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THE PHYSICS OF ELECTRON/POSITRON TRANSPORT IN PENELOPE

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Abstract

PENELOPE is a general-purpose Monte Carlo code system for simulation of coupled electron-photon transport in arbitrary materials and in the energy range from a few hundred eV to ∼1 GeV. In this communication we sketch the physical interaction models implemented in the code as well as recent improvements of the electron/positron transport mechanics (i.e. the numerical algorithm for generating random electron/positron tracks). The energy-dependence correction adopted in the new transport mechanics leads to improved stability under variations of the simulation parameters selected by the user.

1 Introduction

PENELOPE (an acronym for "PENetration and Energy LOss of Positrons and Electrons") is a general-purpose code system for Monte Carlo simulation of coupled electron-photon transport in the energy range from a few hundred eV up to ∼1 GeV[1,2]. The kernel of the code system is a library of FORTRAN subroutines that perform simulation of electron-photon showers in homogeneous materials of arbitrary compositions. Geometry operations and scoring of relevant quantities are performed from the main program, which is to be provided by the user. The complete code system, including the interaction database, auxiliary subroutine libraries and examples of main programs are publicly available through the NEA Data Bank[1] and the RSICC[2].

The simulation of photons is performed by means of the conventional, detailed (interaction by interaction) method and will not be considered here. The simulation of electrons/positrons is much more difficult than that of photons, because of the large number of interactions suffered by high-energy charged particles in the course of their slowing down; this is a direct consequence of the fact that inelastic interactions of charged particles involve preferentially small energy losses (the average energy loss per inelastic collision is of the order of 50 eV). The traditional approach to cope with this problem has been using class I (condensed) simulation methods in which the global effect of multiple interactions along a given path length is described by using approximate multiple scattering theories[3]. This solution is not fully satisfactory due to the approximations

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underlying the multiple scattering theories and/or to the fact that these theories provide only a partial description of the transport (see e.g. Salvat et al., 1996[1]). A differentiating feature of PENELOPE is the use of full class II (mixed) simulation of electrons/positrons, i.e. interactions are classified into hard and soft, and the hard ones are simulated individually. The code also implements a sophisticated transport mechanics algorithm to generate space displacements and energy loss from soft events (the so-called random hinge method), which accounts for the energy dependence of the interaction probabilities in an accurate way.

The models considered here correspond to the version 2001 of PENELOPE, which will be released next November. Some of these models differ substantially from the ones in previous versions of the code. In particular, the random hinge algorithm has been reformulated to account for most of the energy dependence of the interaction probabilities. This largely improves the robustness of the algorithm and minimizes the influence of user-selected parameters on the accuracy of the simulation results.

2 Electron/Positron Interaction Cross Sections

In this section we describe briefly the physical basis of the models used for the simulation of electron/positron interactions. A much more detailed description of these models can be found in the references and in the PENELOPE report[4]. We shall not consider positron annihilation, which is simulated according to the Heitler DCS for two-photon annihilation with free electrons at rest (see Salvat et al., 1996[1]).

2.1 Elastic scattering

Elastic interactions are described by means of the modified Wentzel (MW) model, in which the differential cross section (DCS) is expressed as a mixture of a Wentzel (screened Rutherford) distribution and either a triangle or a delta distribution[4]. The coefficients in the MW model are determined in such a way that the mean free path between elastic collisions and the first and second moments of the angular deflection $\mu = (1-\cos\theta)/2$ in each collision coincide with the results from accurate partial-wave calculations. The analytical form of the DCS facilitates the simulation of random events and the formulation of the mixed algorithm. When transported particles undergo multiple elastic scattering, the results obtained with the MW model do not differ significantly from those simulated from the more accurate partial-wave numerical DCSs.

2.2 Inelastic scattering

Inelastic scattering is described by means of the plane-wave (first) Born approximation. The fundamental feature of this approximation is that the DCS (differential in the energy loss and recoil energy) factorizes into the product of a purely kinematical factor and a structure factor (the so-called generalized oscillator strength or GOS) that is independent of the energy of the projectile (see e.g. Inokuti, 1971[5]). Elementary excitations/ionizations are described by means of the Sternheimer-Liljequist oscillator model, i.e. the GOS is represented as a family of delta-oscillators, with resonance energies adjusted to to give the "correct" (ICRU) stopping power at high energies[1]. For relatively large recoil energies (i.e. large momentum transfers, each oscillator behaves as a set of free electrons and its response is described by means of the Møller and Bhabha DCSs for electrons and positrons, respectively. This GOS model provides values of the stopping power that are essentially equal to those recommended by the ICRU and also yields realistic estimates of the mean free path between inelastic collisions and the energy straggling parameter for the whole energy range from $\sim$100 eV to 1 GeV. The details of the GOS model were selected so as to ensure

accuracy and, at the same time, allow the random sampling of the energy loss and recoil energy by means of purely analytical methods.

