ELSEVIER

Nuclear Instruments and Methods in Physics Research B 100 (1995) 31-46

NIM B
Beam Interactions with Materials & Atoms

PENELOPE: An algorithm for Monte Carlo simulation of the penetration and energy loss of electrons and positrons in matter

J. Baró [a], J. Sempau [b], J.M. Fernández-Varea [c], F. Salvat [c,*]

[a] Serveis Científico-Tècnics, Universitat de Barcelona, Martí i Franquès s/n, 08028 Barcelona, Spain
[b] Institut de Tècniques Energètiques, Universitat Politècnica de Catalunya, Diagonal 647 bis, 08028 Barcelona, Spain
[c] Facultat de Física (ECM), Universitat de Barcelona, Societat Catalana de Física (IEC), Diagonal 647, 08028 Barcelona, Spain

Received 30 September 1994

Abstract

A mixed algorithm for Monte Carlo simulation of relativistic electron and positron transport in matter is described. Cross sections for the different interaction mechanisms are approximated by expressions that permit the generation of random tracks by using purely analytical methods. Hard elastic collisions, with scattering angle greater than a preselected cutoff value, and hard inelastic collisions and radiative events, with energy loss larger than given cutoff values, are simulated in detail. Soft interactions, with scattering angle or energy loss less than the corresponding cutoffs, are simulated by means of multiple scattering approaches. This algorithm handles lateral displacements correctly and completely avoids difficulties related with interface crossing. The simulation is shown to be stable under variations of the adopted cutoffs; these can be made quite large, thus speeding up the simulation considerably, without altering the results. The reliability of the algorithm is demonstrated through a comparison of simulation results with experimental data. Good agreement is found for electrons and positrons with kinetic energies down to a few keV.

1. Introduction

The problem of the penetration and energy loss of fast electrons in matter has attracted great attention since the beginning of this century. Since most of our knowledge about nuclear, atomic, molecular and solid state structure has been, and is being, achieved by using electron beams to probe matter, this problem is of fundamental interest. A detailed description of electron, and positron, transport is required in a number of fields such as beta-ray spectrometry [1,2], electron microscopy [3] and electron and positron surface spectroscopy [4,5]. Accurate information on high energy electron and positron transport is also needed in radiation dosimetry and radiotherapy [6].

Electron multiple scattering processes were first treated on the basis of the transport theory [7,8]. Since the beginning of the sixties, with the increasing availability of fast computers, Monte Carlo (MC) simulation methods have been developed and applied to many experimental situations (see e.g. Ref. [9]). The characteristics of different MC simulation schemes depend mainly on the energy range of interest. "Detailed" MC simulation [10,11] where *all* scattering events experienced by an electron are described in chronological succession, is feasible at low energies. Detailed simulation is virtually exact, i.e. simulation results are identical to those obtained from the exact solution of the transport equation with the same scattering model (except for statistical uncertainties). For progressively higher energies, however, the average number of scattering events per track increases gradually and eventually detailed simulation becomes unfeasible.

For high energies, most of the MC codes currently available (e.g. ETRAN [9], EGS4 [12], GEANT [13]) have recourse to multiple scattering theories which allow the simulation of the global effect of a large number of events in a track segment of a given length (step). Following Berger [14], these simulation procedures will be referred to as "condensed" MC methods. The multiple scattering theories implemented in condensed simulation algorithms are only approximate and lead to systematic errors, which arise mainly from the lack of knowledge about the spatial distribution of the particle after travelling a given path length. These errors can be made evident by the dependence of the simulation results on the adopted step length [9]. To analyze their magnitude, one can perform simulations of the same experimental arrangement with different step lengths. Usually, it is found that the results stabilize when reducing the step length, but the computation time increases rapidly, roughly in proportion to the inverse of the step length. Thus,

* Corresponding author. Tel. +34 3 402 1186, fax +34 3 4021174, e-mail: cesc@ecm.ub.es

0168-583X/95/$09.50 © 1995 Elsevier Science B.V. All rights reserved
SSDI 0168-583X(95)00349-5

for each particular problem, one must reach a compromise between available computer time and attainable accuracy. It is also worth noting that, owing to the nature of certain multiple scattering theories and/or to the particular way they are implemented in the simulation code, the use of very short step lengths may introduce artifacts in the simulation results. For instance, the multiple elastic scattering theory of Molière [15], which is the one used in EGS4 based codes, is not applicable to step lengths shorter than a few times the elastic mean free path [16,17] and multiple elastic scattering has to be switched off when the step length becomes smaller than this value [18]. Evidently, stabilization for short step lengths does not necessarily imply that simulation results are correct. Condensed schemes also have difficulties to properly handle particle tracks in the vicinity of an interface, i.e. a surface separating two media of different compositions [18].

