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Influence of ionization cross-section data on the Monte Carlo calculation of nanodosimetric quantities

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Abstract

In this work, we discuss the effect of cross-section data in the determination of nanodosimetric quantities, such as ionization cluster-size distributions and mean cluster sizes. In particular, two different theoretical approaches to determine secondary electron distributions after proton interactions in nitrogen and propane were tested by means of a Monte Carlo code. The results show that differences of 10–15% in the cross-section data lead to differences of up to 10–20% in the calculated mean cluster sizes, especially at low energies, suggesting the need for new, reliable and consistent experimental cross-section data.

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1. Introduction

Nanodosimetric quantities, such as size distributions of clustered ionization, are important in understanding the radiation-induced damage in biological targets of nanometric size (such as DNA segments). These quantities, however, are not directly measurable in biological targets and our present knowledge is mostly based on theoretical models. A common practice to overcome this problem is to measure cluster-size distributions using a nanodosimeter, which basically consists of a gas-filled counter operating at low pressure. In the last years, several types of nanodosimeters were developed aided by the important contribution of Monte Carlo simulations [1]. These simulations require an accurate, complete and consistent set of scattering cross-sections in the gas of interest. Since experimental results are often fragmentary and contradictory, the use of theoretical models to obtain interaction data becomes crucial.

In this work, we use two different theoretical approaches to determine differential ionization cross-sections for proton interactions in nitrogen and propane, which are the gases most commonly used in nanodosimetry, and we show how the choice of a particular model affects the Monte Carlo calculated cluster-size distribution.

2. Determination of nanodosimetric quantities

The working principle of a nanodosimeter is to evaluate the clustering of radiation-induced ionization by counting the number of charges deposited in a small volume of low-density gas. The cluster-size distribution is defined as the probability P_ν that in a well-defined volume exactly ν ionizations are produced by a single primary particle (including its secondary electrons). If this probability is known, the mean cluster size is given by the first moment M_1 of the distribution

$$M_1 = \sum_{\nu=0}^{\infty} \nu P_\nu \quad \text{with} \quad \sum_{\nu=0}^{\infty} P_\nu = 1. \tag{1}$$

Due to the stochastic nature of the ionization process, it is possible to demonstrate [1,2] that

$$M_1 \propto 1/(\lambda\rho)_{\text{ion}} \tag{2}$$

where ρ is the gas density and λ_{ion} the mean free path length of the primary particle between two ionization events, which is, by definition, inversely proportional to the

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ionization cross section σ_{ion}

$$(\lambda\rho)_{\text{ion}} = (M/N_{\text{A}})\sigma_{\text{ion}}^{-1}$$

where M is the gas molar mass and N_{A} the Avogadro constant.

Eq. (2) therefore points out the importance of the mean cluster size to characterize the radiation quality.

3. Ionization cross-section data for protons

Consistent and reliable interaction data are important for Monte Carlo simulations of particle track structures. In particular, charged particles passing through matter lose most of their energy in ionizing collisions with bound electrons, resulting in energetic free electrons, whose transport has to be followed completely. Therefore, the most important data are ionization cross-sections of primary particles, the spectral and angular distribution of secondary electrons and the data concerning electron degradation via elastic, excitation and ionization processes. The singly differential cross-section (SDCS) of the primary particles gives information about the secondary electron spectral distribution and can be integrated over the electron energy ε to obtain the total ionization cross-section:

$$\sigma_{\text{ion}} = \sum_i \int_0^{T-B_i} \frac{\mathrm{d}\sigma_i}{\mathrm{d}\varepsilon}\,\mathrm{d}\varepsilon \tag{3}$$

where the sum is taken over all target shells. T is the primary particle energy and B_i the ionization threshold of the corresponding orbital.

While some experimental cross-sections are available for proton collisions in nitrogen, those for propane are, up to now, still fragmentary [3,4]. Theoretical models are therefore helpful to obtain the missing information. Here, we present two different approaches for determining secondary electron distributions after proton collisions: the Hansen–Kocbach–Stolterfoht (HKS) model and the Rudd model.

