Article
https://doi.org/10.31489/2024PH4/60-67
UDC 539.184.5

Received: 25.06.2024
Accepted: 19.08.2024

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Final ion formation and energy reemission upon a cascade decay of single vacancies in the *K* and *L* electron shells of atomic platinum

Cascade decay of single vacancies in 1s, 2s, $2p_{1/2}$, and $2p_{3/2}$ subshells of an isolated platinum atom are simulated by the method of construction and analysis of the cascade decay trees. The yields of final ions and the spectra of cascade electrons and photons are calculated. Mean charges of the final ions formed as a result of the cascade decays of 1s, 2s, $2p_{1/2}$, and $2p_{3/2}$ vacancies in the platinum atom are 7.75, 9.82, 7.80, and 7.95, respectively. The energies stored in final cascade ions, and the energies reemitted with cascade electrons and photons are calculated for the decays of each initial inner-shell vacancy. In the case of decay of vacancies in the 2s, $2p_{1/2}$, and $2p_{3/2}$ subshells, most of the energy initially acquired by the atom during the creation of an initial inner-shell vacancy is re-emitted by Auger and Coster–Kronig cascade electrons. In the case of 1s vacancy decay, most of the energy is carried away by cascade photons, predominantly *KL*. The prospects of using platinum-based agents as radiosensitizers in photon activation therapy of cancer are discussed.

Keywords: platinum, vacancy cascade, decay tree, ion yields, cascade energy reemission, radiosensitization, Auger therapy, photon activation therapy.

Introduction

Creation of an inner-shell vacancy in an atom produces a high-energy excited state which then decays through a sequence of radiative and non-radiative transitions into terminal (often highly charged) stable ionic states [1–4]. Cascade decay of vacancies, also called vacancy cascades, is a fundamental atomic process occurring whenever an inner-shell vacancy is created. The energy acquired by the atom upon ionization is reemitted into the environment with numerous cascade electrons and photons. This circumstance makes it possible to use heavy bio-neutral atoms as radiosensitizers in photon activation therapy (PAT) of malignant tumors [5, 6]. Radiosensitizers are the agents introduced into the tumor prior to irradiation in order to increase the damage to cancer cells.

Radiosensitization effect is two-fold. In the first place, due to large photoionization cross sections of the high-Z radiosensitizing atoms, the absorption of energy from an incident ionizing radiation beam is localized in the tumor, so less harm is made to healthy tissues. What is important, the energy absorbed by a radiosensitizing atom does not stay with it, a large portion of the absorbed energy is reemitted with cascade-produced electrons and photons into surrounding tissues causing direct and indirect damage to cancer cells' DNA. Energy reemission following inner-shell ionization has been studied in iron [7], gold [8], silver [9, 10] and iodine [11] atoms by theoretical cascade simulations.

Platinum is a popular radiosensitizer introduced into tumors within chemical compounds or in nanoparticles. It is often contained in chemotherapeutic drugs; a PAT using chemotherapeutic radiosensitizers is called chemoradiotherapy (CRT) [12, 13].

In this work we study the cascade decays of single 1s, 2s, $2p_{1/2}$, and $2p_{3/2}$ vacancies in an isolated platinum atom by straightforward construction of the cascade decay trees. The yields of final cascade ions, and energies *a*) stored in final ions, *b*) reemitted with cascade-produced electrons, and *c*) reemitted with cascade-produced photons are calculated. The prospects of using platinum atoms as radiosensitizers are discussed.

Theory

To simulate the cascade decay of vacancies, we use the method of construction and analysis of decay trees described in detail in [14, 15]. A brief review of the method is given in this Section.

A cascade decay tree consists of branching points and branches connecting them. The branching points are ionic configurations — an initial inner-shell-vacancy one, and those appearing during the cascade transitions. The branches of the decay tree are the cascade transitions — radiative with the emission of photons, and non-radiative (Auger, Coster–Kronig, super-Coster–Kronig) with the emission of electrons.

Cascade decay trees for specific initial inner-shell vacancy states were built as follows. Let $C^{(0)}$ be the starting branching point of the tree, i.e. the initial configuration with a single inner-shell vacancy. It decays into lower-in-energy ionic states which form a set of the first-decay-step configurations $\{C_i^{(1)}\}$. Some of the configurations $C_i^{(1)}$ can still have inner vacancies and can decay further. Their decays form a second-decay-step set of configurations $\{C_j^{(2)}\}$, etc. The tree is completely built when after the n^{th} decay step none of the configurations $\{C_k^{(n)}\}$ can decay further having vacancies only in the uppermost subshells. The decay trees for the cascades with deep vacancies in heavy atoms are very complex. This is illustrated in Table 1 which lists the number of different ionic configurations appearing after each decay step during the cascade decay of single vacancies in 1s, 2s, $2p_{1/2}$, and $2p_{3/2}$ subshells of the platinum atom. One can see that the number of decay steps reaches 23, and tens of thousands of different ionic configurations can appear after several consecutive decay steps. The bottom line of Table 1 shows the total numbers of branches in the decay trees; they amount to tens of millions.

