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Frequency Distributions of Energy Deposition in a Low-Energy Electron Track

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Based on our Monte Carlo calculation model, the frequency distributions of energy deposition in areas of DNA segment and chromatin fiber segment by low-energy electrons are calculated in liquid water. The results are compared with those of OREC code and CPA code. These calculation results provide the theoretical evidence of a soft X ray mechanism, which was suggested by us to explain the physical mechanism of deep biological effects by ultra-low-energy heavy ion implantation.

Key words: low-energy electron, DNA segment, chromatin fiber segment, frequency of energy deposition.

1. INTRODUCTION

Nowadays research on heavy ion biological effects in China is focused on the medium- or high-energy range of heavy ions abroad, but mostly in ultra-low-energy range ($\leq$200 keV). Moreover, the statistical results of low damage, high mutation rate, and broad mutation spectrum have been obtained by the implantation of ultra-low-energy heavy ions into organisms [1]. However, no matter what kinds of irradiation sources such as high-, medium-, and low-energy heavy ions are used, secondary electrons are emitted at a certain probability during the energy and momentum transfer process between energetic heavy ions and organisms. It has been demonstrated that the secondary electrons produced from energetic heavy ions impacting on organisms could cause more than 90% of the breaks

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in chemical bonds that exist in biological macromolecule such as genetic matter DNA in cells [2]. These secondary electrons have low energies less than several thousands of eV. Because the distribution of the spatial energy deposition of low-energy electrons in subcellular structure is extremely important in understanding fundamental mechanisms of direct damage from ionization radiation,[3] the calculation method and results of energy deposition frequency in biological targets of subcellular structure inside a low-energy electron track are presented in this paper. We first found out that by the results of this single-track effect, OREC and CPA codes all support the soft X ray mechanism suggested by us with which deep biological effects caused by ultra-low-energy heavy ion implantation is explained.

2. CALCULATION OF ENERGY DEPOSITION FREQUENCY

2.1 Calculation Method of Energy Deposition Frequency

Liquid water is chosen as the calculation medium because water is the dominant part of live cells and it occupies about 80% to 90% of fresh weight in most organisms. In cells, water exists in two states—combined and free water. A very large part of water is in the free state, which is a solvent where metabolism products interact with each other. Thus, it is reasonably considered that water is not a kind of inactive medium filled in with structural molecule space, but an inseparable part of the subcellular structure system in cells, such as DNA molecules, chromatin fibers, etc., and the structure and function of the cell are decided by this system [4]. For this reason, water is taken as the medium equivalent to the biological targets, such as DNA molecules and chromatin fibers, which are in close connection with the genetic function of cells, and this equivalence has been widely adopted [3,5].

The biological targets suggested by us here are the models of DNA segment and chromatin fiber segments, which are the subcellular structures causing effects after irradiation. Taking their spatial structure into account, the DNA segments and chromatin fiber segments are simplified as two cylinders 2 nm in diameter and height, and 25 nm in diameter and height, respectively. Consequently, the frequency of energy deposition is the probability of deposited energy greater than a given energy threshold E, which is connected with the critical value causing radiation effects, in these cylinders positioned randomly inside a charged particle track.

The electron tracks are simulated with the Monte Carlo calculation model we built [4]. In liquid water each primary or secondary electron is followed from its starting point until its energy is lower than a cutting energy, for example, the ionization energy of atoms in water. Meanwhile, the deposited energy and spatial coordinate where the electron interacts with water molecules are recorded; thus, the track of the incident electron is kept with these parameters. There are great differences among electron tracks because of the random interactions on the electron slowing-down paths, although the incident electrons have the same starting point and incident direction.

The biological target is positioned at random inside an electron track. A great number of statistical sampling experiments need to be done to calculate the frequency distribution of energy deposition. The concrete method is as follows: A virtual sphere is set up, whose radius is the maximum lateral distance for a lot of electron tracks with the same starting point on the three-dimensional coordinate axes. Each track is surrounded by this sphere whose center coincides with the starting point of the track, and the biological target is positioned randomly in the sphere. Then the frequency of energy deposition $f(>E)$ in the target can be obtained with counting deposition energy greater than the threshold E mentioned previously, and this is called the single-track effect. For the sake of good statistical precision, each track should be sampled more than 10^4. In addition, after comparing the ratio of total energy deposited in the sphere to its volume with the ratio of the total energy deposited in all target cylinders to their volume, the calculation precision can also be obtained, because the two ratios should be equal in theory if a numerous sampling is carried out.

