 1A. Moreover, there appear to be only minor differences between the interaction volume representations of figures 1B and 1C. However, the latter was generated with a beam of near-grazing incidence (70 degrees from normal). Physically, the interaction volumes for normal and near-grazing incidences are very different, with the latter generating many more backscattered electrons due to its asymmetry. The conventional representation fails to make this clear.

A more insightful representation of the interaction volume should be independent of the number of simulated electrons and clearly differentiate between a beam of normal and of near-grazing incidence. Figure 1D shows the density of scattering events per volume element, D_V, for the identical simulation parameters as figures 1B and 1C. This alternative representation was constructed for a 2 nm thick slice of the interaction volume parallel to the beam. The slice volume was sampled in 2x2x2nm voxels. The scattering event count was normalized by the number of simulated trajectories divided by 10^6. The asymmetry of the tilted beam interaction volume is easily seen. Moreover, the size of the interaction volume is more accurately represented. The log scale shows both the extent of the interaction and the importance of the region near the impact point. Magnified views of this alternative representation are presented in figure 2, with the same simulation parameters as the corresponding subfigures in figure 1. Although figures 1A and 1B were simulated with a significantly different number of trajectories (5,000 and 100,000, respectively), the size and shape of the high density region ($>10^3$ nm^{-3}) remains constant. Thus, this alternative representation is independent of the number of simulated trajectories. We encourage the adoption of this method of visualization to reduce some of the inherent confusion in the conventional representation of microscopy Monte Carlo data [5].

References

[1] Université de Sherbrooke. "CASINO." http://www.gel.usherb.ca/casino/What.html
[2] Spectel Research. "Metrologia." http://www.spectelresearch.com/metrolog.html
[3] Advanced Microbeam Inc. "Electron Flight Simulator." http://www.advancedmicrobeam.com/efs.htm
[4] D.C. Joy, *Monte Carlo Modeling for Electron Microscopy and Microanalysis*, Oxford University Press, New York, 1995.
[5] Support from DOE, under grant DE-FG02-00ER45819, is gratefully acknowledged.