Table 1

Numbers of different ionic configurations appearing after each decay step during the cascade relaxation of single vacancies in 1s, 2s, $2p_{1/2}$ and $2p_{3/2}$ subshells of an isolated platinum atom, and total numbers of branches (N_{br}) in respective decay trees

Decay step	1s	2s	$2p_{1/2}$	$2p_{3/2}$
1	177	166	153	144
2	1333	1051	950	873
3	5878	4582	3876	3528
4	15079	13374	9695	8477
5	23506	24503	14633	12152
6	27077	31099	16699	13260
7	26766	32711	16009	12554
8	23855	30353	13629	10554
9	19298	25360	10407	7819
10	14288	19345	7111	5198
11	9606	13319	4438	3166
12	6000	8515	2673	1923
13	3624	5164	1686	1289
14	2096	3220	1223	956
15	1418	2163	914	693
16	1006	1593	641	459
17	705	1184	393	281
18	447	791	222	138
19	242	469	97	61
20	110	248	32	18
21	39	109	5	
22		28		
23		2		
N_{br}	2.12E7	1.962E7	8.222E6	5.902E6

The cascade decay tree can be built if for each branching point $C_i^{(m)}$ relative probabilities of all allowed transitions into lower-in-energy ionic states $C_j^{(m+1)}$ are known. These relative probabilities, also known as branching ratios, are calculated with

$$\chi(C_i^{(m)} \to C_j^{(m+1)}) = \frac{\Gamma(C_i^{(m)} \to C_j^{(m+1)})}{\sum_k \Gamma(C_i^{(m)} \to C_k^{(m+1)})}, \quad (1)$$

where Γ are partial transition widths which in atomic units coincide with the probabilities of transitions per unit time. The summation is performed over all energy- and symmetry-allowed radiative and non-radiative transition from $C_i^{(m)}$. Partial transition widths were calculated using the radial parts of bound- and continuous-state atomic wave functions calculated in Pauli–Fock (PF) approximation [16]. They were calculated for single-vacancy ions, and then modified so as to take into account actual electron configurations of decaying ions as described in [14, 15].

Mean energies of cascade transitions $C_i \to C_f$ are calculated using mean total PF energies E_i and E_f of initial and final ionic configurations of the transitions. If the multiplets of C_i and C_f overlapped, only the transitions between the multiplet components allowed by the energy conservation law were considered when calculating mean transition energies and partial transition widths. The multiplets of ionic configurations were simulated with Gaussian probability density distributions using the methods of global characteristics of spectra [17, 18].

In a decay tree, all terminal configurations are those of final ion states with specific ion charges. Let $\{C_i(q)\}$ be the set of terminal ionic states in a $+q$ charge state found in the decay tree. The probability to discover an atom in a specific charge state $+q$ (ion yield) is the sum of probabilities to get from $C^{(0)}$ to each $C_i(q)$ through all possible decay pathways:

$$P_{C^{(0)}}(q) = \sum_i \sum_{\text{pathways}} P_{\text{pathway}}(C^{(0)} \to C_i(q)) \qquad (2)$$

In its turn, the probability of getting from $C^{(0)}$ to $C_i(q)$ along a given pathway is a product of the branching ratios of all the transitions throughout the pathway:

$$P_{\text{pathway}}(C^{(0)} \to C_i(q)) = \chi(C^{(0)} \to C_a^{(1)})\chi(C_a^{(1)} \to C_b^{(2)})...\chi(C_p^{(n-2)} \to C_r^{(n-1)})\chi(C_r^{(n-1)} \to C_i^{n}(q)) \qquad (3)$$

Mean final ion charges upon decays of initial single-vacancy states $C^{(0)}$ are calculated with

$$\langle q_{C^{(0)}} \rangle = \sum_q q P_{C^{(0)}}(q) \qquad (4)$$

The spectra of electrons and photons produced by the cascade relaxation of an inner-shell-vacancy configuration $C^{(0)}$ are the probabilities of emission of electrons $P_{C^{(0)}}^{\text{el}}(i)$ and photons $P_{C^{(0)}}^{\text{phot}}(k)$ against respective electron $E_{C^{(0)}}^{\text{el}}(i)$ and photon $E_{C^{(0)}}^{\text{phot}}(k)$ energies:

$$Sp_{C^{(0)}}^{\text{el}} = \{E_{C^{(0)}}^{\text{el}}(i), P_{C^{(0)}}^{\text{el}}(i)\},\ Sp_{C^{(0)}}^{\text{phot}} = \{E_{C^{(0)}}^{\text{phot}}(k), P_{C^{(0)}}^{\text{phot}}(k)\} \qquad (5)$$