2.3 Bremsstrahlung emission

The energy of bremsstrahlung photons is sampled from the scaled energy-loss DCSs tabulated by Seltzer and Berger[6], which represent the state of the art in theoretical bremsstrahlung data. For a given material, the scaled DCS depends only on the kinetic energy of the projectile E and on the photon energy W, and it is easy to sample the photon energy by using appropriate interpolation/sampling techniques.

The intrinsic angular distribution of bremsstrahlung photons (relative to the direction of the projectile) is sampled from an analytical form that approximates (very closely) the partial wave data tabulated by Kissel, Quarles and Pratt[7]. We have found that the actual angular distribution reduces to a simple analytical form under a Lorentz boost (see e.g. Jackson, 1975[8]) with an appropriate velocity, different from the speed of the projectile). This fact enables us to express the angular distribution by means of an analytical formula (with parameters that vary smoothly with the energies of the projectile and the emitted photon) from which the direction of the emitted photon can be sampled analytically, i.e. in an easy and exact manner (see Salvat et al., 2001[4]).

3 Electron Transport Mechanics

As mentioned above, PENELOPE does class II simulation of electrons/positrons. To clarify the meaning of this, let's assume a projectile electron with kinetic energy E moving in a medium of given composition. The *total* DCS (i.e. the sum of elastic, inelastic and bremsstrahlung contributions) is a function of the energy loss W and the angular deflection $\mu = (1-\cos\theta)/2$. Interactions are classified as "soft" and "hard" by introducing suitable cutoffs $W_{\rm c}$ and $\mu_{\rm c}$ for the energy loss and angular deflection, respectively. It is always possible to select the cutoffs in such a way that the average number of hard collisions along an electron track is small, say of the order of 10. Hard collisions can then be simulated in a detailed way (individually). The soft collisions that occur between a pair of consecutive hard collisions produce gentle energy losses and deflections, which can be accurately described by means of a multiple scattering approach (i.e. using condensed simulation). The strategy used in PENELOPE consists of moving the transported electrons by free steps (where direction and energy remain constant) and simulating interaction events (i.e. energy losses and deflections) at the end of each free step. The lengths of the steps and the kind of events that occur are determined according to the "random hinge method" (Salvat et al., 2001).

Let $\mathrm{d}\sigma^{(\rm h)}/(\mathrm{d}W\,\mathrm{d}\mu)$ denote the total DCS for hard interactions (which vanishes for $W<W_{\rm c}$ and for $\mu<\mu_{\rm c}$). The total "hard" cross section is

$$\sigma^{(\rm h)}(E)=\int_{\mu_{\rm c}}^{1}\mathrm{d}\mu\int_{W_{\rm c}}^{E}\frac{\mathrm{d}\sigma^{(\rm h)}}{\mathrm{d}W\,\mathrm{d}\mu}, \tag{1}$$

and the associated mean free path is $\lambda^{(\rm h)}=\mathcal{N}\sigma^{(\rm h)}(E)$, where $\mathcal{N}$ denotes the density of atoms (or molecules) per unit volume. Notice that the mean free path is a function of the energy E of the projectile, which varies between consecutive hard interactions due to the effect of the soft interactions. As a consequence, $1/\lambda^{(\rm h)}(E)$ is the probability of interaction per unit path length, but $\lambda^{(\rm h)}$ does not represent the average distance between hard events. Similarly, the "soft" interactions are described by the cross section $\mathrm{d}\sigma^{(\rm s)}/(\mathrm{d}W\mathrm{d}\mu)$, which vanishes for $W>W_{\rm c}$ and for $\mu>\mu_{\rm c}$. PENELOPE simulates multiple soft interactions by means of "artificial" distributions that are defined by the first moments of the soft DCS, which again vary with the energy of the projectile.

In previous versions of the PENELOPE algorithm, the energy dependence of these parameters was disregarded. This required limiting the cutoff values so as to have suitably small energy losses

