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A Monte Carlo strategy to simulate positrons and positronium in biological materials

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ABSTRACT

We present an algorithm for Monte Carlo simulations of positron tracks in biological materials. The algorithm takes into account the cross-section data for elastic and inelastic collisions between positrons and molecules and processes like direct annihilation, ionization and positronium formation. In the case of positronium formation, the algorithm considers the interactions of positronium with molecules. The algorithm can be used to identify the processes that are responsible to determine the lifetime of the positrons and their annihilation mechanism (direct or through positronium formation).

KEYWORDS

Monte Carlo Simulation, Positron, Positronium

INTRODUCTION

In recent years a new generation of positron emission tomography (PET) scanners has been developed by Moskal and coworkers [1]. This enables the measurement of positron lifetimes in biological materials and medical applications [2]. From positron annihilation lifetime spectroscopy (PALS), it is possible to deduct the lifetime of positronium, the bound state of one positron and one electron [1, 3]. The lifetime of positronium is influenced by the partial pressure of oxygen [4]. The positronium lifetime, combined with the tomographic information of the position of the annihilation event, can be used to generate spatial images of oxygen concentration in different parts of a patient [5]. Because the partial pressure of oxygen can be 5 times higher in cancer tissue than in healthy tissue, this technique can be used to locate cancer cells in the body.

For a better understanding of the processes that are involved in the production and decay of positronium, computer simulations are necessary. Monte Carlo codes, like Penelope, have been developed to compute positron tracks in biological material [6]. The physical models for the interaction of positrons with the molecules of the

medium are valid only for kinetic energies of the positron above 50 eV. The important physical processes, like the direct annihilation and formation of positronium, happen mainly in the energy range below 20 eV. Therefore, new computational tools are needed that can describe this low-energy part. The low-energy regime can be simulated by the ANTICOOL code by Green [7]. However, the ANTICOOL code is limited to collisions energies below a few eV. It does not take into account inelastic collisions, ionization or positronium formation. Furthermore, it is limited to collisions with one species. In this paper we outline the design of a Monte Carlo strategy to simulate positrons and positronium in biological materials for a large range of energies.

MONTE CARLO STRATEGY

Step length

The step length between two collision events is given by the mean free path

$$\Delta s = -\, r \log(1 - \mu_r) \tag{1}$$

where μ_r is a random number uniformly distributed between 0 and 1 ($0 \le \mu_r < 1$). Here, r is the mean free path between two collisions. In general, the mean free path $r = r(E_{kin})$ is a function of the kinetic energy E_{kin} of the particle and can be written as

$$r(E_{kin}) = \frac{1}{n\sigma_{\mathrm{tot}}(E_{kin})} \,. \tag{2}$$

Here n is the number density of molecules (number of molecules per unit volume) and σ_{tot} is the total cross-section for interactions of the projectile with one molecule. The total cross section depends on the collision partners: the projectile and the target. During the lifetime of the positron, the projectile can be a positron, ortho- or para-positronium. The target of the collision can be any molecule of the molecular species $M_1, M_2, \cdots, M_N$ in the biological material. A general expression for the projectile p in a mixture of molecules can be written as

$$r_p = \frac{1}{\Sigma^p} \tag{3}$$

where we introduce the quantity

$$\Sigma^p = n_1\sigma_{\mathrm{tot}}^{p,M1} + n_2\sigma_{\mathrm{tot}}^{p,M2} + \cdots + n_N\sigma_{\mathrm{tot}}^{p,MN} \,. \tag{4}$$

Here the index p denotes the particle (positron, ortho- or para-positronium), $n_1, n_2, \cdots, n_N$ are the number densities of molecular species, $M_1, M_2, \ldots M_N$. $\sigma^{p,Mi}_{tot}$ are the total cross sections between the projectile p and the various molecular species M_i. All cross sections depend on the kinetic energy of the projectile.

From the step length Δs and the kinetic energy we can compute the time between two collisions. Here we discuss only the case of nonrelativistic energies. For larger kinetic energies, the special theory of relativity has to be used. The time between two collisions can be expressed as:

$$\Delta t = \frac{\Delta s}{v} \,. \tag{5}$$

Here the velocity of the projectile is $v = \sqrt{\frac{2E_{kin}}{m_p}}$. The mass of the projectile, $m_{p,}$ is equal to one electron mass if the projectile is a positron, and to two electron masses, if the projectile is positronium.