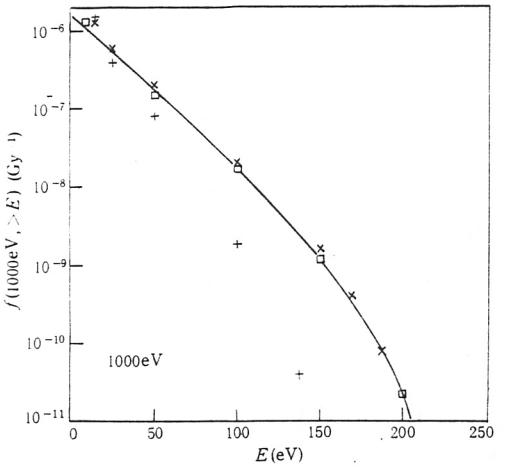

Fig. 1

Absolute frequency of energy deposition in DNA segment inside a 1000 eV electron track.

□ present calculations; × CPA results; + OREC results. These symbols also apply to Figs. 2 to 5.

2.2 Calculated Results of Energy Deposition Frequency Inside the Track of a Low-Energy Electron

Frequency distributions of energy deposition inside the tracks of 1000 eV, 500 eV, and 300 eV electrons are calculated, and the calculation errors are all less than 3%. The absolute frequencies of energy deposition in the DNA segment cylinder inside the tracks of 1000 eV and 300 eV electrons are shown in Figs. 1 and 2, respectively, and that of 1000 eV electrons in a chromatin fiber segment cylinder is shown in Fig. 3. These absolute frequencies $f(>E)$ are all plotted as the integral distributions per target and per unit, that is, as the frequency with which a single target will receive an energy greater than the threshold E if it is positioned at random inside a single electron track and uniformly irradiated with a 1-Gy dose by electrons with a given energy. For 1000 eV electrons, after comparing present results with those of OREC and CPA codes, which are designed by Oak Ridge National Laboratory of the United States and Germany, respectively, it is found that the lower the threshold energy E, the smaller the differences between the three results. The deviation between the results of OREC and CPA is almost beyond an order of magnitude when the threshold energy E is over 50 eV, but our results are between these two and much closer to those of CPA. All results are shown in Fig. 1.

The absolute frequencies obtained previously are all only the results of the single-track effect. They were calculated by treating each track separately, and therefore any overlap of different tracks was ignored. It is mentioned in Ref. [3] that overlap is extremely rare in these small targets except at very high doses, so any overlap effect is not involved in this paper.

The results of relative frequencies of energy deposition are shown in Figs. 4 and 5, which correspond to $E = 50$ eV and $E = 100$ eV, respectively. By taking the absolute frequency of energy deposition f (1000 eV, $>E$) in a DNA segment cylinder inside a 1000 eV electron track as the reference value, the ratio of the absolute frequency of 300 eV or 500 eV electrons, f (300 eV, $>E$), to the reference value is the corresponding relative frequency of energy deposition. There is a great difference among the relative frequency results of us, OREC, and CPA. However, they show the same

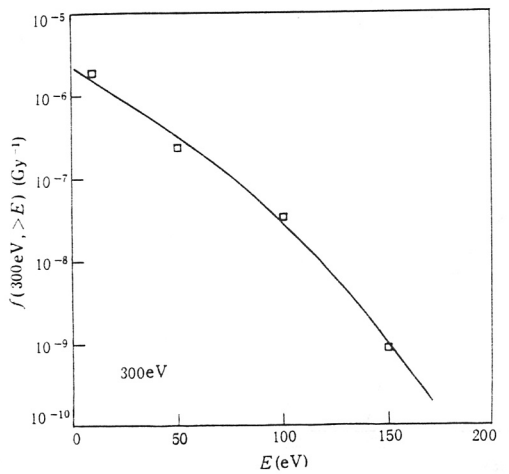

Fig. 2

Absolute frequency of energy deposition in DNA segment inside a 300 eV electron track.

