doi: 10.1017/S1431927609097475
Microsc Microanal 15(Suppl 2), 2009

Visualization and Simulation Optimization of PENELOPE through a Graphical Interface

Philippe T. Pinard*, Hendrix Demers**, Francesc Salvat***, Raynald Gauvin*

* Materials and Mining Eng. Dept., McGill University, 3610 University St., Montreal, Quebec, Canada H3A 2B2

** College of Nanoscale Science and Engineering, SUNY-University at Albany, 251 Fuller Road, Albany, NY, 12203

*** Facultat de Fisica (ECM), Universitat de Barcelona, Diagonal 647, Barcelona, Spain 08028

Monte Carlo codes for simulating the transport of electrons in matter are useful tools for interpreting experimental results in electron microscopy and EPMA. The code PENELOPE [1] uses a detailed scheme to simulate electron and photon histories in complex geometries. Since individual interactions are simulated in chronological succession, the code allows the simulation of X-ray fluorescence in complex geometries, which is not always possible with Monte Carlo models based on the continuous slowing-down approximation. This advantage is counter-balanced by significantly longer simulation times. The efficiency of the simulation can be increased by using variance-reduction techniques. The main program PENEPMA [2] performs simulations of X-ray spectra from samples irradiated by electron beams, for various detector positions and different solid angles; it also provides energy and angular distributions of electrons and photons that emerge from the sample.

To facilitate the use of the code PENEPMA and the interpretation of the results, a cross-platform graphical interface written in Python has been developed. This tool allows to create easily input data sets for specific simulations, by offering the user a set of common geometries and corresponding default parameters. For instance, common geometries such as a bulk substrate, couples with vertical and horizontal boundaries, or a spherical inclusion in a substrate can easily be defined, and the various phases can be assigned arbitrarily complex compositions. The positions of X-ray detectors are automatically determined according to the geometry, to give fast and precise results. Problems that require long simulation times, such as line scans or simulations for multiple electron energies can be run in batch mode. The characteristics of the electron beam (Gaussian energy distribution, angular divergence) are set by the user; the allowed degrees of freedom can be used for spatial resolution studies. While tracking the progress of the simulation the interface offers a live preview of the results. Finally, simulations can be run directly from the interface or saved as input files of PENEPMA to be run from the command line.

PENEPMA makes extensive use of interaction forcing, a variance-reduction technique that consists of artificially increasing the probability of occurrence of those interactions that are relevant to the considered problem. In the case of EPMA simulations, the interactions that can be forced are electron bremsstrahlung emission, inner-shell ionization by electron impact, Compton scattering of X-rays and photoelectric absorption. Depending on the geometry and composition, there is an optimal value of the forcing factor, which maximizes the efficiency of the simulation and, consequently, minimizes the simulation time (see ref. [2]). Figure 2 shows the variation of the efficiency of a hemispheric detector when only electron interactions (bremsstrahlung emission and inner-shell ionization) are forced. For all elements, the maximum efficiency is found for $F_{\text{int}}(e)$ values between about 40 and 100. The effect of forcing interactions of X-rays was then studied using electron forcing factors equal to 40 and 100 (Figure 3). The effect of forcing interactions of X-rays does not improve the efficiency of the EPMA spectrum appreciably. However, it does have an effect on the calculation of fluorescence corrections. For all simulations, the difference between the intensity calculated with and without interaction forcing is less than 1% in the region near the maximum efficiency, which is less than the statistical uncertainties of the simulation results. That is, the use of interaction forcing does not alter the final results, and reduces the simulation times needed to attain a given accuracy significantly. More simulations are underway to verify the effects of complex composition and geometry on the efficacy of interaction forcing.

As an output from the simulations, $\varphi(\rho z)$ curves can be obtained from the probabilities of generated and emitted X-rays (Figure 4). The fluorescent contribution can be evaluated separately as shown in Figure 5. Another feature of our interface is the visualization of the interaction volume by tracking primary and second generation electrons, a useful tool to evaluate the resolution near interfaces of different densities as shown in Figure 6.

[1] F. Salvat, J.M. Fernández-Varea and J. Sempau, "PENELOPE. A Code System for Monte Carlo Simulation of Electron and Photon Transport"' (OECD/NEA Data Bank, Issy-les-Moulineaux, France, 2006).

[2] X. Llovet and F. Salvat (2008), PENEPMA, a Monte Carlo code for the simulation of x-ray emission spectra using PENELOPE, 38 pp.

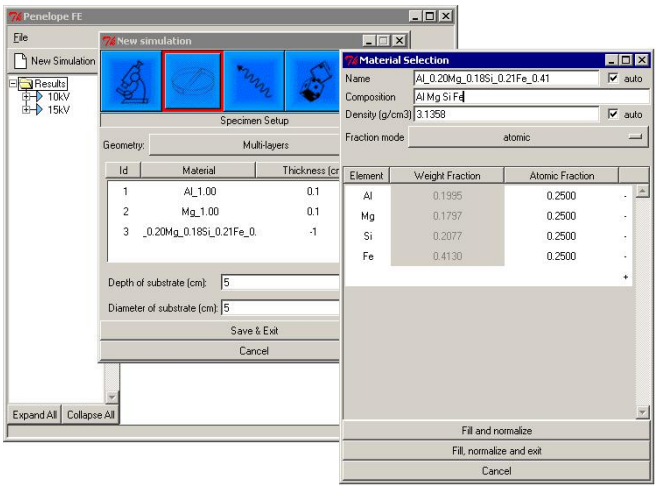

Fig. 1: Screen shot of the graphical interface showing how different material composition can be entered for a multi-layers geometry.

