ROLE OF PHOTO- AND CASCADE ELECTRONS IN PHOTON ACTIVATION THERAPY USING HIGH-Z RADIOSENSITIZERS

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Emission of electrons and photons during the cascade decay of vacancies in the electron shells of the Ag, Gd and Pt atoms are simulated by straightforward construction and analysis of the cascade decay trees. The energies reemitted with cascade photons, cascade electrons and photoelectrons after photoionization of Ag, Gd and Pt atoms in the 0.1–100 keV incident photon energy range are calculated. It is shown that the cascade electrons and photoelectrons are the most effective local energy depositors when the high-Z atoms are used as radiosensitizers in photon activation therapy.

Keywords: photoionization; cascade relaxation; energy reemission; radiosensitization; radiotherapy.

Introduction

Bio-neutral atoms with high nucleus charges Z, such as Ag, I, Gd, Hf, Pt, Au, are widely used as radiosensitizers in a branch of radiation therapy of cancer called photon activation therapy (PAT). Such atoms, contained in chemical compounds or nanoparticles are injected into a tumor prior to its irradiation with high-energy photons which increases the damage to the tumor under irradiation. The radiosensitization effect is two-fold. First, the high-Z atoms having large photoionization cross sections allow localizing the energy absorption from the incident photon beam inside the tumor, and thus less harm is made to healthy tissues. Second, the cascade decay [1] of inner-shell vacancies created by photoionization leads to the reemission of energy with cascade electrons and photons which eventually cause direct and indirect damage to the tumor cells' DNA.

Cascade reemission of energy has been studied in the cases of the cascade decay of inner-shell vacancies in atomic Fe [2], Ag [3], I [4], and Au [5]. In this work we simulate the cascade decays of vacancies in Ag, Gd and Pt, and analyze the energies reemitted after photoionization of these atoms in the 0.1-100 keV incident photon energy range. Relative role of cascade electrons, cascade photons and photoelectrons in targeted energy deposition to the environment is discussed.

Method of calculation

Cascade decays of vacancies in inner electron subshells of the Ag, Gd, and Pt atoms were simulated by the method of straightforward construction of and analysis of decay trees (CADT) described in detail in refs. [6,7]. The following approximations were used in the simulations:

–Transition probabilities are calculated in Pauli–Fock (PF) approximation [8] with taking into account actual electron configurations of the decaying multivacancy ionic states;

–Transition energies are calculated as differences of total energies of the initial- and final-state ions;

–Multiplet splitting of ionic configurations are accounted for by the method of global characteristics of the atomic spectra.

Photoionization cross sections are calculated using the PF approximation for the core and continuous spectrum wave functions with accounting for the core relaxation in the field of an inner vacancy as described in [5].

Calculated spectra of cascade electrons $P^{\mathrm{el}}_{nlj}(E_i)$ and photons $P^{\mathrm{phot}}_{nlj}(E_k)$ emitted during the decay of the nl_j-vacancy are the transition probabilities against respective transition energies. As an example, electron and photon spectra emitted during the cascade decay of the 1s vacancy in Gd are shown in Fig. 1.

The energies reemitted with cascade electrons and cascade photons during the decay of an nl_j vacancy are calculated using respective spectra:

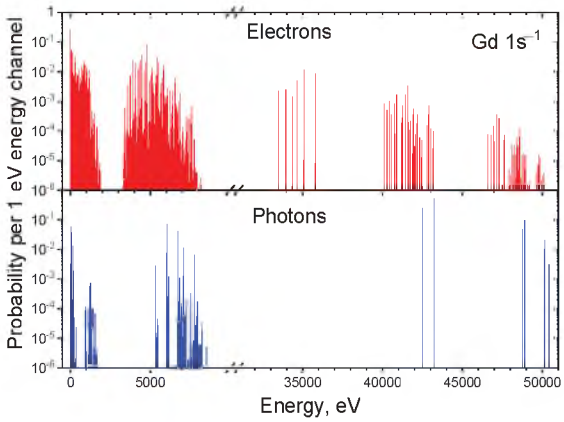

Fig. 1. Spectra of electrons and photons emitted during the cascade decay of the 1s vacancy in atomic Gd

$$E^{\mathrm{el}}_{\mathrm{reem}}(nl_j) = \sum\nolimits_i E_i P^{\mathrm{el}}_{nlj}(E_i)\,, \qquad (1)$$

$$E^{\mathrm{phot}}_{\mathrm{reem}}(nl_j) = \sum\nolimits_k E_k P^{\mathrm{phot}}_{nlj}(E_k)\,. \qquad (2)$$

The energies of photoelectrons after nl_j photoionization are

$$E^{\mathrm{PE}}_{\mathrm{reem}}(nl_j) = h\nu - I_{nlj}\,, \qquad (3)$$

where $h\nu$ is the incident photon energy, and I_{nlj}, the nl_j-subshell ionization threshold.

At a given incident photon energy, many electron subshells can be ionized, which should be taken into account. Let $\sigma_{nlj}(h\nu)$ be partial photoionization cross sections of a radiosensitizer atom. Then one can introduce the following normalized values:

$$\varepsilon^{x}_{\mathrm{reem}}(h\nu) = \frac{dE^{x}_{\mathrm{reem}}}{dV d\Phi dn} = \\ = \sum\nolimits_{nlj} \sigma_{nlj}(h\nu) E^{x}_{\mathrm{reem}}(nl_j), \qquad (4)$$

where $x = $ el, phot or PE. These are the energies reemitted by radiosensitizing atoms in unit volume per unit incident photon flux density, unit atomic concentration of radiosensitizer atoms, and unit time.