In the above notations, i and k number spectral components, i.e. cascade transitions during the cascade relaxation of $C^{(0)}$. Probability of any cascade transition $P(C_i \to C_f)$ is the product of the probability of the initial-state configuration C_i to appear, and the transition branching ratio:

$$P(C_i \to C_f) = P(C_i)\chi(C_i \to C_f) \qquad (6)$$

The appearance probabilities $P(C_i)$ are calculated in the same way as the probabilities to discover the configurations of final ions, see (2), (3).

Upon nl_j ionization, the atom acquires the energy $E_{\text{in}}(nl_j)$ equal to the threshold ionization energy of the nl_j orbital. We split the acquired energy $E_{\text{in}}(nl_j)$ into the following redistribution channels: *a*) mean energy stored in final cascade ions $E^{\text{ion}}(nl_j)$, *b*) mean energy reemitted with cascade electrons $E_{\text{out}}^{\text{el}}(nl_j)$, and *c*) mean energy reemitted with cascade photons $E_{\text{out}}^{\text{phot}}(nl_j)$. $E_{\text{out}}^{\text{el}}(nl_j)$ and $E_{\text{out}}^{\text{phot}}(nl_j)$ are calculated using electron and photon spectra emitted upon the decay of respective single-vacancy states $C^{(0)} = nl_j^{-1}$:

$$E_{\text{out}}^{\text{el}}(nl_j) = \sum_i P_{nl_j^{-1}}^{\text{el}}(i) E_{nl_j^{-1}}^{\text{el}}(i), \quad E_{\text{out}}^{\text{phot}}(nl_j) = \sum_k P_{nl_j^{-1}}^{\text{phot}}(k) E_{nl_j^{-1}}^{\text{phot}}(k) \qquad (7)$$

Evidently,

$$E^{\text{ion}}(nl_j) = E_{\text{in}}(nl_j) - E_{\text{out}}^{\text{el}}(nl_j) - E_{\text{out}}^{\text{phot}}(nl_j) \qquad (8)$$

Note that when a cascade relaxation of an atom happens within an organism tissue as in the case of PAT, the energy of the cascade ions $E^{\text{ion}}(nl_j)$ will be also eventually deposited to the environment via ions neutralization.

Results and Discussion

Calculated final ion yields (ion charge spectra) upon the decay of 1s, 2s, $2p_{1/2}$ and $2p_{3/2}$ initial single vacancies in the platinum atom are shown in Figure 1. Mean final ion charges are given in respective panels. One can see that quite large degree of cascade ionization can be reached: the ions with charges up to +18 are produced. Mean final ion charges are also large, e.g. in the case of the 2s vacancy relaxation mean ion charge is 9.82.

Note that the charge spectra upon the decay of 1s, $2p_{1/2}$ and $2p_{3/2}$ vacancies are very much alike. This is because the main channels of the first-step decay of the 1s vacancy are the radiative transitions into $2p_{1/2}$ and $2p_{3/2}$ states with the emission of KL_{23} ($K\alpha_{12}$) photons. According to our calculations, a combined branching ratio of this transition is 0.78, and the decay trees for $2p_{1/2}$ and $2p_{3/2}$ initial vacancies do not differ much. In the case of the initial 2s vacancy, the cascade is more complex. Its decay tree contains additional $L_1L_{23}N$ and $L_1L_{23}O$ Coster–Kronig branches causing additional emission of electrons. The charge spectra of the cascades in platinum are very much the same as those of the cascades in gold. The latter are discussed in detail in ref. [19].

