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Microscopic Dosimetry around Silver Core Gold Nanoparticle: Monte Carlo Study

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1. Introduction

One of the most widely used methods for tumor treatment is radiation therapy. When conducting radiation therapy, the dose to the normal organ must be minimized to reduce side effects, and the dose to the interest region, such as the tumor, must be maximized to increase the therapeutic effect. However, in conventional external beam radiotherapy (EBRT), the dose to the tumor is limited due to the neighboring normal organ.

Nowadays, attempts to use high-Z metal nanoparticles (MNP) to increase the dose delivered to tumors are promising [1]. When external radiation interacts with high-Z MNPs and releases many secondary electrons, such as auger electrons and photoelectrons, these low-energy secondary electrons can increase the energy delivered to the tumor. As a result, the therapeutic effects of RT can be further enhanced using high-Z MNPs.

Targeted radionuclide therapy (TRT) is another approach to achieving a more localized dose. MNPs can be labeled with radionuclides to use RT. It uses radiation generated from radionuclides without external radiation, so it can further reduce the dose to the normal organ. EBRT irradiates external radiation for tumor treatment; as a result, unnecessary doses are delivered to the normal organ. However, TRT injects radionuclides through blood vessels or directly into the tumor; as a result, radionuclides with MNPs accumulated in the tumor region and are delivered dose locally only to the tumor.

Before using radiolabeled NPs, an investigation of the dose enhancement effect must be preceded. Monte Carlo (MC) study allows the evaluation of the dose enhancement effect of radiolabeled NPs [2]. Herein, we investigated the dose enhancement of silver core gold nanoparticles (GNP) using MC simulations. Especially, microscopic dosimetry around GNPs was compared using MCNP6.2 and Geant4.

2. Materials and Methods

2.1 MC simulation geometry

Fig.1 shows the silver core GNP geometry simulated in MCNP6.2 and Geant4. A totally 50 nm diameter gold or water nanoshell with a 20 nm silver core was designed for microscopic dosimetry around GNP. We obtained the dose enhancement factor (DEF) by calculating the radial energy deposition at intervals of 5-1000 nm up to a distance of 1 mm from the water spherical shell around the GNP. Photon and electron volume source was isotropically generated in the silver core. The simulated energy of photon and electron was 5-30 keV.

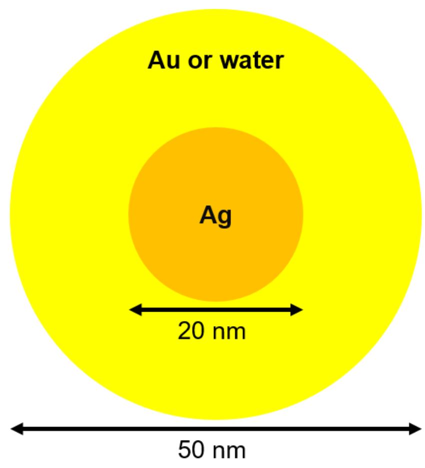

Fig. 1. Illustration of MC simulation geometry in MCNP6.2 and Geant4.

MCNP6.2 using the physics library of Electron-Photon-Relaxation data 14, is based on the ENDF/B. And Geant4 version 11 was used. In this version, Geant4-DNA physics has cross-section data of gold and water. However, for silver core, use Geant4-Livermore physics because Geant4-DNA physics does not have cross-section data of silver. In order to make the simulation setup as similar as possible, Both MC codes set an energy cutoff of 100 eV for photon and electron, and a single-event electron transport method was used for precise calculation for the nanoscale level.

3. Results and Discussion

3.1 Simulation results

Fig. 2 shows the radial energy deposition along the radial distance from the surface of GNP. For 5 keV, the difference between the two MC codes was significant. In particular, in the case of the electron with a gold nanoshell, it can be seen that the difference is more extensive. As the particle energy increased, the difference between MCNP6.2 and Geant4 became smaller. In the case of water nanoshell, it can be seen that the results between both MC codes are almost overlapped. However, in the gold nanoshell case, the MCNP6.2 was always greater than Geant4 at distances within 100 nm, where the influence of low-energy electrons was dominant.