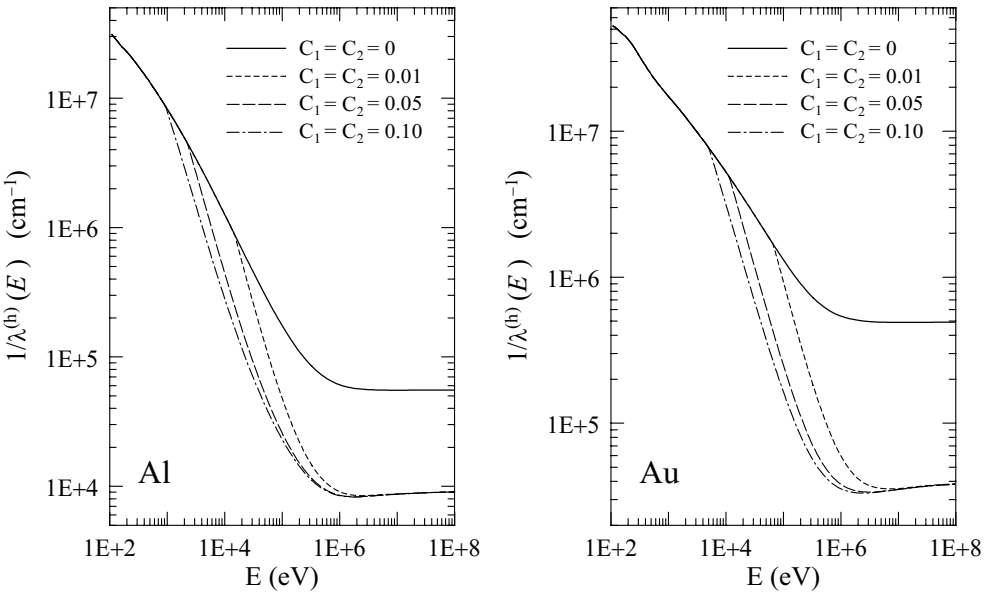

Figure 1: Inverse mean free path (interaction probability per unit path length) for hard interactions of electrons in Al and Au for various values of the simulation parameters (which correspond to different cutoff deflections μ_c). In al cases, the cutoff energy loss was $W_c = 100$ eV.

along each step and, therefore, it set a limit on the simulation speed. In the 2001 version of the code, this energy dependence is accounted for in a quite accurate manner, which is to the advantage of code accuracy and stability. The adopted solutions are described in detail in the PENELOPE manual (Salvat et al., 2001). Essentially, they make use of two facts. First, our energy straggling model allows us to set an effective upper limit for the energy loss along a step of given length. And, second, the inverse hard mean free path (as a function of E) does not have maxima[3] (see fig. 1). This implies that the energy dependence of the hard mean free path can be accounted for *exactly* and very efficiently. The energy variation of the moments of the soft interaction DCS are described by means of a linear approximation, which is accurate enough to permit step lengths of the order of 10 per cent of the Bethe range, which is conveneient for efficient class II simulation.

The transport mechanics adopted in PENELOPE is very accurate and stable under variations of the simulation parameters, due mostly to the effectiveness of the energy-dependence corrections. This is illustrated in fig. 2, which displays results from simulations of 511 keV electrons in aluminium (infinite medium); with radiative events switched off. Electrons started off from the origin of coordinates moving in the direction of the z axis. The simulation of each track was discontinued when the electron had travelled a path length s equal to 200 μm, and the distributions of the final electron energy and position coordinates were tallied; no secondary radiations were followed. Crosses represent results from detailed (interaction by interaction) simulations, continuous curves are results from class II simulations with relatively large cutoffs, which are 55 times faster than detailed simulation. Both calculations agree almost exactly, which proves that our class II simulation is indeed very accurate.

[3]This is so because our hard interaction mechanism includes elastic scattering. The inverse mean free path for hard (restricted) inelastic scattering and bremsstrahlung emission has a maximum at intermediate energies.

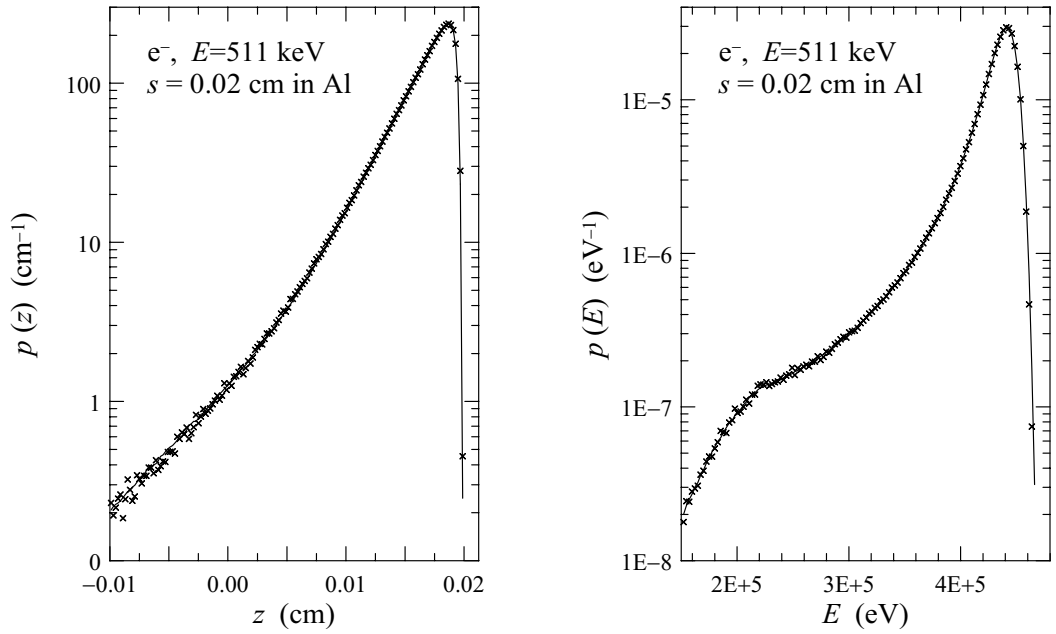

Figure 2: Results from the simulations of 511 keV electrons in aluminium described in the text. Crosses, detailed simulation; continuous curves, mixed simulation. $p(z)$ and $p(E)$ are the distributions of the z-coordinate and the energy E of the electron, after traveling the prescribed 200 μm.

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