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Study of Particle Interactions and Cross Sections for Modeling Energy Deposition and Cell Response

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Abstract: *Microscopic interactions between particles and tissue elements were investigated to predict biological phenomena in the cell response by the energy transfer. Calculated results were demonstrated on cross sections and energy-angular distributions of secondary particle productions. The flux of terrestrial neutrons was also investigated for a study of the error rate of an implantable device.*

Keywords: *Cross section, Secondary particles, Energy deposition, Cell response, Terrestrial neutrons*

1. Introduction

Charged particles cause DNA damages and may possibly lead to chromosome damage, mutation and cell transformation due to energy transfers through radiation tracks. Particle radiation therapy, which uses protons or heavier ions of relativistic energies has revealed to be highly effective against a variety of cancers, thanks to its excellent dose distribution around the tumor and potentially lower whole body dose compared with photon or electron therapy [1]. The number of such hospital-based facilities worldwide is increasing rapidly. The dose prediction algorithms used today for particle therapy treatment planning rely on parameterizations of measured proton dose distributions, whose predictive capabilities are inherently limited by severe approximations and simplifications in modeling the radiation transport physics. In contrast, the Monte Carlo radiation transport technique can offer sufficiently accurate estimations.

The Monte Carlo technique can, in principle, provide accurate predictions by taking into account all the physical processes involved, including electronic energy loss, energy straggling, multiple Coulomb scattering, elastic and inelastic nuclear interactions, and the transport of secondary particles. Biophysical models have provided essential predictions [2,3] on biological phenomena, such as qualitative differences in radiation interactions in terms of linear energy transfer (LET). There has been a conclusion that the Monte Carlo technique is most promising for developments in both biomedical physics and hospital-facilitated medical treatments. To widen its applicable regime and also to deepen the insights, more basic information is indispensable [4] in physical quantities. For instance, the radial dose distribution needs information of secondary electrons momentum and angular distribution. And for the depth dose, secondary particles from nuclear reactions must be included. Experimental data on these quantities are limited. Studies on proton data have started [2] recently. However, no efforts have been paid for heavier ions such as alpha and carbon ions of relativistic energies.

The effect of neutrons also has become serious today. Device therapy using an implantable cardioverter defibrillator or a programmable pacemaker has revealed its usefulness in recent years, and the number of patients receiving the therapy has risen exponentially. Since such devices contain microcomputers that run sophisticated programs, they are susceptible to hit of charged radiations [5,6]. Recent studies on modern electronics [7] show that the use of boron-based glasses in integrated circuits makes them very sensitive to terrestrial neutrons causing $^{10}B(n, \alpha)$ reactions. An understanding of the soft-error rate induced by environmental neutrons is vitally important for the high reliability requirements and life-supporting nature of the application. Although several measurements have been performed for terrestrial neutron fluxes over the world, they limited themselves outside buildings. There is no data inside buildings in spite of its importance.

In the present article, we investigate the

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primary process and discuss some of selected aspects of biological significance of particle-cell interactions. In the context of biophysics, particle-induced electron-production cross sections, and angular distributions of secondary electrons are presented for alpha and carbon ions. We also investigate typical results regarding heavy-ion-induced nuclear reactions through comparison with the modern Monte Carlo simulation. Moreover, the status of the environmental neutron flux study is discussed with respect to device therapy.

2. Secondary electron productions

Space and momentum densities of secondary electrons are of particularly importance for detailed interpretation of radial dose distributions in nano-meter scale. Simulation tools used widely cannot be applied to investigate nano-meter size phenomena. That is because they are based on the condensed history method, which include a step-size parameter artificially adjusting the energy degradation rate and smearing individual interaction events out. The fully-microscopic Monte Carlo calculation is the only candidate for this aim. We therefore need cross sections of electron-production cross sections and angular distributions of secondary electrons.

2.1. Ionization Cross Sections

The ionization cross sections for the particle impact on molecule were calculated by referring to the electron ionization cross section. Following an energy scaling [8], the ionic particle cross section at a kinetic energy is given by the electron cross section at the energy, where the velocity is the same as that of the ion. In the relativistic kinematics, the relation between the kinetic energy T and the velocity v is given by

$$T = m_0 \frac{1}{\sqrt{1-(v/c)^2}} . \tag{1}$$

The prescription formulated by Seltzer [9] gives electron ionization cross sections on a water molecule. The energy-differential cross sections in terms of electron kinetic energy ε ejected from the j-th orbital of the molecule are written in two terms,

$$\frac{d\sigma^{(j)}}{d\varepsilon} = \frac{d\sigma_c^{(j)}}{d\varepsilon} + \frac{d\sigma_d^{(j)}}{d\varepsilon} . \tag{2}$$