A third class of simulation schemes, the so-called "mixed" simulation methods [14,19,20], combines detailed simulation of hard events, i.e. events with polar scattering angle θ or energy loss W larger than previously selected cutoff values θ_S and W_c, with condensed simulation of soft interactions with $\theta < \theta_S$ or $W < W_c$. Owing to the fact that, for high-energy electrons, the differential cross sections (DCS) for the various interaction processes decrease rapidly when θ or W increase, cutoffs can be selected such that the mean number of hard events per track is sufficiently small to allow their detailed simulation (i.e. a few hundred at most). Hard events cause large angular deflections and energy losses, which can only be properly reproduced through detailed simulation. On the other hand, soft interactions have a mild effect on the evolution of the track, which can be accurately simulated by using a multiple scattering approach. Mixed simulation is preferable to condensed simulation because i) spatial distributions are more correctly simulated, ii) tracks in the vicinity of interfaces are properly handled, and iii) possible dependencies of the results on user-defined parameters are largely reduced.

In this paper we describe a mixed simulation algorithm called PENELOPE (an acronym that stands for PENetration and Energy LOss of Positrons and Electrons). The adopted single scattering DCSs for inelastic collisions and bremsstrahlung emission have been described by Salvat and Fernández-Varea [21]. Approximate simulation methods for elastic scattering have been considered in previous works [16,22]; here we adopt the W2D model introduced in Ref. [22].

In Section 2 we consider various aspects of the adopted single scattering DCSs and pertinent sampling techniques not covered in Refs. [21] and [22]. Mixed simulation strategies to speed up the simulation of high-energy particles are presented in Section 3. The complete simulation algorithm is described in Section 4. Section 5 contains an analysis of the stability of the simulation results under changes in the adopted cutoff values of the angular deflection and the energy loss. Finally, the reliability of this simulation scheme is demonstrated by comparing simulation results and experimental data.

2. Single scattering model

Let us consider a fast particle, electron or positron, with kinetic energy E moving in a single-element medium of atomic number Z. The extension to compounds and mixtures will be treated below. The number of atoms per unit volume is given by

$$N = \frac{N_A \rho}{A_w}, \tag{1}$$

where N_A is the Avogadro number, ρ is the mass density of the material and A_w is the atomic weight.

The possible interactions of the particle with the medium are elastic scattering, inelastic collisions and bremsstrahlung emission (and annihilation in the case of positrons). Each kind of interaction is characterized by a single scattering atomic DCS, which determines the associated mean free path and the probability density functions of the scattering angle θ and the energy loss W in each individual interaction. The DCSs adopted in PENELOPE are sufficiently accurate for most practical simulation purposes and permit the random sampling of the scattering angle and the energy loss completely analytically, so that sampling errors that could originate from numerical interpolation are readily avoided. It is worth pointing out that *multiple* scattering distributions are quite insensitive to the fine details of the single scattering DCSs. If the adopted DCSs have a physically reasonable shape, only a few quantities, obtained by integrating the DCS over θ or W, have a direct influence on the simulation results [16,23]. As a consequence, a general purpose simulation procedure can be made much simpler by using analytical approximate DCSs leading to the correct values of these relevant integrals.

The transport of photons is not included in the present simulations. A code for the simulation of electron-photon showers, which combines PENELOPE with a conventional procedure to follow photon histories [24], is currently being checked and will be described elsewhere.

2.1. Elastic scattering

Single elastic collisions are determined by the values of the polar and azimuthal scattering angles, θ and ϕ respectively. Assuming that the scattering potential has spherical symmetry, single and multiple scattering angular distributions are axially symmetrical about the direction of incidence, i.e. they are independent of the azimuthal scattering angle ϕ. For our purposes, it is convenient to measure angular deflections produced by single scattering events in terms of the variable

$$\mu \equiv \frac{1 - \cos\theta}{2} \tag{2}$$

instead of the scattering angle θ.

