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Monte Carlo Simulation of EPMA Measurements on Complex Specimens Using PENELOPE

F. Salvat* and X. Llovet**

* Facultat de Física (ECM), Universitat de Barcelona. Diagonal 647. 08028 Barcelona. Spain.
** Serveis Científico-Tècnics. Universitat de Barcelona. Lluís Solé i Sabarís, 1-3. 08028 Barcelona. Spain.

PENELOPE [1] is a general purpose Monte Carlo code system for the simulation of coupled electron-photon transport in complex geometries. The modeling of particle interactions is based on the most accurate interaction data available, limited only by the required generality of the code. For the sake of generality, it is assumed that molecular binding effects are negligible and, consequently, the molecular cross sections are obtained by summing the contributions from all the atoms in a molecule. This additivity approximation is valid for electrons with energies larger than about 1 keV. Nevertheless, the numerical interaction database covers the energy range from 50 eV up to 1 GeV.

The simulation of electron (and positron) histories is based on a flexible mixed algorithm. In the energy range of interest in EPMA applications, the code can be run in the detailed mode, where all interactions undergone by the transported electrons are simulated individually. Photons are also followed using the conventional detailed simulation scheme. The considered interaction mechanisms for electrons are elastic scattering, inelastic collisions and bremsstrahlung emission. The relevant interaction processes for photons are Rayleigh (coherent) scattering, Compton (incoherent) scattering and photoelectric absorption. Individual interactions are described according to the adopted differential cross sections, which are usually given in numerical form. In the interactions of a transported particle, secondary knock-on electrons can be generated and, when the interaction produces a vacancy in an inner atomic shell, the emission of characteristic x rays and Auger electrons is simulated. Secondary particles are stored in memory and transported after completion of the current particle history. Thus, each electron impinging on the specimen generates a shower of electrons and photons; all particles are followed until they reach a predefined "absorption" energy.

The code system includes the geometry subroutine package PENGEOM, which simulates the transport of radiation through material systems consisting of uniform bodies limited by quadric surfaces. PENGEOM is able to handle very complicated geometries, with up to 5,000 bodies and 10,000 limiting surfaces. The geometry is defined through an input file, to be prepared by the user. The geometry routines allow "cloning" previously defined bodies and groups of bodies, and the easy generation of large quasi-periodic structures. If certain simple rules are followed, the simulation speed is practically independent of the complexity of the system. This geometry tool permits the simulation of multilayers, inclusions, lamellae and other structures usually found in EPMA specimens.

Finally, PENELOPE allows the user to apply a number of variance reduction techniques, which

effectively speed up the simulation of specific quantities without biasing the results. In particular, the simulation of x-ray spectra, which is very slow when the code operates in the detailed mode, can be accelerated by using interaction forcing.

Detailed simulation of electrons consistently accounts for the effect of geometrical inhomogeneities on the angular and energy distributions of backscattered electrons. By tracking individual photons (characteristic x rays and bremsstrahlung quanta), the emission of fluorescent x rays is properly accounted for. Therefore, simulations of EPMA measurements with PENELOPE provide a consistent description of backscattering and fluorescence corrections, for the specific geometry of the simulated sample.

PENELOPE is structured as a set of subroutine packages; the user is supposed to provide a steering main program adapted to his/her specific experiment, which controls the evolution of simulated histories and scores the relevant quantities. A dedicated main program for the simulation of EPMA experiments, named PENEPMA is available from the authors [2,3]; this program is not part of PENELOPE. To simulate x-ray spectra from a given sample, the user must provide the corresponding geometry definition file, define the energy and direction of the incident electron beam and specify the position of the photon detectors (up to ten different detectors can be defined). For each detector, PENEPMA generates the energy spectrum of detected photons, as well as the spectrum of characteristic x-ray lines (with the bremsstrahlung background removed).

Practical examples of simulated spectra for specimens with complex geometries will be presented. Results will be discussed from the perspective of conventional quantification procedures.

References

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