Collision partner

At the end of each step of the projectile p a decision has to be made about the collision partner and about the type of collision. It is helpful to introduce the quantity

$$\Sigma_{\mathrm{k}}^{\mathrm{p}} = \frac{1}{\Sigma_{\mathrm{p}}} \sum_{\{i=1\}}^{k} n_i \, \sigma_{tot}^{p,M_i} \tag{6}$$

In order to choose the collision target, a random number μ_M (uniformly distributed, $0 \le \mu_M < 1$) is generated.

- If $0 \le \mu_M < \sum_1^p$, the projectile p interacts with species M_1.
- If $\sum_1^p \le \mu_M < \sum_2^p$, the projectile p interacts with species M_2.
- ...
- If $\sum_{N-1}^p \le \mu_M < 1$, the projectile p interacts with species M_N.

Collision process

After the collision partners are determined, the type of the collision process has to be determined. The possible types of collisions depend on the projectile p and the molecular species M_i. The processes between a positron as a projectile and a molecule are elastic collisions, inelastic collisions (rotational, vibrational and electronically), positron-impact ionization of the molecule, the formation of ortho- or para positronium, direct annihilation and many other processes (for example, positron-induced chemical reactions). Some of the processes have a threshold energy. Below this threshold the process cannot occur. If the projectile is ortho-positronium it can decay into 3 gamma-rays or can be converted into para--positronium. Furthermore, it can have elastic or inelastic collisions with the molecule, undergo pickoff annihilation or can dissociate into a positron and an electron. If the projectile is para-positronium it can decay into 2 gamma-rays or be converted into ortho-positronium. In addition, it can undergo the processes mentioned for ortho--positronium. It is helpful to calculate the quantities:

$$\Pi_d^{p,M_i} = \frac{1}{\sigma_{tot}^{p,M_i}} \sum_{\{c=0\}}^{d} \sigma_c^{p,M_i} \,,$$

where the sum is over the different collision processes c, which can occur between the projectile p and the molecular species M_i. These quantities depend on the collision energy and have to be

computed at the end of the step. In order to choose the type of the collision process, a random number μ_c (uniformly distributed, $0 \le \mu_c < 1$) is generated.

- If $0 \le \mu_c < \prod_1^{p,Mi}$, collision process 1 will occur.
- If $\prod_1^{p,Mi} \le \mu_c < \prod_2^{p,Mi}$, collision process 2 will occur.
- ...

Depending on the projectile and the scattering process, a number of additional steps are required. If the process is an elastic collision, the new direction of the projectile has to be determined on the basis of the differential-elastic cross section. This procedure is outlined in chapter 5 of Dapor's book [8]. If the collision is inelastic, the kinetic energy of the projectile has to be changed, according to the energy transfer to or from the target molecule. In addition, the scattering angle has to be determined. If the projectile is a positron and the process is the formation ortho- or para-positronium, the projectile in the following steps is ortho- or para-positronium.

Calculation of observables

In PET applications the concentration of positrons is rather small. Therefore, it is justified to simulate the trajectory of each positron individually. In a Monte Carlo simulation we compute the trajectories of many millions of positrons and analyse the results statistically. Interesting quantities are the lifetime and range of positrons from their creation until their annihilation (either directly or by decay of positronium). The lifetime can be computed by summing up the times between the various collisions. We assume that the collision process itself does not take any time. The range of the positron is given as the distance between the location of its creation and its annihilation. Other quantities of interest are the rate coefficients for the formation of positronium, the conversion between ortho- and para-positronium and the lifetime of ortho- and para-positronium. These quantities can be obtained by analysis of the point-of-time for the formation of positronium and the point-of-time of a conversion or decay event.

CONCLUSIONS

We outlined a Monte Carlo strategy to simulate positrons and positronium in biological materials. Our formalism is nonrelativistic. This seems to be justified because for energies larger than 100 eV, the annihilation probability is much smaller than the probability for slowing down (see, e.g., chapter 1 in [9]). The procedure requires cross section data for collisions of positrons and positronium with various molecules of biological interest. A collection of cross sections of positrons with molecules is compiled in the review by Ratnavelu et al. [10]. Currently, we are working on the implementation of the algorithm.

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