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MONTE CARLO TRACK SIMULATIONS

Michael Dingfelder
East Carolina University
Greenville, North Carolina

1.0 Introduction

Monte Carlo track structure simulations follow the primary as well as all produced secondary particles event-by-event, from starting or ejection energy down to total stopping. Simulation codes require both transport models and reliable interaction cross sections for the primary and secondary particles with the material under consideration. In general, charged particles can scatter elastically (they change direction, but do not lose energy) and can ionize or excite the target material. In addition, if the primary particle is an ion, i.e., an atomic system, it can change its charge state by electron capture and electron loss at low energy as it slows down. Different charge states of the same atom will have different ionization and excitation probabilities.

MC (Monte Carlo) track structure simulations determine the location, type, and energy deposition of each event. The physical stage describes the energy deposition distribution; the chemical stage starts with the final locations of the thermalized (totally stopped) electrons and the locations of ionizations and excitations, and simulates the creation and transport of radical species, mainly from the water radiolysis. The physical stage and the general calculation of interaction cross sections needed for this type of simulation will be described in section 2.0 Section 3.0 discusses some of these models applied to (liquid) water and biomolecules, which are of special importance. Chemical and biological consequences are further discussed in the article by Plante (Plante, 2010).

2.0 Cross Section Models (Physical Inputs)

2.0.1 Track structure simulation

Track structure simulations follow the primary as well as all produced secondary particles in an event-by-event manner, until the particles leave the area of interest or are completely stopped. Track-structure codes rely on interaction cross sections of charged particles with the matter under consideration, and require total and differential cross sections of all ionization or excitation processes considered. This is different from the commonly used *continuous slowing down approximation* (csda or also called condensed history) where the only ingredient is the stopping power, or energy loss per track length (LET_∞). In track structure simulations, the mean free path of the particle determines the position of the next interaction; relative total cross sections of all considered processes determine the type of interaction. Depending on the type of interaction, energy and/or angular (momentum) dependent differential cross sections determine the energy loss and change in direction relative to the direction before the interaction. Furthermore, in case of ionizations, information about secondary electron emission energies and directions are needed. In the following, we will discuss methods to calculate or obtain all necessary information, for the charged particles under consideration. We will first focus on electrons and protons, and will then discuss heavier ion interactions.

2.0.2 Elastic scattering

Charged particles can scatter *elastically*, i.e., transfer momentum but not energy from one particle to the other. This will lead to a change in direction of the primary particle without losing any energy in the collision. Since the scattering angle in elastic scattering depends on the masses of the two involved partners, large angle scattering (up to 180 degrees) can appear in electron-electron scattering. However, small angle forward scattering is more probable. Proton-electron elastic scattering normally leads to very small angle proton scattering (typically on the order of millirads) because of the very large difference in the masses of the two particles. Therefore, elastic scattering for protons is in general neglected and it is assumed that the protons travel in a straight line. Angular differential and total elastic scattering cross sections for electron-electron scattering are in general calculated theoretically using a partial wave expansion phase shift calculation in an atomic (or single atom) picture. However, since matter in general is in the condensed phase, corrections in the interaction potential addressing periodic (or non-free) boundary conditions need to be considered. Details to the state-of-the-art calculations and tabulated data for electron and positron elastic scattering can be found in ICRU Report 77 (ICRU, 2007).

2.0.3 Inelastic scattering

Charged particles can excite or ionize the target material. Both processes transfer energy and momentum from the primary particle to the target electron. Therefore, they are considered *inelastic*. Other inelastic processes can include phonon, vibrational or rotational (in case of free atoms or molecules) interactions. However, the energy transfer in these processes is small compared to electronic excitations and ionizations. They are sometimes called sub-excitation processes and are neglected in track structure simulations. We will focus on electronic excitation and ionization processes. When dealing with condensed matter instead of a single atom picture, it is also common to use the inverse mean free path (IMFP) $\Sigma = N\sigma$ (N is the number density of the target material), instead of the microscopic cross section, σ. The unit of Σ is 1/length while the unit for σ is area. Excitation and ionization cross-sections or inverse mean free paths for charged particles are most commonly calculated within the framework of a first Born approximation. This approximation is traditionally realized as plane wave Born approximation (PWBA) which assumes that the incoming particle is sufficiently fast compared to the bound target electrons and can be represented by a plane wave of a free particle. Within this approximation, the double differential (differential in energy transfer $E = \hbar\omega$ and momentum transfer $q = \hbar k$) inverse mean free path Σ is proportional to the energy loss function $\eta_2(E, k)$ and a kinematic factor:

