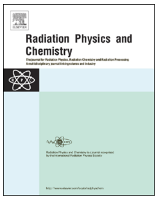
Radiation Physics and Chemistry 96 (2014) 211–216

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

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



Radial dose calculation due to the irradiation of a heavy ion: Role of composite electric field formed from the polarization of molecules and molecular ions

Kengo Moribayashi [a,b,*]

[a] *Quantum Beam Science Directorate, Japan Atomic Energy Agency, 8-1-7, Umemidai, Kizugawa-city 619-0215, Japan*
[b] *Faculty of Life and Medical Sciences, Doshisha University,1-3 Tatara Miyakodani, Kyotanabe City 610-0394, Japan*

HIGHLIGHTS

- This paper analyses the radial dose due to the irradiation of an ion.
- Some electrons are trapped due to electric field of ions and polarizations.
- Electrons trapped near the track of an incident ion form plasma.
- The relationship between energies of an incident ion and radial dose.

ARTICLE INFO

Article history:
Received 9 August 2013
Accepted 30 September 2013
Available online 12 October 2013

Keywords:
Radial dose
Heavy ion irradiation
The motion of free electrons
Electric field
Electron temperature
Plasma

ABSTRACT

This paper discusses the role of composite electric field on radial doses through simulations due to the irradiation of a heavy ion. This composition electric field is formed from molecular ions, the polarization of molecules, and free electrons. Free electrons as well as these molecular ions are produced from the impact ionization of an incident ion or the other free electrons. The motions of the free electrons are simulated using a simulation model shown by Moribayashi, 2011. Phys. Rev. A. 84, 012702-1–012702-7 and Moribayashi, 2013a. Rad. Phys. Chem. 85, 36–41. This simulation model employs an isolated atom model that additionally may be able to treat the advantage of the free electron gas model. Some free electrons are trapped near the track of this incident ion and form plasma. The results obtained here show that this plasma plays a role of bringing about higher radial doses with increasing impact ionization cross sections of incident ions.

1. Introduction

In the theoretical study for the interaction of swift heavy ions with matter, two types of models have been developed (Ziegler et al., 2008). In these two models, the targets are treated as free electron gases and a collection of isolated atoms, respectively. Therefore, we name these two models 'free electron gas model' and 'isolated atom model', respectively in this paper. More accurate data such as stopping powers or LET (linear energy transfer) (Kraft et al., 1992), track structures (Uehara and Nikjoo, 2002), radial doses (or local doses) (Kraft et al., 1992) can be calculated in the isolated atom model through simulations (Kraft et al., 1992; Nikjoo et al., 1998; Uehara et al., 2000; Uehara and Nikjoo, 2002). On the other hand, collective and single motions of free electrons, which are ionized from atoms or molecules, can be treated separately in the electron gas model (Lindhard and Winther, 1964). As computers progress and accurate data of collisions between an ion (or an electron) and an atom (or a molecule) are accumulated, isolated atom models excluding the collective motions have more often been employed (Kraft et al., 1992; Nikjoo et al., 1998; Uehara et al., 2000; Uehara and Nikjoo, 2002). On the other hand, we have been developing a simulation model that employs an isolated atom type model, which additionally incorporates the collective motions (Moribayashi, 2011, 2012, 2013a, 2013b). In this paper, we apply this simulation model to radial dose calculation.

Using the electron gas model, Lindhard and Winther (1964) found that two kinds of waves, i.e. plasma resonance waves and essentially single electron waves are produced by the interaction of a passing ion with free electrons. They also concluded that these two waves moving carry an equal amount of the energy according to the equipartition rule. From a classical point of view, we can

---

* Tel.: +81 774 71 3337; fax: +81 774 71 3316.
E-mail address: moribayashi.kengo@jaea.go.jp

0969-806X/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.radphyschem.2013.09.016

explain their models as follows. The Hamiltonian H, which corresponds to the physical quantity of the total energy in a free electron gas as functions of places, momentums, and times, is given by

$$H=\frac{1}{2m_e}\sum_{i=1}^{N}p_i{}^2+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1,j\neq i}^{N}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}-U_0, \tag{1}$$

where m_e, N, e and p_i are the mass of an electron, the number of electrons, the charge of an electron, and the momentum of the i'th electron, respectively. The first to the third terms of the right hand side of Eq. (1) are the kinetic energies of free electrons, the Coulomb forces between free electrons, and the uniform positive potentials formed from charges of ions, respectively. When the second term is ignored, we call it 'a free electron gas'. In the free electron gas, the interaction of a passing ion increases energies of free electrons and changes the space distribution for these free electrons. Then, the positive potential U_0 used in Eq. (1) plays a role of restoring forces acting on these free electrons. As a result, some of these free electrons create plasma waves, that is, collective motions. According to Ziegler et al. (2008), the free electron gas model is applicable for hard close collisions but its use should be avoided for weak scattering. Here, they define the "hard" and "weak" as the amount of the energy transferred. We expect that the collision between an incident ion and a target atom becomes harder with decreasing incident ion energies. This expectation comes from the facts that the interaction time between an incident ion and a target atom is an important determinant of the hardness of this collision and that its time becomes shorter with increasing ion energies. Ziegler et al. (2008) also reported that the Bethe solutions using the first Born approximation, which can be applied only for the collision processes of high energy ions, is valid only for the weak scattering. This may mean that the 'weak scattering' corresponds to an incident ion with a high energy.