Results and discussion

Fig. 2 shows calculated $\varepsilon^{x}_{\mathrm{reem}}(h\nu)$ for photon-irradiated Gd atom. One can see that at incident photon energies under Gd *K* threshold, most of the energy acquired by the Gd atom on photoionization is reemitted into environment with cascade electrons and photoelectrons.

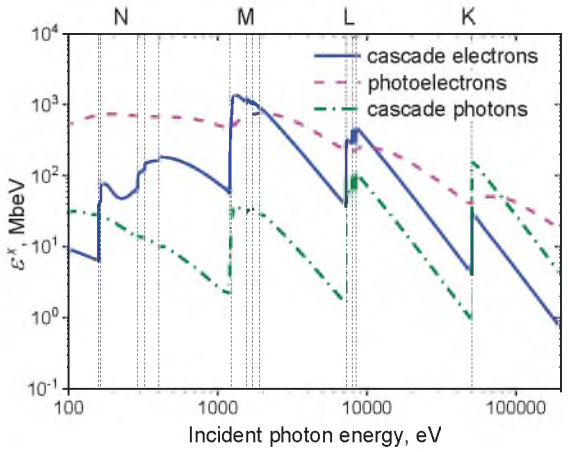

Fig. 2. Energies reemitted with photoelectrons, cascade electrons and cascade photons in unit volume per unit incident photon flux and unit Gd concentration. Vertical dashed lines show the positions of ionization thresholds

The energy carried away by cascade photons is dominant on the 51–80 keV interval above the *K* threshold. Anyway, most of the cascade photons are of little importance in radiosensitization since their mean free paths in tumor tissues are orders of magnitude larger than a typical cell size *D* of 10^4-10^5 nm [5]. This means that they will depose their energy in the surrounding medium in large volumes and with rather small doses.

On the contrary, the mean free paths of photoelectrons, and especially cascade Auger, Coster–Kronig and super Coster–Kronig electrons, are much smaller than *D*. These electrons will depose energy to the tumor tissues in small volumes in the nearest vicinity of the emitting atom, and with large doses.

In Fig. 3, combined normalized contributions to reemitted energy from cascade electrons and photoelectrons

$$\varepsilon^{\mathrm{el,PE}}_{\mathrm{reem}}(h\nu) = \varepsilon^{\mathrm{el}}_{\mathrm{reem}}(h\nu) + \varepsilon^{\mathrm{PE}}_{\mathrm{reem}}(h\nu) \qquad (5)$$

for the Ag, Gd, and Pt atoms are compared. Expectantly, $\varepsilon^{\mathrm{el,PE}}_{\mathrm{reem}}$ peak near respective ionization thresholds; their approximate positions are marked in Fig. 1. If tunable-energy photon sources are available in clinical practice, the energy of irradiating photons should be chosen to be able to ionize the radiosensitizer atoms near thresholds.

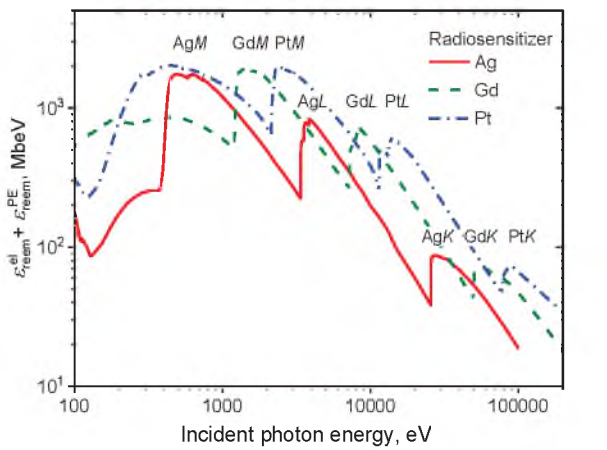

Fig. 3. Energies reemitted with photoelectrons and cascade electrons in unit volume per unit incident photon flux and unit atomic concentration of the radiosensitizing atom (Ag, Gd and Pt)

An approximate tuning of irradiating photon energy can be achieved even when using the X-ray tubes by choosing the anode material and voltage.

Maximal energy reemission is seen at incident photon energies near the *M* thresholds of Ag, Gd and Pt. However, irradiation at this photon energy range will be effective only in the case of close-to-body-surface tumors as the depth of penetration of the incident photon beam is too small.

Using energies near *L* and *K* thresholds makes it possible to reach deeper-sitting tumors. But in this case, larger photon fluxes are needed to obtain desirable therapeutic doses as normalized reemission energies $\varepsilon^{el,PE}_{reem}$ are substantially smaller at those energies.

Conclusion

The mechanisms energy deposition when using silver, gadolinium and platinum atoms as radiosensitizers in PAT are studied. Cascade electrons and photoelectrons are found to be the main local energy depositors when high-Z atoms are used as radiosensitizers. Calculated normalized energies reemitted with cascade-produced electrons and photoelectrons as functions of incident photon energy can serve a theoretical base in developing the strategies of PAT. Theoretically-based choice of radiosensitizing atoms concentration, the energy and flux of irradiating photons can provide desired therapeutic doses in tumors of various sizes and location.

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