$$\frac{d^2\Sigma}{dE\,dk} = \frac{1}{\pi a_0 T}\frac{1}{k}\eta_2\left(E,k\right) \qquad (1)$$

Here, $a_0 = \hbar^2/me^2$ is the Bohr radius (with m being the electron rest mass, and e the elementary charge), and $T = mv^2/2$ the non-relativistic kinetic energy of the projectile.

The energy loss function fully describes the target material ($n = NZ$, where N is the number density of the material, and Z the number of electrons per atom/molecule). It is related to the dielectric response function ε(E, k) in condensed media, or the generalized oscillator strength df(E, k) / dE in a single atom picture as follows:

$$\eta_2(E,k) = \mathrm{Im}\left(\frac{-1}{\varepsilon(E,k)}\right) = \frac{\pi}{2}\,\frac{E_p^2}{Z}\,\frac{1}{E}\,\frac{df\,(E,k)}{dE} \tag{2}$$

Here, Im(.) denotes the imaginary part (the dielectric response function ε(E, k) is, in general, a complex function), and $E_p = \hbar(4\pi ne^2/m)^{1/2}$ is the plasmon energy of free electrons.

Energy differential and total cross sections or IMFPs can be calculated by integration taking into account kinematical considerations. In case of electron impact, exchange effects need to be considered. More details can be found in the literature, e.g., in Dingfelder et al. (1998, 2000, 2008b).

2.0.4 Relativistic expansion

Since track structure simulations historically started with low-energy electrons, non-relativistic descriptions were used for simplicity. However, for electrons above 5 keV of kinetic energy, relativistic kinematics should be used. In a fully relativistic description, not only the instantaneous Coulomb interaction (longitudinal part of the interaction) but also the exchange by virtual photons (transverse part of the interaction) has to be considered. It is also common to use the recoil energy Q instead of the momentum transfer $q = \hbar k$. The recoil energy is defined by $Q(Q + 2mc^2) = (cq)^2$ where c is the velocity of light in vacuum. Within a fully relativistic theory, the double differential (differential in energy transfer E and recoil energy Q) can be written in a similar form as in the non-relativistic case:

$$\frac{d^2\sigma}{dE\,dQ} = \frac{2\pi e^4}{mv^2}\left(\frac{1}{EQ\left(1+\frac{Q}{2mc^2}\right)} + \frac{\beta^2 \sin^2\theta_r\,\frac{E}{2mc^2}}{\left[Q\left(1+\frac{Q}{2mc^2}\right) - \frac{W^2}{2mc^2}\right]^2}\right)\frac{df(E,Q)}{dE} \tag{3}$$

Here, $\beta = v/c$, and θ_r is the angle between the initial momentum of the projectile and the momentum transfer. It is given by

$$\cos^2\theta_r = \frac{\frac{E^2}{\beta^2}}{Q(Q+2mc^2)}\left(1 + \frac{Q(Q+2mc^2) - E^2}{2E(T+mc^2)}\right)^2 \tag{4}$$

Within the relativistic theory, the generalized oscillator strength df/dE is related to the dielectric response or energy loss function by

$$\frac{df(E,Q)}{dE} \equiv E\left(1+\frac{Q}{mc^2}\right)\frac{2Z}{\pi E_p^2}\,\mathrm{Im}\left(\frac{-1}{\varepsilon(E,Q)}\right) \tag{5}$$

A detailed description of the relativistic approach can be found in Fernández-Varea et al., (2005) and references cited therein.