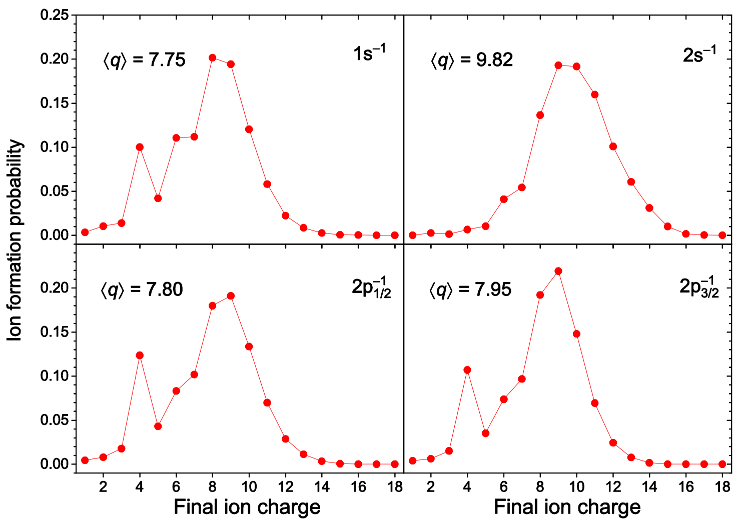

Figure 1. Final ion yields upon the cascade decay of single 1s, 2s, $2p_{1/2}$ and $2p_{3/2}$ vacancies in atomic Pt

As an example, Figure 2 shows the spectra of electrons and photons emitted during the cascade decay of the 1s vacancy in the platinum atom. A typical feature of all the deep-initial-vacancy cascade spectra is their complex multicomponent structure caused by the fact that the cascade transitions occur in a multitude of different multivacancy ionic configurations.

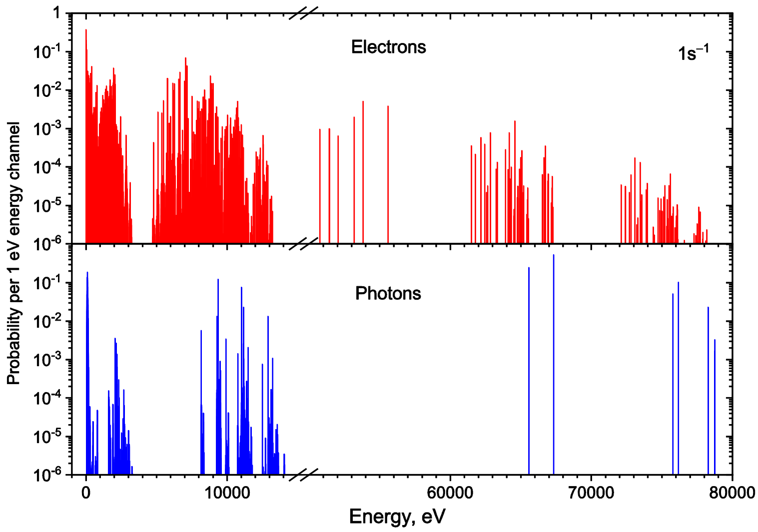

Figure 2. Spectra of electrons and photons emitted during the cascade decay of 1s vacancy in an isolated Pt atom. Energy bin is 1 eV

Table 2 shows calculated energies acquired by the platinum atom on ionization of its 1s, 2s, $2p_{1/2}$ and $2p_{3/2}$ subshells, and the energies stored in final cascade ions and reemitted with cascade electron and photons after cascade relaxation of vacancies. Also shown in the Table are relative weights of energy redistribution channels (in parentheses). It is seen from Table 2 that upon *K* and *L* ionization of Pt, only a small portion of the acquired energy rests with the platinum ions. Most of the energy is reemitted into the environment by cascade electrons and photons. Energy reemitted by electrons is the principal energy redistribution channel in the case of *L* ionizations making 59 to 66 % of the acquired energy. In the case of 1s ionization, most of the energy is carried away by cascade photons, predominantly KL_{23}.

To be able to draw conclusions about the role of cascade electrons and photons in PAT, it is necessary to analyze their mean free paths in organism tissues. Most effective in causing damage to tumor cells will be the particles with small inelastic free paths in the organism tissue medium. They will depose their energy to tumor cells in the nearest vicinity of the emitting atom, and with large doses. The particles with large free paths will spread their energy in larger volumes and with smaller doses.

Table 2

Energies acquired upon nl_j ionization of atomic platinum $E_{in}(nl_j)$, energies stored in final platinum ions $E^{ion}(nl_j)$, and energies reemitted with cascade electrons $E^{el}_{out}(nl_j)$ and cascade photons $E^{phot}_{out}(nl_j)$

nl_j	$E_{in}(nl_j)$, eV	$E^{ion}(nl_j)$, eV	$E^{el}_{out}(nl_j)$, eV	$E^{phot}_{out}(nl_j)$, eV
1s	78814	614 (0.8 %)*	7827 (10.0 %)	70373 (89.2 %)
2s	13917	939 (6.8 %)	9039 (65.0 %)	3939 (28.2 %)
$2p_{1/2}$	13236	534 (6.8 %)	7762 (58.7 %)	4939 (37.3 %)
$2p_{3/2}$	11492	525 (4.6 %)	7621 (66.3 %)	3346 (29.1 %)
*Note – Relative weights of energy redistribution channels				