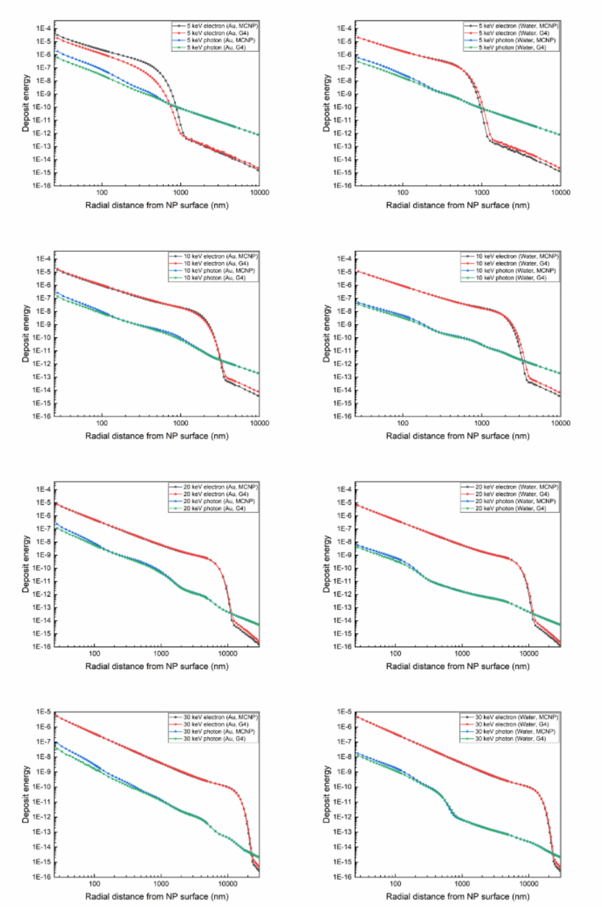

Fig. 2. Radial energy deposition alone the radial distance from the surface of GNP. The left rows show the radial energy deposition with gold nanoshell, and the right rows show the radial energy deposition with water nanoshell.

Fig. 3 shows the DEF around GNP. Similar to the trend of radial energy deposition, the difference between both MC codes was large when the particle energy was low. However, as the energy increased, the difference decreased significantly. In particular, the DEF of the photon, where several peaks occur due to photoelectron, also confirmed a similar tendency.

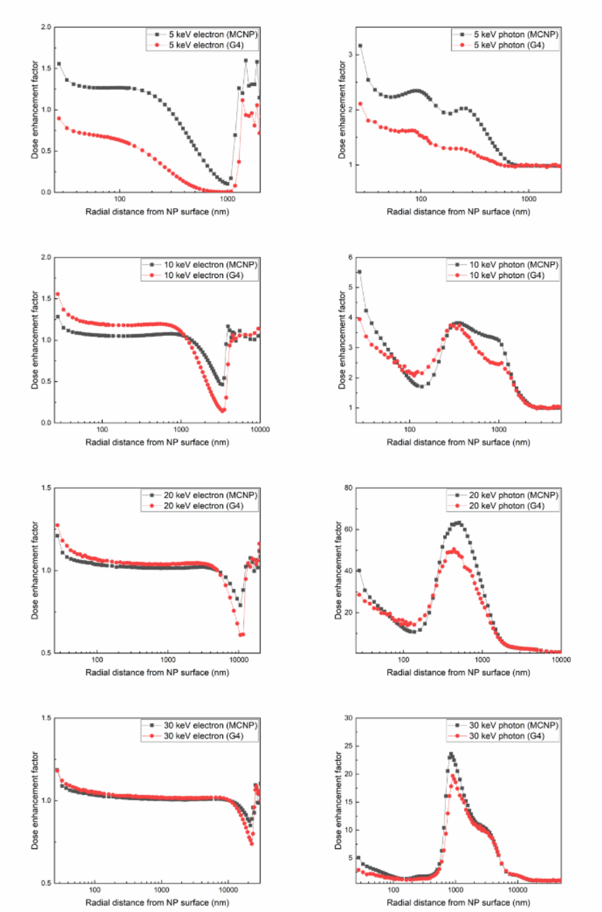

Fig. 3. DEF around GNP. The left rows show the DEF of the electron, and the right rows show the DEF of the photon.

4. Conclusions

We investigated the microscopic dosimetry around GNP using MCNP6.2 and Geant4. Except for 5 keV, both MC simulation codes obtained similar radial energy deposition and DEF. This is because MCNP6.2 and Geant4-DNA physics have different cross-section data for low-energy electrons and photons. MCNP6.2 uses cross-section data based on the Livermore library like Geant4-Livermore physics. Nevertheless, using the single-event electron transport method, we confirmed that MCNP6.2 could also be accurately calculated at the nanoscale. In the future, we will perform simulations to determine the radionuclide and GNP structures suitable for TRT.

Acknowledgements

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REFERENCES

[1] Kwatra, D, Venugopal, A, and Anant, S, Nanoparticles in radiation therapy: A summary of various approaches to

enhance radiosensitization in cancer. Transl. Cancer. Res., Vol. 2, p. 330-342, 2013.
[2] Sung, W, Jung, S, and Ye, S. J, Evaluation of the microscopic dose enhancement for nanoparticle-enhanced Auger therapy. Phys. Med. Biol., Vol. 61, p. 7522-7535, 2016.