2.0.5 Bethe approximation

The main disadvantage of the PWBA is that the energy-loss function or the generalized oscillator strength needs to be known for the whole E,q plane, i.e, over the Bethe ridge. There exist only two exact solutions: the hydrogen atom and the free electron gas (i.e, the Lindhard solution). It is therefore also common to use the Bethe approximation (for details, see e.g., Inokuti 1971) instead of the PWBA. The Bethe approximation and the PWBA share the same asymptotic behavior. Furthermore, the Bethe approximation only requires knowledge of the optical oscillator strength, or the energy-loss function in the optical limit, i.e., for momentum transfer q = 0. Within the Bethe approximation, the single differential (differential in energy transfer) inverse mean free path in a relativistic formulation (and without any corrections) is given by

$$\frac{d\Sigma}{dE} = \frac{1}{\pi a_0 T^*}\left[A(E)\left(\ln\left\{ \frac{\beta^2}{\left(1-\beta^2\right)} - \beta^2 \right\} \right) + B^*(E) \right] \qquad (6)$$

where $T^* = mv^2/2$ (not the relativistic kinetic energy). A(E) and B(E) are the Bethe coefficients, and $B^*(E) = B(E) + A(E)\ \ln(\hbar c/e^2)^2$. The Bethe coefficients depend only on the optical oscillator strength or the dielectric response function in the optical limit, i.e, for momentum transfer $\hbar k = 0$. Further information and explicit formulas to calculate the Bethe coefficients can be found in Inokuti 1971 (general notation), or in Dingfelder et al. 1998 (this notation).

2.0.6 Semi-empirical models

Semi-empirical models take advantage of general properties of cross sections and of asymptotic behaviors of the PWBA and Bethe approximations. They provide simple analytical formulas depending on materials properties and parameters. Parameters can include binding energies; they can be obtained in general fits to available experimental data – mainly from the gas phase – and use analogies, inter- or extrapolation techniques to expand them to other materials. Semi-empirical models are available for single differential and total cross sections, for electron, or ion impact. Widely used is the Rudd Model for differential cross sections for secondary electron production by proton impact (Rudd 1988). For electron impact, successful models include the Binary Encounter Dipole (BED) model, and its simplified version, the Binary Encounter Bethe (BEB) model, both introduced by Kim and Rudd (1994). Like the Bethe approximation, the BEB model uses optical oscillator strength information. Further information on these types of cross section models can be found, e.g., in the ICRU Report 55 (ICRU, 1995).

2.0.7 Optical data models

The generalized oscillator strength (GOS) or energy loss function can be modeled using the optical oscillator strength (OOS) or dielectric response function in the optical limit and simple collision kinematics like the binary collision theory. The OOS is often available for materials, or can be obtained from photon interactions, where the GOS is unavailable. Most commonly used is the Ashley delta-oscillator model which assumes a collision between free electrons. It relates the energy transfer E and the momentum transfer $q = \hbar k$ as in a free collision: $E^2 = q^2/2m$. Therefore, the GOS or dielectric response function can be modeled and the equations for the PWBA and Bethe approximations simplified. Further information to optical data models can be found, e.g., in Fernández-Varea et al. (1993, 2005).

2.0.8 Beyond PWBA

With the availability of modern computers more sophisticated models and calculations become feasible. Molecular wave-functions and binding energies can be obtained more easily, as well as complicated matrix elements evaluated. Condensed phase properties can be simulated as well as free molecule behavior. All this allows a more detailed description of the scattering process and provides better multiple differential (i.e, in energy transfer, momentum transfer, and ejection direction of secondary electrons) cross sections. Main target materials are water, both in the liquid and vapor phase, and bio-molecules up to DNA constituents. More information can be found, e.g., in Champion et al. (2006, 2010), and Champion (2010).