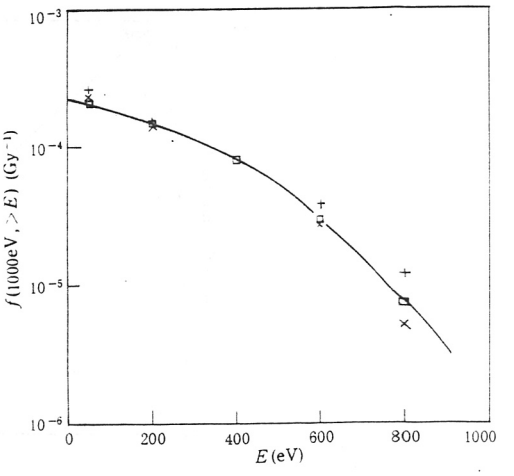

Fig. 3

Absolute frequency of energy deposition in a chromatin fiber segment inside a 1000 eV electron track.

trend, that is, when electron energy changes from several hundreds to several thousands of eV, the lower the energy of the electron, the higher the absolute and relative energy deposition frequencies in the case of threshold energy E. We think that the calculation discrepancy among the three is caused by lack of authoritative interaction cross sections between electron sand water molecules in liquid water at present.

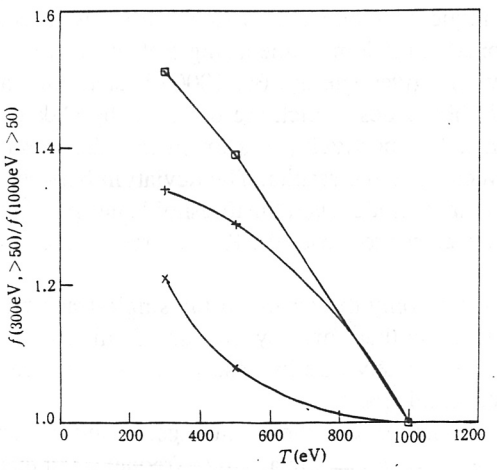

Fig. 4

Relative frequency of energy deposition corresponding to energy threshold E = 50 eV.

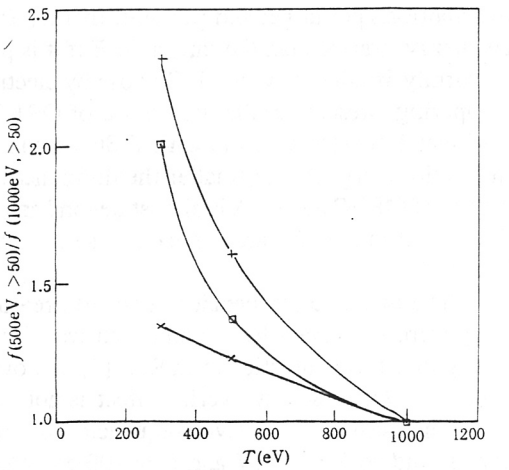

Fig. 5

Relative frequency of energy deposition corresponding to energy threshold E = 100 eV.

3. DISCUSSION

The calculated results indicate that the biological efficiency of low-energy electrons is larger than that of the higher-energy ones because the frequency of energy deposition is proportional to the biological efficiency. They coincide with the experimental results [6].

At present, it has been discovered by many researchers that ultra-low-energy ion implantation can also induce deep biological effects on plant seeds. But the limited range of ultra-low-energy ions themselves cannot reach the depth of observed biological effects; therefore, we suggest an indirect action mechanism, soft X ray mechanism [7,8]. It is considered that ultra-low-energy ions are the source of the inducing characteristic soft X ray. The X ray can penetrate to a great depth into seeds and cause deep biological effects. Finally, it is the low-energy electrons coming from Compton scattering or the photoelectric effect between soft X rays and cells that will act on biological tissue. For example, when the characteristic soft X rays of carbon, the content of which is very high in biological tissue, interact with atoms in seeds, low-energy electrons about 280 eV will be produced. So these calculated results all support the soft X ray mechanism. Furthermore, the intensity of the soft X rays attenuates steeply when they penetrate to a greater depth. Therefore, action on organisms by induced low-energy electrons is approximately the single-track effect, which supports the physical mechanism suggested by us.

The research into low-energy electron track structure is helpful in explaining the mechanism of deep biological effects by ultra-low-energy heavy ions and establishing a corresponding model.

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