Monte Carlo Modeling of Electron Backscattering from Carbon Nanotube Forests

Md. Kawsar Alam and Alireza Nojeh[1]
Department of Electrical and Computer Engineering, University of British Columbia, Vancouver BC V6T 1Z4, Canada

[1]Corresponding Author: anojeh@ece.ubc.ca

Given the nanoscale and hollow structure of carbon nanotubes, their interaction with electron beams [1-3] and imaging mechanisms in electron microscopy [4-7] are expected to be quite different than those of bulk materials. However, to the best of our knowledge, there has been no report on the modeling of electron trajectories in carbon nanotubes or nanotube-based structures such as forests of vertically aligned nanotubes, and their secondary and backscattered electron coefficients.

In our recent experiments, we have observed unusual electron backscattering behavior from cylindrically shaped nanotube forests with diameters of a few hundred micrometers (figure 1 inset): The backscattering yield first decreases and then increases as a function of primary beam energy (figure 2). We attribute this to the porous nature of the structure that leads to unusually high electron range.

Monte Carlo methods have been used extensively to model electron-solid interaction. A nanotube forest, on the other hand, is a semi-regular array of a large number of sub-structures (individual nanotubes) with empty space in-between them. This forms an inhomogeneous and anisotropic structure and cannot be treated in the same manner as a regular bulk material. We present a new Monte Carlo tool, capable of simulating the electron trajectories in nanotube forests, taking into account the underlying nanostructured nature of the material. The theoretical framework is based on the one described in [8]; however, we adaptively modify the scattering angle distribution at each step of the simulation process according to the local neighborhood (how the nanotubes are positioned, their diameters, inter-nanotube distances, etc). This provides additional degrees of freedom in the Monte Carlo program that can be directly related to the internal structure of the nanotube forest. Figure 1 shows 100 electron trajectories through a 500-μm-diameter cylindrical forest of vertically aligned carbon nanotubes obtained using the program. Figure 2 shows a comparison between experimental backscattering data and the Monte Carlo simulation results for an example set of structural parameters of the forest. The program was implemented in Matlab and, despite treating the internal nanoscale aspects of the forest, the simulation time scales linearly with the overall dimensions of the structure. This allows the simulation of even macroscopically-sized structures in reasonable time on a regular computer. The approach can also be used to investigate super structures made from other nanoscale elements.

References

[1] A. Rivacoba and F. J. Garcia de Abajo, Physical Review B **67**, 085414-1—085414-8 (2003)
[2] A. Nojeh *et al.*, Physical Review Letters **96,** 056802-1—056802-4 (2006)
[3] M. K. Alam *et al.*, Physica E **42**, 124-131 (2009)
[4] T. Brintlinger *et al.*, Applied Physics Letters **81,** 2454-2456 (2002)
[5] Y. Homma *et al.*, Applied Physics Letters **84**, 1750-1752 (2004)
[6] W.K. Wong *et al.*, Scanning **28**, 219-227 (2006)
[7] P. Finnie *et al.*, Nanotechnology **19**, 335202-1—335202-6 (2008)
[8] R. Browning *et al.*, Scanning **17**, 250-253 (1995)

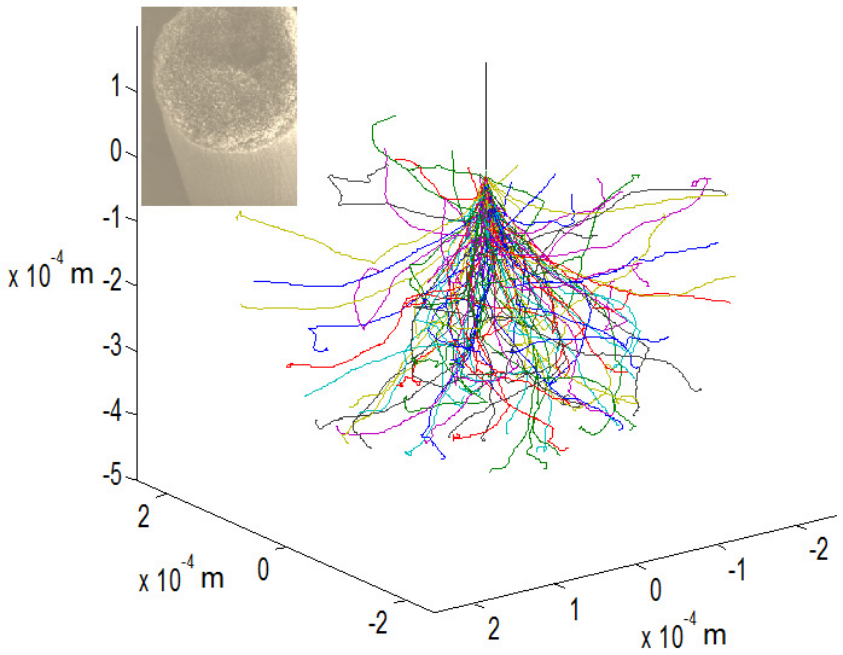

Figure 1. 100 electron trajectories (primary energy: 20 keV) through a 500-µm-diameter cylindrical forest of vertically aligned carbon nanotubes, obtained using the described Monte Carlo program (Inset: Scanning electron micrograph of the forest)

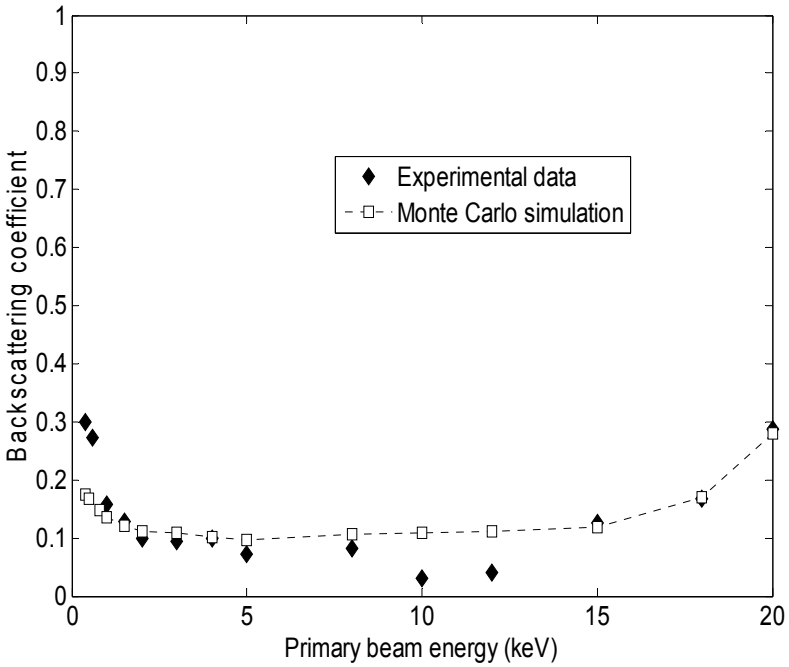

Figure 2. Comparison of experimental and simulation results for the electron backscattering coefficient from the 500-µm-diameter cylindrical nanotube forest. 10,000 electron trajectories were simulated at each primary energy to obtain the coefficient.