2.0.9 Heavy ions (helium and heavier)

Scaling laws can be applied for bare, i.e., fully ionized ions. Within the plane wave Born approximation interaction cross sections for particles with the same velocity v scale with the square of the nuclear charge of the projectile z_0^2. Therefore, interaction cross sections for ions are obtained from interaction cross sections for protons using this scaling:

$$\frac{d\sigma_{ion}}{dEdQ}(v) = z_o^2 \frac{d\sigma_{proton}}{dEdQ}(v) \qquad (7)$$

For sufficiently fast dressed ions, i.e., not fully ionized ions traveling with considerable speed, an effective charge z* can be used to account for the partial shielding of the nuclear charge by the orbital electrons. Most commonly, the Barkas formula is used:

$$z^* = z_0 \left[1 - \exp\left(-125 z_0^{-3/2} \beta\right)\right] \qquad (8)$$

Ions are atomic systems. When they slow down, charge transfer interactions can take place: a proton, for example, can pick up an electron (electron capture) from the target and become a neutral hydrogen atom. The neutral hydrogen atom itself can excite and ionize the target, or lose its electron (electron loss, or stripping) and become again a proton. Neutral hydrogen has different interaction probabilities than protons, i.e., excitation and ionization cross sections are different. In case of an alpha particle, three charge states need to be considered: He^{2+}, He^{+}, and neutral helium He^{0}. For heavier particles, this scheme complicates quickly. For protons and alpha particles charge changing events become important below several 100 keV/n of energy. More information can be found in, e.g., Dingfelder et al. (2000, 2005).

2.0.10 Transport models

Cross sections alone do not suffice for successful MC track structure simulations. Often, supplemental information about energy depositions, excitation and de-excitation modes, scattering angles, secondary electron emission spectra, or inner shell vacancy fill ups (Auger processes, x-ray emission, etc.) is needed. The whole transport model needs to be consistent, i.e., the cross sections and the other information must fit together. Exchange of parts of the model may be difficult without adjusting other parts of the model.

3.0 Simulation of Energy Deposition in Water and Biomolecules

In this section we describe cross sections and transport models for water and biomolecules implemented in Monte Carlo simulation codes and summarize results on the energy depositions.

3.0.1 Why Water?

Water is the major constituent of a human body and serves as substitute for biological soft tissue. Water surrounds the DNA in cells. Water exists in three phases: vapor, liquid, and frozen (ice). However, at room temperature or within a human body, water only exists in the liquid phase. Scattering experiments with liquid water are very difficult to perform, and experimental data are few. Cross sections for liquid water mainly rely on scarce measurements of optical and dielectric constants and theoretical model calculations. Water vapor and ice, especially amorphous solid water (ASW) are better accessible by experiment; a variety of experimentally obtained interaction cross sections exist in the literature.

Another argument for the use of liquid water as transport substance is that the mean energy loss of liquid water is approximately the same as for dry DNA.

3.0.2 Liquid Water Models

Ionization and excitation cross sections for charged particles with liquid water are commonly calculated using an optical data model within the first Born approximation as described in section 2. There are three major models available in the literature: the PARTRAC model (GSF, now Helmholtz Zentrum Munich - Paretzke, Dingfelder, see, e.g., Dingfelder et al., 2008a), the NOREC model (Oak Ridge National Laboratory - Richie, Turner, Hamm, see, e.g., Dingfelder et al., 2008a), and the Nikjoo and Emfietzoglou model (see e.g., Emfietzoglou et al., 2005, Emfietzoglou and Nikjoo, 2006). The first two models are based on the optical reflectance measurement on a liquid water surface (Heller et al., 1974) while the latter is based on a measurement using synchrotron radiation (Hayashi et al. 2000).

All three models parameterize the optical oscillator strength or the dielectric response function in the optical limit as a linear combination of functions representing discrete excitation and ionization levels. Parameters are fitted to experimental data, taking into account theoretical constraints like sum rules. All models consider 5 electronic excitation levels and 5 ionization shells. The NOREC model considers in addition to the 5 electronic excitations, the Plasmon excitation level, a collective excitation of the medium. All three models use slightly different excitation and ionization energies: excitation energies range from around 6 eV to 15 eV, while the ionization threshold is around 10.7 eV. The PARTRAC model, e.g., uses the following excitation and ionization energies: excitation: 8.17eV, 10.13eV, 11.31eV, 12.91eV, and 14.50eV; ionizations: 10.79eV, 13.39eV, 16.05eV, 32.30eV, and 539eV (Dingfelder et al., 1998).