The first term is the close collision between two electrons, and expressed in the form:

$$\frac{d\sigma_c^{(j)}}{d\varepsilon} = \frac{2\pi r_e^2 m_e c^2 n_j}{\eta^2} \frac{T}{T+B_j+U_j} \cdot \left\{ \frac{1}{E^2} + \frac{1}{(T-\varepsilon)^2} + \frac{1}{T^2}\left(\frac{\tau}{\tau+1}\right)^2 - \frac{1}{E(T-\varepsilon)} \frac{2\tau+1}{(\tau+1)^2} + G_j \right\} \tag{3}$$

with

$$G_j = \frac{8U_j}{3\pi}\left\{\frac{1}{E^2} + \frac{1}{(T-\varepsilon)^3}\right\}\left\{\tan^{-1}\sqrt{\xi} + \frac{\sqrt{\xi}(\xi-1)}{(\xi+1)^2}\right\}$$

and

$$\eta^2 = 1-(\tau+1)^{-1},$$
$$\tau = T/m_e,$$
$$\xi = \varepsilon/U_j .$$

Here we used $r_e = 2.81794\times10^{-13}$ cm, and m_e is the electron rest mass, n_j the number of electrons in the orbital, B_j the orbital binding energy, U_j the mean kinetic energy of the orbital electron, and T the kinetic energy of incident electron. The energy transfer E is given by $E = \varepsilon + B_j$.

The second term comes from the interaction with the equivalent radiation field, and is written by

$$\frac{d\sigma_d^{(j)}}{d\varepsilon} = n_j\, I(E)\, \sigma_{PE}^{(j)}(E) , \tag{4}$$

where $\sigma_{PE}^{(j)}$ is the photoelectric cross sections per orbital electron for the incident photon of energy E ($= \varepsilon + B_j$). The virtual photon spectrum integrated over impact parameters $b_{\min} < b < b_{\max}$ is given by

$$I(E) = \frac{2}{137\pi\beta^2 E}\{H(x_{\min}) - H(x_{\max})\}, \tag{5}$$

with

$$H(x) = xK_0(x)K_1(x) - \frac{x^2}{2}\{K_1^2(x) - K_0^2(x)\},$$

where

$$x = \frac{Eb}{\hbar}\frac{\sqrt{1-\eta^2}}{\eta},$$

and K_0 and K_1 are the Bessel function of the order of 0 and 1, respectively.

The partial ionization cross section for the molecular orbit j is written as

$$\sigma^{(j)} = \int_0^{(T-B_j)/2} d\varepsilon \frac{d\sigma^{(j)}}{d\varepsilon} . \tag{6}$$

The total ionization cross section is given by

$$\sigma_{ion} = \sum_{j=1}^{5} \sigma^{(j)} . \tag{7}$$

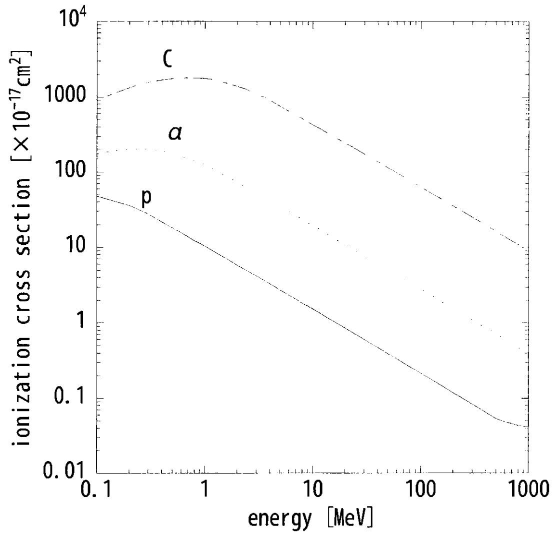

Fig. 1 Total ionization cross sections for H_2O molecule with impact of proton, alpha and carbon.

As an example of the formalism, the ionization cross sections for water vapor were calculated for proton, alpha and carbon bombardment in an energy range from 0.1 to 1000 MeV. We show the resultant cross sections in Fig. 1 for alpha- and carbon-interactions with H_2O molecule as well as proton-H_2O interactions.

