AbstractID: 8923 Title: Elastic scattering of electrons in gold: an event-by-event simulation algorithm based on the NIST cross-section data

Purpose: An increasing number of studies report on new approaches to detection and therapy of cancer based on the use of gold nanoparticles. Interaction of these nanoparticles with ionizing radiation, used either for diagnostic or therapeutic purposes, distorts the radiation field, especially on a microscopic scale. Monte Carlo calculation of dose distributions on such a scale, and microdosimetric analysis require event-by-event algorithms. The purpose of this study was to develop an event-by-event algorithm for simulation of electron elastic scattering in gold that is based on accurate cross sections from the NIST data base, Version 3.1.

Method and Materials: Angular dependencies of the NIST singly differential cross sections were fitted with a linear combination of the Wentzel cross section and Legendre polynomials of up to the 11th order. An algorithm was developed for sampling a scattering angle from the distribution represented by this linear combination. The algorithm is based on a rejection scheme. An angle is sampled from a simple distribution that has three components represented by Wentzel, isotropic, and backscatter (peak at π) terms. The sampled angle is rejected with a probability depending on the ratio of this simple distribution and the desired one. For some applications the three component distribution can be a sufficiently accurate representation of the NIST cross sections.

Results: Fitting parameters have been determined for electron energies in the range from 50 eV to 1 keV. Total cross sections calculated with these parameters agreed with the NIST data within 2×10^{-4} % and transport cross sections agreed within 0.5%. The algorithm has been implemented in a computer code and tested. The probability of accepting an angle in the rejection scheme was in the range of 0.25 to 0.54 depending on electron energy.

Conclusion: An algorithm has been developed for accurate simulation of electron elastic scattering in gold.