The energy loss function or Bethe surface is obtained by using an extension algorithm to account for the momentum dependence (Dingfelder and Inokuti, 1999). The extension algorithms are based on binary collision theory, simple quantum mechanics considerations, and experimental data (e.g., Watanabe et al, 1997).

3.0.3 Water Vapor

Scattering experiments of charged particles with gas phase targets are more feasible than with high density (condensed phase) materials. Therefore, a good database for experimental information on water vapor exists in the literature. This led to the development of semi-empirical models for the calculation of interaction cross sections; experimental information was used to fit parameters. Examples for commonly used models are the model by Miller and Green (1973) for excitations by protons, or the models by Rudd (Rudd 1988), the Binary Encounter Dipole (BED) and Binary Encounter Bethe (BEB) models for ionization cross sections, both introduced by Kim and Rudd (1994). An overview of the most commonly used models can be found in the ICRU report 55 (ICRU, 1995).

Paretzke developed a transport model for electrons in water vapor which is based on the optical oscillator strength (OOS) distribution and the Bethe/Born theory. The OOS model is based on experimental information and theoretical constraints. Details can be found in Paretzke (1987, 1988).

The main difference between the OOS of water vapor and liquid water is the excitation spectrum. A free single molecule (in water vapor) has more degrees of freedom (e.g., rotations) than the molecule bound in the condensed phase. Furthermore, transition energies are sharply peaked and clearly separated from each other in the gas phase, while smeared out in the condensed phase. Another difference between the vapor and liquid phase is the ratio between excitation and ionization events as indicated by the optical oscillator strength distributions: in the vapor phase, one gets around 30% excitations and 70% ionization events, while for liquid water this ratio changes to 12% excitations and 88% ionizations. Effectively, this creates more secondary electrons in liquid water than in water vapor for the same charged particle passing through. Also, excitation and ionization energies are around 1-2 eV higher in the vapor phase than in the liquid phase.

3.0.4 Amorphous Solid Water (ASW)

Below a temperature of 53°K, water vapor freezes in an amorphous state, called amorphous solid water (ASW). ASW has no lattice nor long range order, a porous surface, and a density of around 0.6 g/cm^3. The energy loss function peaks at around the same mean energy loss as liquid water, and excitation spectra are similar. Excitation and ionization energies are also similar to liquid water, maybe up to 0.5 eV smaller. Thin layers (nanometer size) of ASW can be used in scattering experiments. Leon Sanche and co-workers have measured electron induced excitation cross sections, including low-energy phonon, vibrational and electronic excitations, in ASW for electron energies below 100 eV (Michaud et al., 2003). These cross sections can be used to model the low-energy (below 100 eV) electron transport in liquid water, ASW and other materials of biological interest. Toburen, et al. (2010) measured doubly differential secondary electron emission yields emitted from thin layers (0.1 micrometer and thicker) from ASW and other frozen gases after proton and light ion impact. Dingfelder, et al. (2008b) modeled these experiments using the MC track structure code PARTRAC to evaluate the low-energy electron transport model implemented. Preliminary results show that electron transport above around 50 eV is satisfactorily described, while below 50 eV, theoretical simulations overestimate experimentally produced secondary electron yields (Toburen et al., 2010).

3.1 Biomolecules and DNA

Cells also contain proteins, histones, DNA, and other biomolecules. It is common to use liquid water as a substitute and scale it with density to a value slightly above unity, i.e, around 1.06 – 1.08 g/cm^3. In recent years, however, effort is made to calculate basic interaction cross sections for biomolecules and the constituents of DNA, like the bases adenine, guanine, cytosine, and thymine, using simple semi-empirical models like the Binary-Encounter-Bethe model, or the Deutsch-Märk model. Basic quantities of the molecules, such as binding energies, ionization potentials, electronic configurations (occupied orbitals) which are necessary for these semi-empirical models, are typically calculated for single molecules using quantum chemistry codes like Gaussian. Ionization potentials for the DNA bases are on the order of 8.0 to 9.0 eV, around 2.0 to 2.5 eV lower than for liquid water. Examples for such calculations are found in Bernhard and Paretzke (2003), Blanco and García (2007), and Możejko and Sanche (2005).

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