Radiation Physics and Chemistry 146 (2018) 68–72

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Effect of the track potential on the motion and energy flow of secondary electrons created from heavy-ion irradiation

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ARTICLE INFO

Keywords:
Heavy ion beam
Secondary electron
Track potential
Energy deposition

ABSTRACT

Using simulations, we have evaluated the effect of the track potential on the motion and energy flow of secondary electrons, with the goal of determining the spatial distribution of energy deposition due to irradiation with heavy ions. We have simulated this effect as a function of the mean path τ between the incident ion-impact-ionization events at ion energies E_{ion}. Here, the track potential is the potential formed from electric field near this incident ion path. The simulations indicate that this effect is mainly determined by τ and hardly depends on E_{ion}. To understand heavy ion beam science more deeply and to reduce the time required by simulations, we have proposed simple approximation methods that almost reproduce the simulation results here.

1. Introduction

Cancer therapy using heavy ions is more body-friendly than treatments using any other types of radiation, such as γ-rays or protons, because the relative biological effectiveness (RBE) of heavy ions is higher; that is, smaller dose is required with this therapy (Kraft et al., 1999; Kase et al., 2008). In an effort to determine the reason for the higher RBE of heavy-ion beams, Ward (1994) and Goodhead (1994) have postulated that heavy-ion irradiation creates more clustered DNA damage, which raises the rate of cell death. Here, clustered DNA damage is defined as multiply damaged sites within a region corresponding to a DNA length of several nanometers. Experiments have confirmed that clustered DNA damage has a great effect on a cell (Shikazono et al., 2009) and that more clustered DNA damage is produced by irradiation using heavy ions (Akamatsu et al., 2015). However, it is still unclear when, where, and how such clustered DNA damage is created. We have therefore been studying the motions of secondary electrons using simulations (Moribayashi, 2011a, 2013, 2014, 2017a) in order to determine the spatial distribution of energy deposition created by heavy-ion irradiation. Here, a secondary electron is defined as an electron created by the incident-ion impact ionization. Since secondary electrons carry the energies deposited from the incident ion into the target, we expect the spatial distribution of the energy deposition produced by the secondary electrons to be related to the spatial distribution of DNA damage due to heavy-ion irradiation. In other words, we expect this spatial distribution to enable us to determine the amount of clustered DNA damage.

During irradiation by heavy ions, numerous molecules in a target are ionized along the heavy-ion path, and strong electric field is formed by the positive charges of the molecular ions near this path (Borovsky and Suszcynsky, 1991; Moribayashi, 2011a, 2013). The potential produced from this electric field has been called the “track potential” (Rothard et al., 1998; Schiwietz and Xiao, 1996; Kimura et al., 2002). Kimura et al. (2002) concluded from their measurements of the secondary-electron yield that slow secondary electrons are trapped by the track potential. That is, the track potential affects the motion of the secondary electrons and thus changes the spatial distribution of energy deposition. However, as far as we know, no simulations have treated the track potential (Katz and Kobetich, 1969; Kraft et al., 1992; Nikjoo et al., 1998; Uehara and Nikjoo, 2002; Wang and Vassiliev, 2017) etc., except for ours (Moribayashi, 2011a, 2013, 2017a). Wang and Vassiliev (2017) called the effect of the positively charged ions that accumulate along the particle track a “non-linear transport effect”, that is, in fact the track potential that affects the motions of the secondary electrons. They noted that this effect is not necessarily negligible and that all the Monte Carlo simulations they discussed were based on the linear transport model (approximation). They also simply explained our simulations (Moribayashi, 2014) in which the non-linear transport effect was incorporated.

We have derived a formula for the electric field producing the track potential from our simulation results. We find that this electric field decreases as $1/r$ (Moribayashi, 2017b), where r is the perpendicular distance from the path of the incident heavy ion. On the other hand, the Coulomb force of a point charge on a molecular ion decreases as $1/r'^2$, where r' is the distance from the point charge. Therefore, the track potential provides a longer-range force than that from a point charge,

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https://doi.org/10.1016/j.radphyschem.2018.01.017
Received 18 December 2017; Received in revised form 10 January 2018; Accepted 17 January 2018
Available online 03 February 2018
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and slow secondary electrons are easily to be trapped by this longer-range force. Note that we succeeded in reproducing the trend of the secondary-electron yield measured by Kimura et al. (2002) (Moribayashi, 2017a).

We incorporated the track potential into a simulation model and demonstrated that secondary electrons are trapped by the track potential (Moribayashi, 2011a, 2013). Using this model, we simulated radial dose that is the dose as a function of r (Moribayashi, 2014, 2015). There are two types of radial dose distributions, which are employed in the treatment planning system for heavy particle cancer therapy (Kase et al., 2008) as well as in the estimation of cluster DNA damage. However, there is a different feature in the region near the incident ion path between these distributions although this region is the most important to produce high RBE, that is, to estimate the cell survival (Katz and Kobetich, 1969; Chatterjee and Schaefer, 1976; Kase et al., 2008). The former one, which we call 'Katz type', is obtained from the conventional model ignoring track potential mentioned above (Katz and Kobetich, 1969). In the latter one calling ' Chatterjee type', track potential is considered, however, the target is free electron gas that is far from the reality because this model is produced from theoretical treatments without simulations (Chatterjee and Schaefer, 1976). From the simulations using our model that overcomes weak points of the models producing the two types of conventional radial dose distributions mentioned above, we proposed another distribution (Moribayashi, 2014, 2015). When the stopping power (or LET) is weak where the effect of the track potential is also weak, our distribution agrees well with the Katz type. On the other hand, in strong stopping power, our distribution near the incident ion path becomes close to the Chatterjee type. Further, in order to verify that our model is valid, we compare our simulations with the measurements for the number of secondary electrons escaping the track potential when $E_{ion} = 500$ keV/u, where E_{ion} is the energy of the incident ion (Moribayashi, 2017a). In the present paper, we treat cases with $E_{ion} = 3 - 10$ MeV/u and determine not only the number of secondary electrons but also the energy flow escaping the track potential with the aim of elucidating the spatial distribution of energy deposition due to heavy-ion irradiation. The energy flow simulations shown here are expected to enable us to quantitatively understand how our model produces the space distribution of energy deposition and the radial dose distribution due to the irradiation of heavy ions.