Let $\mathrm{d}\sigma_{el}/\mathrm{d}\mu$ denote the single scattering DCS. The mean free path λ_{el} between elastic events is given by

$$\lambda_{el}^{-1} = N\sigma_{el} = N \int_0^1 \frac{\mathrm{d}\sigma_{el}}{\mathrm{d}\mu}\,\mathrm{d}\mu, \tag{3}$$

where σ_{el} is the total elastic cross section. The first and second transport mean free paths, λ_1 and λ_2, are defined by (see Ref. [16])

$$\lambda_1^{-1} = N \int_0^1 2\mu \frac{\mathrm{d}\sigma_{el}}{\mathrm{d}\mu}\,\mathrm{d}\mu \tag{4}$$

and

$$\lambda_2^{-1} = N \int_0^1 6(\mu - \mu^2) \frac{\mathrm{d}\sigma_{el}}{\mathrm{d}\mu}\,\mathrm{d}\mu. \tag{5}$$

We consider that accurate values of the mean free path, λ_{el}, and transport mean free paths λ_1 and λ_2 are known. These can be directly obtained from partial wave calculations for low energies, and from suitable approximations for high energies. In the simulations reported below, for electrons and positrons with kinetic energies less than 1.5 MeV, we have adopted the values of these quantities obtained from partial wave calculations, using the PWADIR code described in Ref. [25] with the analytical Dirac–Hartree–Fock–Slater atomic scattering potential [26] (including solid-state effects, and exchange effects in the case of electrons). For higher energies, transport mean free paths have been calculated from the screened Mott formula described in Ref. [27]. This formula is not accurate for very small scattering angles; hence, a different approach should be used to obtain the mean free path or, equivalently, the total elastic cross section σ_{el}, which strongly depends on the small-angle behaviour of the DCS. The total cross section for $E > 1.5$ MeV has been computed from the optical theorem, using the forward scattering amplitude for the free atom analytical Dirac–Hartree–Fock–Slater potential obtained from the eikonal approximation [28]. The mean free paths and transport mean free paths used in the simulations are expected to be reliable for energies from ~ 1 keV up to several hundred MeV. These quantities are tabulated for a grid of kinetic energies, and transformed into continuous functions of the energy by means of cubic spline interpolation on a log-log scale.

Elastic scattering is simulated here by using the W2D model described in Ref. [22]. Essentially, this is a model DCS which yields multiple scattering distributions that do not differ significantly from those obtained from the actual scattering process. The W2D single scattering DCS is given by (cf. Eq. (3))

$$\frac{\mathrm{d}\sigma_{el}^{(W2D)}}{\mathrm{d}\mu} = \frac{1}{N\lambda_{el}} p_{ap}(\mu), \tag{6}$$

where λ_{el} is the tabulated mean free path and

$$p_{ap}(\mu) \equiv (1 - B)\frac{A(1 + A)}{(\mu + A)^2} + B\delta(\mu - \mu_0). \tag{7}$$

The parameters A (> 0), B ($0 \le B < 1$) and μ_0 ($0 \le \mu_0 \le 1$) are determined in such a way that the mean and variance of the approximate distribution $p_{ap}(\mu)$ are the same as those obtained from the actual DCS or, equivalently,

$$\int_0^1 \mu p_{ap}(\mu)\,\mathrm{d}\mu = \frac{1}{2}\frac{\lambda_{el}}{\lambda_1} \tag{8}$$

and

$$\int_0^1 \mu^2 p_{ap}(\mu)\,\mathrm{d}\mu = \frac{1}{2}\frac{\lambda_{el}}{\lambda_1} - \frac{1}{6}\frac{\lambda_{el}}{\lambda_2}. \tag{9}$$

Thus, the average path length between collisions and the mean and variance of the angular deflection μ in each elastic collision obtained from the W2D model are identical to the values obtained from the actual DCS (i.e. the DCS calculated as described above). A detailed analysis of the reliability of the W2D model has been presented in Ref. [22], where explicit analytical formulas for random sampling of the angular deflection μ in single elastic events are given. Notice that the model parameters are completely determined by the quantities λ_{el}, λ_1 and λ_2. In principle, it can be applied to any scattering law.

2.2. *Inelastic collisions*

Inelastic collisions of electrons and positrons in dense media are simulated in terms of the analytical DCSs described in Ref. [21]. The basis of this treatment is a generalized oscillator strength model where each electron shell is replaced by a single oscillator with strength f_i equal to the number of electrons in the shell and resonance energy $W_i = aU_i$, where U_i is the ionization energy of the shell [29]. Excitations of the conduction band are accounted for by a single oscillator with oscillator strength f_{cb} and resonance energy W_{cb} ($U_{cb} = 0$). The semi-empirical adjustment factor a is introduced to obtain agreement with the adopted mean excitation energy I, which is taken from Ref. [30]. Its numerical value is given by

$$\ln a = (Z - f_{cb})^{-1}\left[Z \ln I - f_{cb} \ln W_{cb} - \sum f_i \ln U_i\right]. \tag{10}$$

The DCS for inelastic scattering is a function of the energy loss W and the polar scattering angle θ of the projectile.