3.1. Hansen–Kocbach–Stolterfoht (HKS) model

This model is based on a semi-classical approximation and gives a simple expression for the SDCS of each target shell [3,5]

$$\frac{\mathrm{d}\sigma_i}{\mathrm{d}\varepsilon} = \frac{4Z_1^2 a_0^2}{Rv^2\alpha_i k_{c,i}^3 \tilde{k}_{t,i}} \left\{ \frac{5(\tilde{K}_{m,i}+\tilde{k}_{t,i}) + 3(\tilde{K}_{m,i}+\tilde{k}_{t,i})^3}{3[1+(\tilde{K}_{m,i}+\tilde{k}_{t,i})^2]^2} - \frac{5(\tilde{K}_{m,i}-\tilde{k}_{t,i}) + 3(\tilde{K}_{m,i}-\tilde{k}_{t,i})^3}{3[1+(\tilde{K}_{m,i}-\tilde{k}_{t,i})^2]^2} + \arctan\left(\frac{2\tilde{k}_{t,i}}{1+\tilde{K}_{m,i}^2-\tilde{k}_{t,i}^2}\right) \right\} \tag{4}$$

where $a_0 \approx 5.29\times10^{-11}\,\text{m}$ is the Bohr radius, Z_1 the primary particle's charge, $v = (T/R)^{1/2}$ its velocity parameter, $R = 13.606\,\text{eV}$ the Rydberg energy, $\alpha_i = (B_i/R)^{1/2}$ the initial momentum parameter and

$$\tilde{K}_{m,i} = (\alpha_i^2 + k^2)/(2v\alpha_{c,i})$$
$$\tilde{k}_{t,i} = \left[k^2 + 0.2\alpha_i^2\sqrt{v/\alpha_i}\right]^{1/2}/\alpha_{c,i}$$
$$k_{c,i} = \left[k^2 + 2\alpha_i^2/\ln(2v^2/\alpha_i^2)\right]^{1/2}$$
$$\alpha_{c,i} = \alpha_i\left[1 + 0.7v^2/(v^2+k^2)\right]$$
$$k = (\varepsilon/R)^{1/2}.$$

The advantage of using Eq. (4) is that it depends only on parameters related to the kinematic of the collision (like momentum and kinetic energy of protons) and on the target's binding energies. Nevertheless, a thorough investigation of its applicability to any target is still lacking [3] and would be desirable.

3.2. Rudd model

Rudd et al. [4] based their semi-empirical theory on the classical binary-encounter approximation at high proton energy and on the molecular promotion model at low energy [6]. The resulting SDCS is given by

$$\frac{\mathrm{d}\sigma_i}{\mathrm{d}\varepsilon} = \frac{(S_i/B_i)(F_1+F_2w_i)(1+w_i)^{-3}}{1+\exp\left[\chi(w_i-w_{c,i})/v\right]}. \tag{5}$$

Here, χ is an adjustable parameter and

$$S_i = 4\pi a_0^2 N_i (R/B_i)^2$$
$$w_i = \varepsilon/B_i$$
$$w_{c,i} = 4v^2 - 2v - R/(4B_i)$$
$$F_1 = L_1 + H_1$$
$$F_2 = L_2H_2/(L_2+H_2)$$

with N_i being the electron occupation number in a shell and

$$L_1 = C_1 v^{D_1}/[1+E_1 v^{(D_1+4)}]$$
$$H_1 = A_1\,\ln(1+v^2)/(v^2+B_1/v^2)$$
$$L_2 = C_2 v^{D_2}$$
$$H_2 = A_2/v^2 + B_2/v^4.$$

Although the Rudd model needs 11 parameters (A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2, E_1, E_2, χ) to be adjusted on the basis of experimental results, it allows to cover a wide energy range and to extrapolate missing data.

4. Monte Carlo calculation

Cluster-size distributions in propane and nitrogen were calculated with an *ad hoc* code developed at PTB [7,8], which simulates the geometry of an ion-counting nanodosimeter developed in collaboration with the Weizmann Institute (Rehovot, Israel) [7]. The binding energies and occupation numbers for nitrogen and propane were taken from Hwang et al. [9] and the fitting parameters for the Rudd model from Rudd et al. [4]. The proton energy was