2.2 Energy and Momentum Transfer

The emission angles of secondary electrons were investigated by calculating the time evolution in momentum P_i and coordinate R_i space of the i-th particle. The Newtonian equation derived from the time dependent variational principle has the form:

$$\frac{\partial R_i}{\partial t} = \frac{\partial H}{\partial P_i}, \text{ and } \frac{\partial P_i}{\partial t} = -\frac{\partial H}{\partial R_i}. \tag{8}$$

Here, the Hamiltonian H is the sum of the kinetic and the Coulomb potential energies. We assumed the electron is rest at the coordinate origin initially, and is approached by the incident particle as illustrated in Fig. 2. One of the typical results is shown in Fig. 3, in which both trajectories of an electron and a proton are presented for the whole calculated region. In the micrometer scale both trajectories are almost straight lines. The detailed picture in pico- to femt-meter scale of the crossing region is in Fig. 4, which demonstrates that the electron firstly moves to the left from which the particle is approaching. Then it changes its direction when the incoming particle passes away due to their attractive interaction. As the result, the momentum of scattered electron is nearly perpendicular to the initial ion direction. More calculation results implied that most of all the ejected electrons move toward the vertical direction with respect to the incident particle direction. This information is very important to estimate the radial dose distribution.

In Fig.5 is shown the energy transfer as function of kinetic energy of incident proton up to 15 MeV at an impact parameter in Fig. 2. Since the interaction time decreases with increasing the particle speed, the transferred energy also decreases from 4 meV down to almost zero. These quantities are essential for the Monte Carlo simulation to investigate the energy deposition and the cell response.

The energy-differential cross sections are also needed to execute the Monte Carlo simulation. The ICRU report [10] has presented a form of the cross section on the bases of the binary-encounter approximation with the Rutherford scattering formula. The cross sections are summarized [4] as follows:

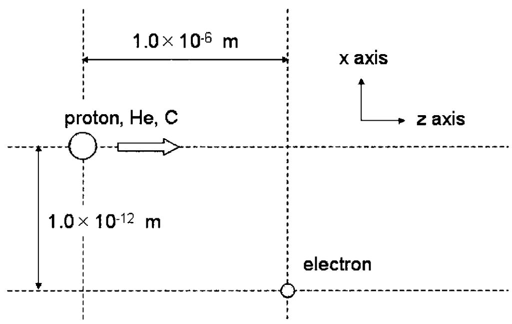

Fig. 2 Coordinate system of calculation.

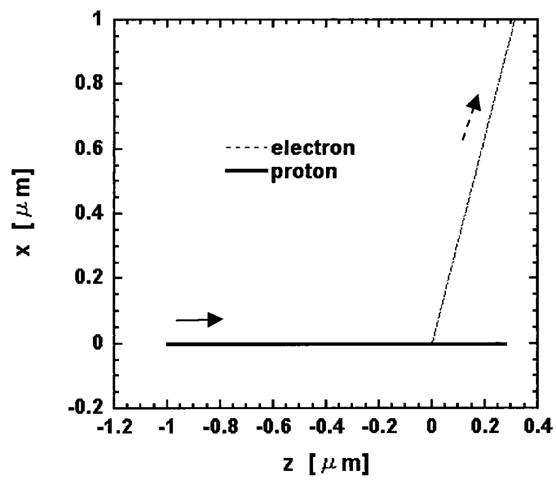

Fig. 3 Trajectories of an electron and a proton.

$$\frac{d\sigma}{d\varepsilon} = \frac{d\sigma_{Ruth}}{d\varepsilon} \cdot \left(1 + \frac{4U}{3E}\right) \quad \text{for } E < E_-,$$

$$\frac{d\sigma}{d\varepsilon} = \frac{d\sigma_{Ruth}}{d\varepsilon} \cdot \frac{U}{6E}.$$

$$\left\{\left(\frac{4T}{U}\right)^{3/2}+\left[1-\sqrt{1+E/U}\right]^{3}\right\}$$

$$\text{for } E_{-}<E<E_{+},$$

$$\frac{d\sigma}{d\varepsilon}=0 \qquad \text{for } E>E_{+},$$

and the Rutherford scattering cross section of

$$\frac{d\sigma_{Ruth}}{d\varepsilon}=\frac{4\pi a_0^2}{T}\left(\frac{R}{E}\right)^2,$$

where ε is the emission energy of the secondary electron, T the kinetic energy of an electron having the same speed as the incident particle, a_0 the Bohr radius, R the Rydberg energy (13.6 eV), and E the energy transfer, U the kinetic energy of the target electron and $E_{\pm}=4T\pm 4\sqrt{TU}$.

