Photoelectronic processes when irradiating magnetite nanoparticle with a monochromatic X-ray beam

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Abstract
Magnetite (Fe₃O₄) nanoparticles possess several properties that can make them a tool for targeted delivering of radiation to tumors for the purpose of brachytherapy. First, they are biodegradable. Second, due to their magnetic properties they can be fixed near desired location inside body using external magnets. Finally, they can emit secondary radiation when irradiated by an external source, such as X-ray tube or synchrotron. We consider two mechanisms for generation of such secondary radiation: photoelectronic processes and Mössbauer effect (in the latter case the particles must have a substantial part of ⁵⁷Fe isotope). In the present work we consider photoelectronic processes only. The work on Mössbauer effect is under way.

Motivation
● to develop a method of tumor irradiation that does not require radioactive isotopes. The method must allow targeted delivering of radiation to tumor. Only biodegradable materials must be used.

The specific aims of this study are:
● to calculate the dose enhancement ratio around magnetite particle irradiated by photon beams of different energies. Estimate optimal energy.
● to calculate spectra going out from the particle.

Background
The ferrofluid, based on ⁵⁷Fe isotope enriched Fe₃O₄, was synthesized, investigated by Mössbauer spectroscopy method and injected transcranially in the ventricle of the rat brain. The comparison of the Mössbauer spectra of the initial ferrofluid and the rat brain measured in two hours and one week after the transcranial injection allow us to state that the synthesized magnetic ⁵⁷FeO₄ nanoparticles undergo intensive biodegradation in live brain and, therefore, can be regarded as a promising target for a new method of radionuclide-free Mössbauer brachytherapy.

Computational details
The simulations were done using Geant4 package version 10.0.0.p1 with low energy data pack G4MLOW which includes data from EPDL97 (Evaluated Photon Data Library from Livermore). This library is among the recommended for medical computations by the AAPM (American Association of Physicists in Medicine) in TG-43U1 protocol. Water was used as a phantom for absorbed dose calculations.

Spherical magnetite particle of 10 nm diameter was placed at the center of a cube with 100 nm edge size either filled with water (for obtaining tracks and dose distributions) or empty (for obtaining spectra going out from the particle).

The particle was irradiated by monochromatic photon beams. Absorbed doses were accumulated in 2D histograms with ring-shaped cells of 1 nm size by the both directions (by height and radial). Histogram bin for obtaining secondaries spectra was 100 eV.

Results
By means of the Monte Carlo method we have simulated the dose distribution in water around a 10 nm diameter magnetite particle irradiated by monochromatic X-ray beams of different energies.

First, we considered an idealistic case when the particle is irradiated by a narrow beam of the same diameter as the particle (see Figures 1-3). This allows us to see that optimal beam energy is about 8 keV (Iron Kα is 6.4 keV). At lower energies the primary beam strongly interacts with water while at higher energies the total outcome reduces due to weak interaction of the beam with the particle material.

Finally, we calculated dose enhancement ratio for irradiation by wide beam of 8 keV photons.

Conclusion
The magnetite particle was shown to increase the dose absorbed by surrounded water. However, if we want to increase twice or higher the dose deposited to cell DNA, we need to transport the particles into cell nucleus.

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For notes etc.