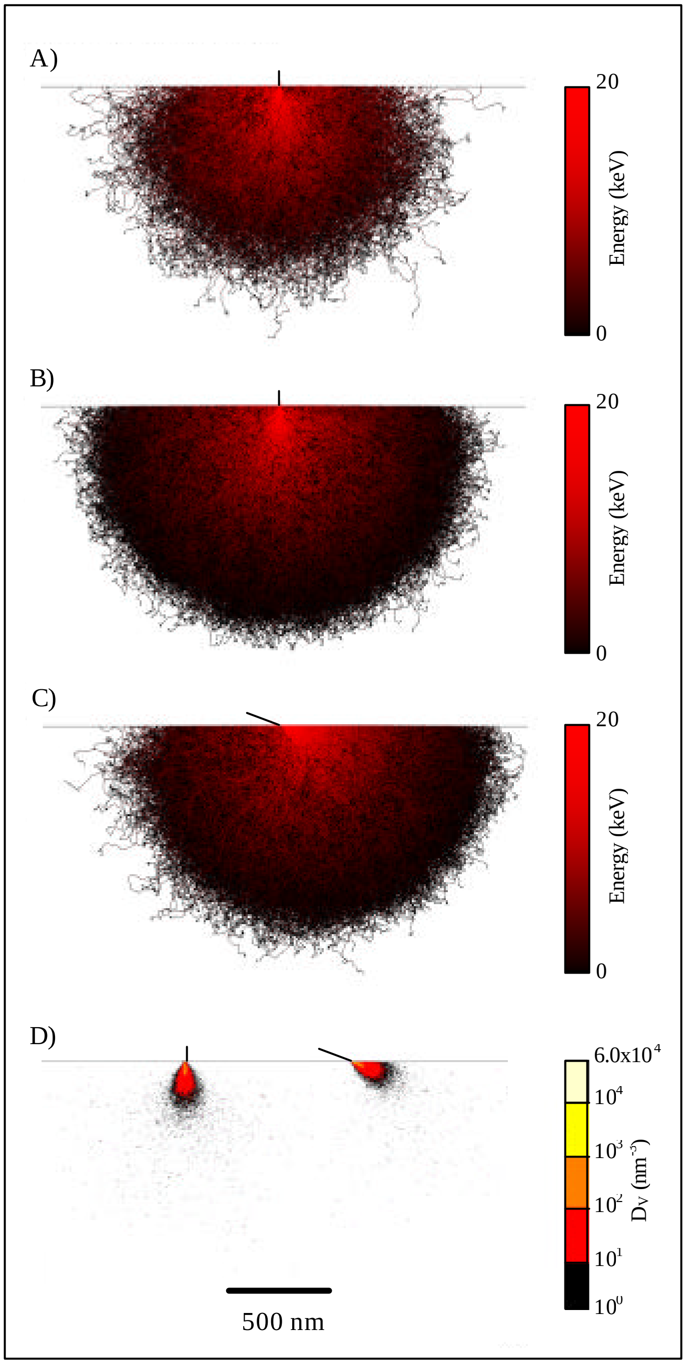

FIG. 1. Visualizing a 20kV beam on Ni. Conventional representations: A) 0^o tilt, 5k trajectories B) 0^o tilt, 100k trajectories C) 70^o tilt, 100k trajectories. Alternative representation: D) 0^o and 70^o tilt, 100k trajectories

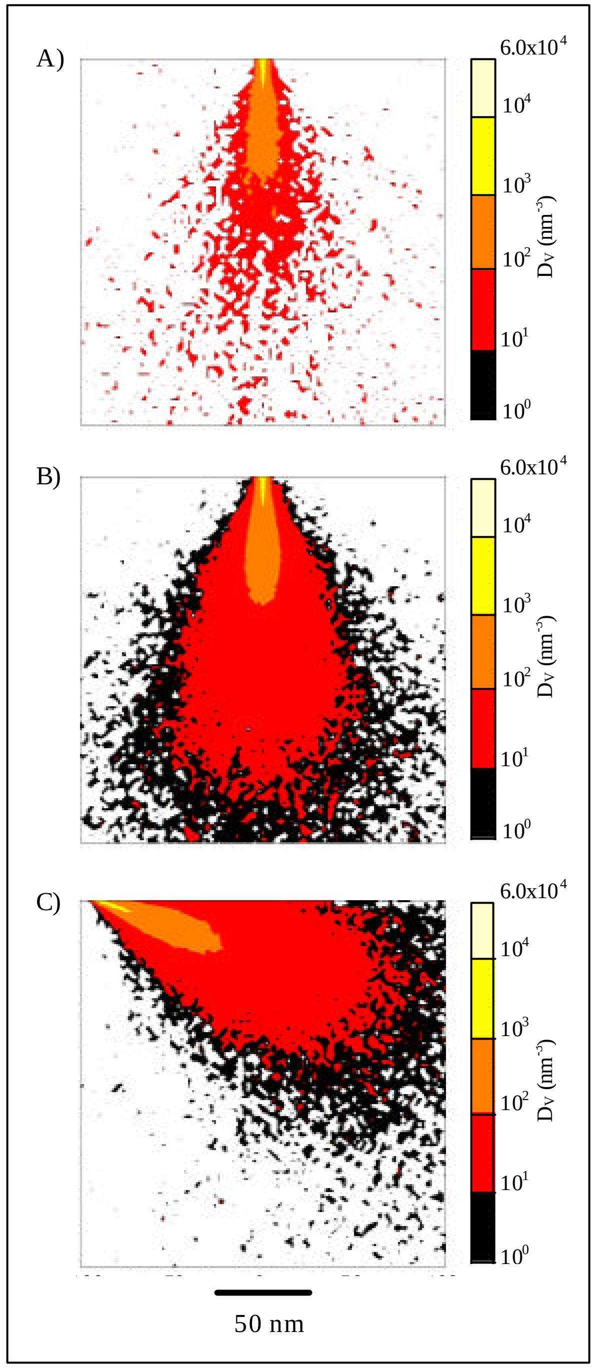

FIG. 2. Magnified alternative representations. Letters match conventional representations in figure 1: A) 0^o tilt, 5k trajectories B) 0^o tilt, 100k trajectories C) 70^o tilt, 100k trajectories