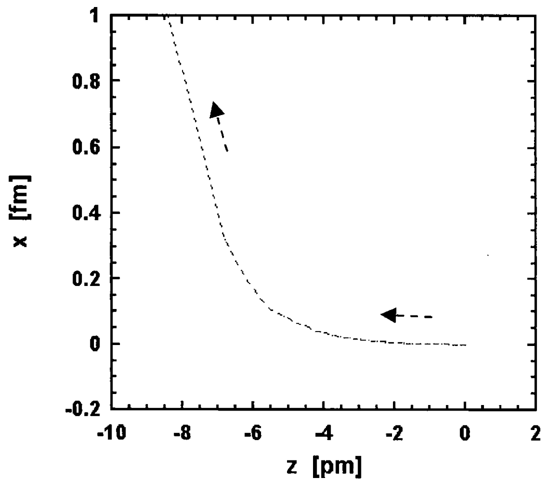

Fig. 4 Close view of electron trajectory near the coordinate origin of Fig.3

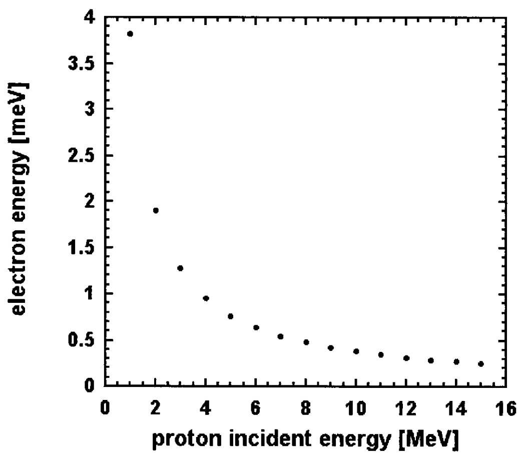

Fig. 5 Kinetic energy of an emitted electron as a function of proton incident energy.

3. Secondary particle productions

3.1. Charged Particle Interaction

Secondary ions emitted from ion-nucleus interactions can possibly affect on the dose distribution. Phits [11] and Geant4 [12] codes are useful for this purpose. We investigated the interaction by measuring proton spectra from the Carbon-Carbon reaction at 290 MeV/u and examining the predictive ability of the Phits code.

The measurement was carried out with 290 MeV/u carbon beam from HIMAC (Heavy Ion Medical Accelerator in Chiba) of the National Institute of Radiological Sciences in Japan. The spectra were obtained by the combination of a multi wire proportional chamber (MWPC) and a GSO(Ce) spectrometer. The emission angles of protons from the graphite target were determined by two dimensional positions measured with the MWPC. The GSO(Ce) spectrometer was used for the energy measurement and particle identification. The spectrometer consists of four cubic crystals of $43\times43\times43$ mm^3 and one cylindrical crystal of 62 mm diameter by 120 mm length. The spectra were obtained in the proton energy region from 200 MeV to 550 MeV three angles covering from zero to three deg. More detailed explanations of the experiment are available in Ref. [13].

In Fig.6, the measured proton energy distributions are displayed. Since more corrections might be needed in data reduction, these results are still preliminary. However, it appears that the Phits simulation results tend to underestimate the experimental data at near 0-degree and in the low energy region. These discrepancies would be serious in estimating the depth dose distributions as well as radial dose distribution. Therefore, further investigations are necessary to develop a more reliable simulation.

3.2. Neutron Flux in a concrete Building

It has been known that neutrons can induce bit-flip in memory devices. Environmental neutrons recently appeared to possibly cause soft-errors in therapeutic devices. To assess the soft-error rate in implantable device therapy, we measured neutron flux as floor variation in an eleven-story building. The measurements were carried out with a gaseous ^{3}He counter and a neutron dose meter. Cosmic muons were also measured with a parallel scintillator plate counter. Details of the experiment are described in Ref. [14]. The resultant fluxes are shown in Fig. 7 after some corrections, and compared with Phits calculation. The neutron flux $f(x)$ after attenuation by a concrete floor of thickness, x is written as

$$f(x)=\phi_n^0\exp(-x/\lambda_n), \qquad (9)$$

where ϕ_n^0 is the neutron flux before absorption by concrete slabs, and λ_n the neutron attenuation length. The results of both neutrons and muons can be accounted by eq. (9).