2. Simulation model

The main advantage of our model (Moribayashi, 2011a, 2013, 2014, 2015, 2017a) is that it can incorporate the track potential. To incorporate it, we treat individual neutral molecules, individual molecular ions, and individual free electrons in the target. In our model, the track potential is produced from the Coulomb interactions between individual charged particles (molecular ions and the other electrons) and individual free electrons (see Section 2.3). In contrast, conventional simulations employ a continuum target, and the track potential is ignored (Katz and Kobetich, 1969; Kraft et al., 1992; Nikjoo et al., 1998; Uehara and Nikjoo, 2002; Wang and Vassiliev, 2017), to the best of our knowledge. We believe that our simulation model employed in this paper has become possible in the 21st century because it takes a few days to simulate the irradiation of one heavy ion even using the present super computers.

2.1. Parameters

In studies of heavy-ion irradiation, the parameter S_p has often been employed for a fixed value of E_{ion} (Kimura et al., 2002), where S_p is the stopping power. In our studies of heavy-ion irradiation, instead of S_p we use as parameters the mean path τ between ion-impact-ionization events and the initial energies E_{is} of the secondary electrons (Moribayashi, 2017a). The two sets of parameters are equivalent because

$$S_p \sim N_m \sigma (V_{ia} + E_{isa}) = \frac{V_{ia} + E_{isa}}{\tau}, \quad (1)$$

where σ, N_m, E_{isa}, and V_{ia} are the ion impact ionization cross section, the number density of molecules in the target, the average value of E_{is}, and the average ionization energy of the molecules, respectively. Note that V_{ia} has a fixed value that depends upon the target. Here, we treat the target as water, which is the main component of cells; that is, we take the density of the target to be 1 g/cc ($N_m \sim 3.3 \times 10^{22}$ /cm^3).

We do not need to consider types of incident-ion species, for the following reasons. Schiwietz and Grande (2001) derived simple equations that reproduce well the measurements of $< q^2 >$ as a function of E_{ion}, the incident ion species, and the target materials, where q is the charge of the incident ion and $< q^2 >$ is the average value of q^2. From their equations, we can approximately estimate $< q^2 >$ for different incident-ion species from E_{ion} alone; that is, from σ or τ, because $S_p \propto \sigma \propto < q^2 >$ is approximately satisfied at a fixed value of E_{ion} (Kimura et al., 2002; Moribayashi, 2017a).

In our previous paper (Moribayashi, 2017a), we considered incident ions with charge states from $q = 1$ (protons) to $q = 6$ (carbon ions), because we had found no data for the distributions of secondary electrons $f(E_{is})$ for $q > 6$. Cappello et al. (2009) estimated that the maximum value of σ is about 10^{-14} cm^2, which corresponds to $\tau \sim 0.03$ nm in a collision of C^{6+}. In order to compare among various values of E_{ion}, we here treat $\tau \geq 0.03$ nm.

2.2. Targets and heavy ion irradiation

We consider a rectangular volume of size 10 nm × 10 nm (the area of the bottom and top) × 30 nm (height) as the target. Within the target, we arrange the molecules in proportion to the density. The positions of the molecules are assigned randomly, subject to the condition that the distances between molecules are greater than 2.7 Å. A heavy ion with energy E_{ion} passes from the center of the top to the center of the bottom area. We assume that E_{ion} and the direction of motion of the heavy ion do not change during its passage through the target, because the target size is too small. We show the results averaged over a few 100 ions, for various positions of the target molecules and for various emission energies (E_{is}) and angles (θ and ϕ) of the secondary electrons, where θ and ϕ are the polar and azimuthal emission angles of the secondary electrons, respectively.

2.3. Production of molecular ions and secondary electrons

Using σ, our simulations generate secondary electrons and molecular ions along the heavy-ion path. The center of the cross-section σ is located at the center of the individual molecules in the target. We assume that heavy-ion impact ionization occurs only when the heavy-ion crosses the area σ and then, E_{is}, θ, and ϕ are then determined from the following equations (Moribayashi, 2015):

$$\frac{\int_0^x f(x')dx'}{\int_0^{x_{max}} f(x')dx'} = R_n \quad (2)$$

where $x' = E_{ie}$, θ, or ϕ, and $f(x')$, x_{max}, and R_n are the distribution function, the maximum value of x, and a random number, respectively. For $f(E_{ie})$, we employ the Rudd model (Rudd et al., 1992), which reproduces well the measurement data for proton-impact ionization. This model also reproduces well $f(E_{ie})$ for impact ionization by C^{6+} and C^{4+} ions (Cappello et al., 2009; Ohsawa et al., 2013). We therefore conclude that the Rudd model can be applied for $q = 1$–6. For $f(\theta)$, we have employed measured data (Cappello et al., 2009; Moribayashi, 2015), and we take $f(\phi)$ to be isotropic. On the other hand, in the conventional model, S_p determines total energy deposition. Using single differential cross sections, this total energy deposition is divided according to E_{is}.

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