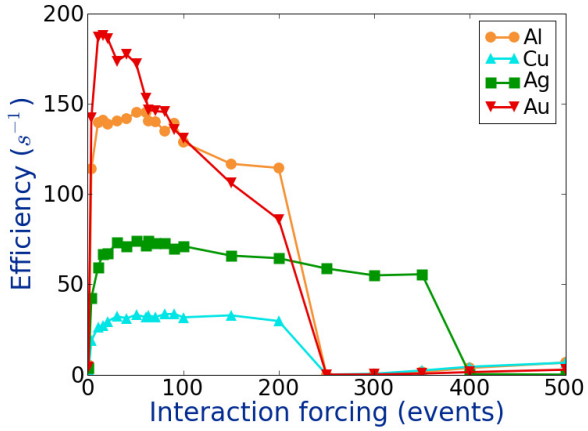

Fig. 2: Effect of electrons interaction forcing on the average efficiency of a hemispheric detector. The same factor was used for hard bremsstrahlung emission and inner-shell ionization. Each simulation was run for 12 hours (more than 10 millions electrons). Accelerating voltage of 15kV, normal incident beam, bulk substrate.

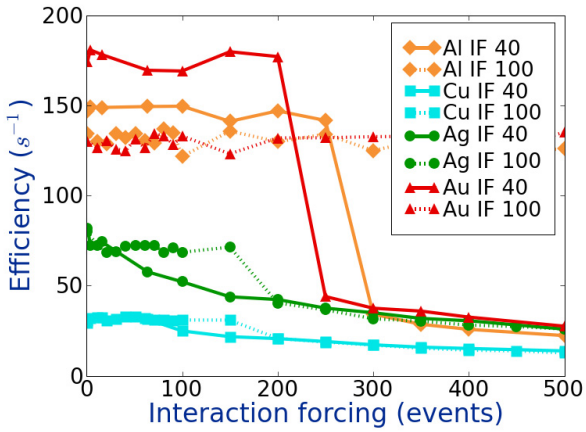

Fig. 3: Effect of X-rays interaction forcing on the average efficiency of a hemispheric detector with electrons interaction forcing indicated in the legend. The same factor was used for Compton scattering and fluorescence. Same conditions as Fig. 2.

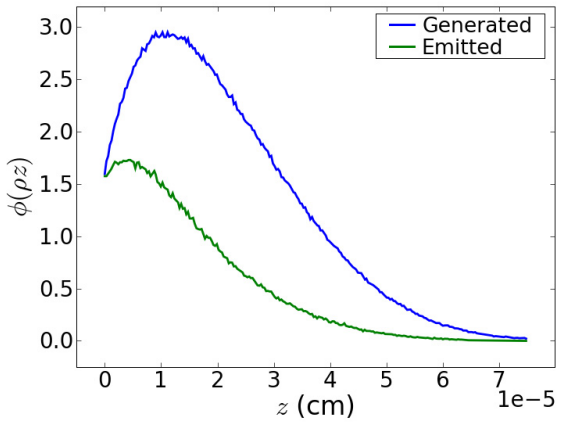

Fig. 4: Distribution of generated and emitted Cu L_α X-rays in a pure Cu substrate at 15kV and a thin-film of 20nm.

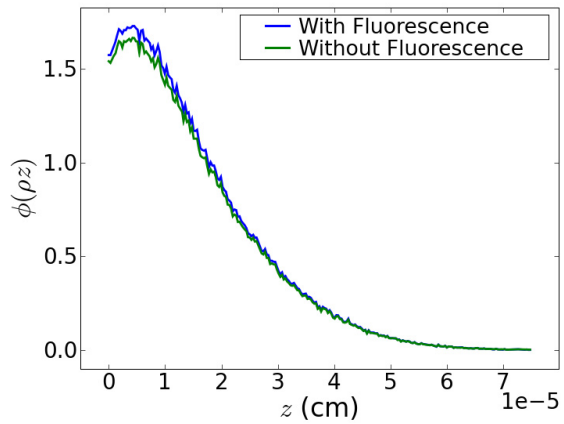

Fig. 5: Distribution of emitted Cu L_α X-rays with and without fluorescence X-rays. Same conditions as Fig. 4.

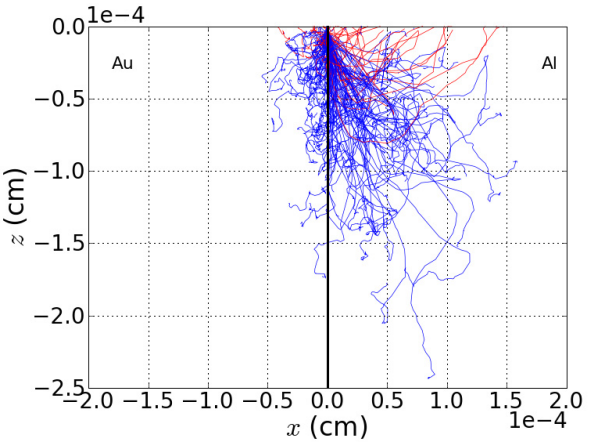

Fig. 6: Electrons interaction volume of an Au-Al couple showing the absorbed (blue) and backscattered (red) electrons at 15kV with a beam diameter of 10nm. 500 trajectories are shown.

https://doi.org/10.1017/S1431927609097475 Published online by Cambridge University Press