In the isolated atom models, collision processes between an incident ion (or an electron) and an atom (or a molecule) such as impact ionization are employed. As mentioned before, more accurate data such as stopping powers can be calculated using Monte Caro simulations (Kraft et al., 1992), however, the collective motions of free electrons, that is, plasma had never been treated. The progress of computers and the accumulation of accurate data of collisions between a charged particle and a molecule promote to employ isolated atom models. These Monte Carlo simulations have concluded that radial doses obey the $1/r^2$ law, that is, decrease according to r^{-2} (Kraft et al., 1992), where r is the distance from the track of an incident ion.

Chatterjee and Schaefer (1976), Magee and Chatterjee (1980) approximately formulated this radial dose as a function of r by incorporating the advantages of not only the isolated atom models but also the free electron gas models . They classified regions where the free electrons move into two groups, that is, the 'Core' and the 'Penumbra' regions, which are located near and far from the track of an incident ion, respectively. Using the equipartition rule employed in free electron gas models (Lindhard and Winther, 1964), they proposed that almost the equal amount of the energy transferred from an incident ion to the media is deposited in the Core and Penumbra regions through impact processes of free electrons. In Penumbra region, the energy deposition mainly comes from impact ionization processes of energetic secondary electrons and the $1/r^2$ law (Kraft et al., 1992) is adapted for the radial doses. On the other hand, in the Core region where energy deposition occurs mainly in processes of excitation and electron plasma oscillations, high radial doses are brought about there.

In practical application to radiation biology, such high radial doses are expected to increase the production number of clustered DNA damage. Here, the clustered DNA damage is defined as multiply damaged sites within a region corresponding to DNA length of several nanometers (Ward, 1994; Goodhead, 1994; Nikjoo et al., 1998; Hada and Georgakilas, 2008; Shikazono et al., 2009) and is expected to lead us to understand why relative biological effectiveness (RBE) in the case of the irradiation of carbon ions is much higher than that of protons or γ-rays (Blakely and Kronenberg, 1998; Tanaka et al., 2010; Hase et al., 2012). The evidence on the biological significance of clustered DNA damage has been accumulated (Hada and Georgakilas, 2008; Shikazono et al., 2009), however, it remains unknown how clustered DNA damage results after irradiation (Shikazono et al., 2009). The study of the collective motion of free electrons, that is, plasma may become a key to understand production processes of clustered DNA damage because this plasma is expected to bring high radial dose in the Core region. Higher radial doses are expected to produce higher density of DNA damages, which corresponds to the larger production number of clustered DNA damage.

The difficulty to measure this plasma and clustered DNA damage has promoted us to perform simulation studies for motions of free electrons, which are ionized from molecules (Moribayashi, 2011, 2012, 2013a). Before our studies, in the simulation studies where isolated atom models have been the most often employed (Kraft et al.,1992; Nikjoo et al., 1998; Uehara et al., 2000; Uehara and Nikjoo, 2002), no plasma was produced as mentioned before. By developing the Monte Carlo simulation model, we have found that the plasma may be produced as follows. We have treated each individual molecule and the motion of each individual free electron controlled by the interaction of individual charged particles (ions or the other free electrons etc.) in water (Moribayashi, 2011, 2012, 2013a) or a bio-molecule (Jurek et al., 2004; Moribayashi, 2009, 2010). We employ (i) accurate data for the collision processes between an incident ion (or a free electron) and a target molecule and (ii) electric field formed from molecular ions for the calculation of motions of free electrons. The terms (i) and (ii) correspond to the advantages of the isolated atom model and the free electron gas model, respectively. Using this simulation model, we have found for the irradiation of a C^{6+} ion by comparing the irradiation of a proton that (i) the stronger composite electric field [which corresponds to U_0 in Eq. (1)] is created from molecular ions, which are produced from incident impact ionization, and that (ii) the larger number of electrons is trapped near the track of this incident ion (Moribayashi, 2011, 2012, 2013a). We expect that these trapped electrons form plasma. In this paper, we study the role of the trapped free electrons due to composite electric field, that is, plasma on radial dose.

2. Simulation model

We apply our simulation model shown by Moribayashi (2011, 2012, 2013a) to radial dose calculations by treating up to 100 fs on and after the irradiation of ions and employing C^{6+} ions with the energies of 3 MeV/u–100 MeV/u and protons with 200 keV/u–1 MeV/u as incident ions. Here, we only mention the summary of our simulation model.

We employ water as a target and treat individual water molecules and individual free electrons. We consider the following impact processes of an ion or a free electron. (i) The incident ion interacts with a H_2O molecule and a secondary electron, which is one of free electrons, is emitted through ion impact ionization processes ($A^{z+}+H_2O\rightarrow A^{z+}+H_2O^{+}+e^{-}$) (Uehara et al., 2000; Cappello et al., 2009). (ii) By the interaction of this electron with a H_2O molecule, ionization ($e^{-}+H_2O\rightarrow e^{-}+H_2O^{+}+e^{-}$) (A free electron is emitted) (Orient and Srivastava, 1987) and electronic and vibrational excitation