We also estimated the neutron flux by using the code Phits under an assumption that the flux is ascribed by only the cosmic neutrons, and other sources can be negligible. The Phits result is shown in Fig. 7 for comparison, and show a much steeper fall off than measurements. This inconsistency may be ascribable to the poor assumption. Probably, the code Phits needs to be improved to include other neutron sources. One of the possible sources should be nuclear interactions induced by cosmic muons. And neutron interactions with soil and the reflection might be additional sources of terrestrial neutrons.

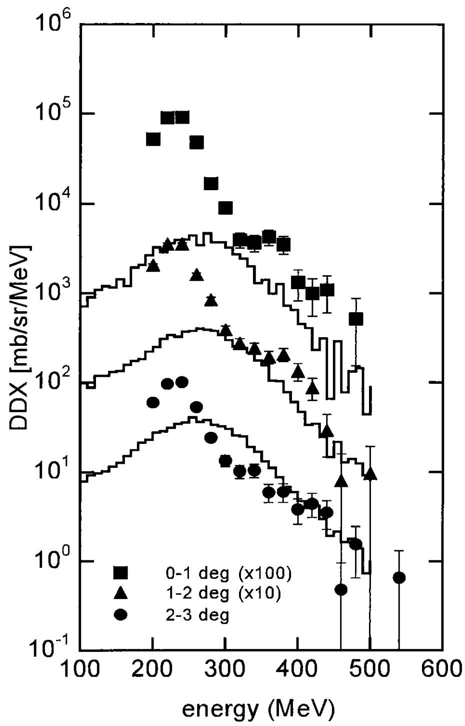

Fig. 6 Proton energy distributions from the C+C reaction at 290 MeV/u.

4. Conclusions

We investigated interactions between particles with cell elements to predict energy deposition and cell response for biomedical modeling in radiation therapy. Several calculations were carried out on cross sections and angular distributions for productions of secondary electrons, protons and heavier particles. Electron production cross sections of protons, alphas and carbons incidence were calculated in an energy range from 0.1 up to 1000 MeV. These high-energy cross section data have been determined for the first time.

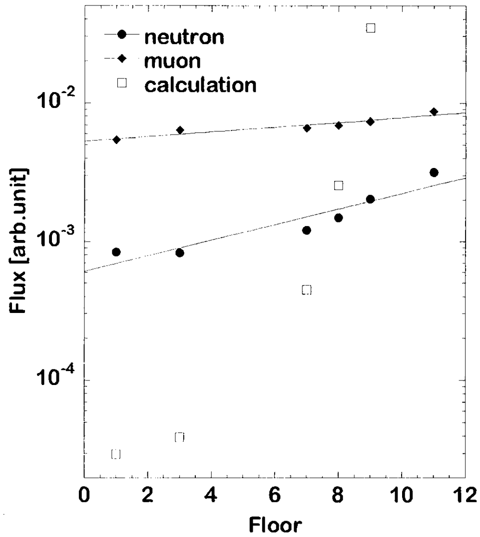

Fig. 7 Floor variation of fluxes of measured neutron (circle), measured muon (diamond) and calculated neutron (square).

And, it was demonstrated that ejected electrons from the interaction are in mostly vertical directions with respect to the incident ion direction. We also investigated the energy transfer and the energy-differential cross section, which are indispensable for the Monte Carlo simulation of the energy deposition and the cell response. Proton production reactions were also investigated with carbon-carbon reaction at the beam energy of 290 MeV/u. One of the most popular simulation tools, Phits has appeared to suffer from a large discrepancy in the energy distribution at the most forward direction. These data obtained in this study is essential to develop a reliable Monte Carlo code for heavy-ion therapy. In addition to these basic studies, the flux of terrestrial neutrons was also investigated for assessment of soft-error rates in implantable device therapy. It is the first time to measure the flux in a concrete building as function of floor, and demonstrated a serious inconsistency between the data and Phits simulation results.

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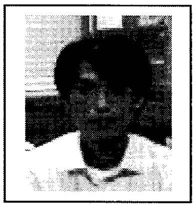

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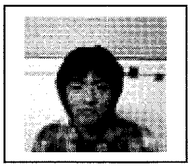

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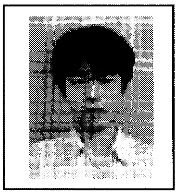

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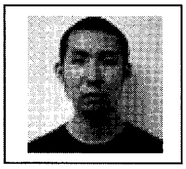

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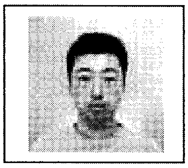

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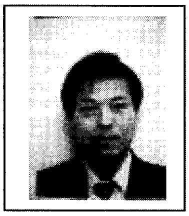

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