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PENELOPE-2005. A MONTE CARLO CODE SYSTEM SUITABLE FOR SIMULATION OF X-RAY SPECTRA

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Monte Carlo (MC) simulation of x-ray spectra emitted from targets bombarded by electron beams is of interest in x-ray microanalysis, especially for the quantitative interpretation of measurements under unconventional conditions. Examples are the analysis of non-homogeneous samples (at the micron scale) such as particulate matter, multilayer films or samples with rough surfaces, the analysis at grazing-angle incidence or at very-low incident electron energies. The usefulness of MC simulation stems from its ability to incorporate realistic interaction models devoted to describing the evolution of electrons in the sample and to track not only primary electrons but also all secondary radiations (electrons and photons) generated within the sample.

PENELOPE is a general-purpose MC code that allows the simulation of coupled electron-photon transport in targets consisting of bodies with arbitrary composition, for an energy range from 100 eV to 1 GeV [1]. The interaction models implemented in the code are based on the most reliable information available at present, limited only by the required generality of the code. These models combine results from first-principles calculations, semi-empirical models and evaluated data bases. PENELOPE is coded as a set of FORTRAN subroutines that perform the random sampling of interactions and the tracking of electrons and photons. Hence, the user must provide a main program so as to follow the particle tracks through the target and keep score of the quantities of interest.

The latest public version of PENELOPE was released in 2003 and it is available from the OECD Nuclear Energy Agency Data Bank (`http://www.nea.fr`). We are now preparing a new version 2005 of the code that contains substantial improvements in the interaction models and in the geometry routines, which will be released in a few months. Namely, it incorporates numerical differential cross sections for elastic scattering obtained from partial-wave analysis using Dirac-Fock atomic electron densities and the exchange potential of Furness and McCarthy. These cross sections were obtained by using the code ELSEPA [2]. Another improvement is that it allows the simulation of characteristic x rays and Auger electrons that result from vacancies produced in M-shells. The structure of the code is still flexible enough to enable the use of alternative, more elaborate interaction models when available. For instance, the cross sections for ionization of inner shells (by electron impact) implemented by default, which were evaluated using the method of virtual quanta, are reliable only for electrons with kinetic energies well above the ionization threshold. In the present simulations we have replaced these cross sections by more accurate values calculated from the distorted-wave Born approximation [3].

As in previous versions of PENELOPE, the tracking of particles in the target can be done automatically with the aid of the subroutine package PENGEOM, provided the target is defined as a

set of bodies limited by quadric surfaces. PENGEOM-2005 allows the use of previously-defined bodies to define new bodies and the grouping of bodies into modules, which in turn can form part of larger modules. This modular structure makes it possible a substantial reduction of the computation time of the geometry routines. Version 2005 of PENELOPE also includes a generic main program PENMAIN that is devised to allow occasional users to employ PENELOPE without having to do any programming work. Indeed, the operation of PENMAIN is completely controlled from the input file. Although it is impossible to cover all possible applications with a closed program, PENMAIN is flexible enough to address a broad class of practical problems, including the simulation of x ray spectra from samples irradiated by electron beams.

In this communication, we describe the interaction models and simulation algorithms implemented in PENELOPE-2005 and we show the capabilities of PENMAIN as a tool for quantitative x-ray microanalysis, particularly for interpretating x ray spectra obtained under unconventional conditions.

References

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