Figure 3 shows mean inelastic free paths of electrons and photons in liquid water calculated in [8]. Water is a commonly accepted simulation of organism tissues. As seen from Figures 3 and 4, mean inelastic free paths of cascade electrons are rather small; they are three to four orders of magnitude less than typical cell size, it is shown in Figure 4 with horizontal lines. This means that all the cascade electrons will contribute to the PAT effect. As for photons, their free paths in most cases are by orders of magnitude greater than the cell size which makes them hardly effective in PAT. Only a small portion of emitted cascade photons have free paths smaller than the cell size. Proportions of the energy reemitted with such PAT-prospective photons are 0.2 %, 2.5 %, 1.4 % and 1.7 % in 1s- 2s- $2p_{1/2}$- and $2p_{3/2}$-cascades, respectively.

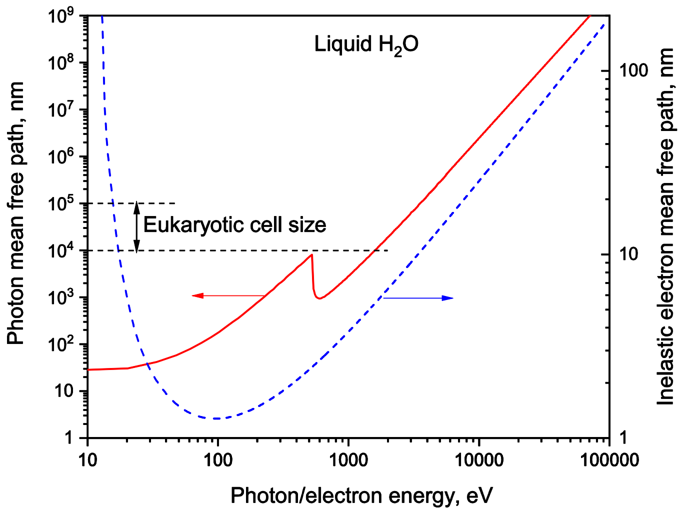

Figure 5. Electron and photon inelastic free paths in water calculated in [8].

The studies on cascade energy reemission in gold [8], silver [9, 10] and iodine [11] atoms have shown that photoelectrons can also contribute to the PAT effect giving contribution to the emitted energy comparable to that from cascade electrons. Although we did not address the role of photoelectrons in this study, we believe that in the case of platinum, they will give considerable contribution to the PAT effect, too.

Conclusions

The method of construction and analysis of the decay trees is applied to simulate cascade decay of single 1s, 2s, $2p_{1/2}$ and $2p_{3/2}$ vacancies in an isolated platinum atom. Final ion charge spectra and the spectra of cascade electrons and photons are calculated. It is shown that most of the energy acquired by the atom upon ionization is reemitted by cascade electrons and photons. All the cascade electrons having rather short inelastic mean free paths are effective in photon activation therapy of cancer when platinum is used as a radiosensitizing agent. Only a small portion of cascade photons is PAT effective.

Acknowledgments

This research was funded by the Russian Science Foundation (project no. 23–22–00222, https://rscf.ru/project/23-22-00222/).

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Ақырлы иондардың түзілуі және платина атомының K және L электронды қабықшаларындағы жалғыз бос орындардың каскадты ыдырауы кезінде энергияның қайта шығарылуы

Каскадты ыдырау ағаштарын құру және талдау әдісімен оқшауланған платина атомының 1s, 2s, $2p_{1/2}$ және $2p_{3/2}$ ішкі қабықшаларындағы бір жұмыс орындарының каскадты ыдырауын модельдеу жүргізілді. Соңғы иондардың шығуы және каскадты электрондар мен фотондардың спектрлері есептеледі. PT атомындағы 1s, 2s, $2p_{1/2}$ және $2p_{3/2}$ қуыстарының каскадты ыдырауынан пайда болған соңғы иондардың орташа зарядтары сәйкесінше 7,75, 9,82, 7,80 және 7,95 құрайды. Әрбір бастапқы ішкі қуыстың ыдырауы үшін соңғы каскадты иондарда жинақталған энергия және каскадты электрондар мен фотондар қайта шығаратын энергия есептеледі. 2s, $2p_{1/2}$ және $2p_{3/2}$ ішкі қабықшаларындағы бос орындар ыдыраған жағдайда, бастапқы ішкі қуысты жасау кезінде атом қабылдаған энергияның көп бөлігі каскадтың Оже және Костер–Крониговски электрондары арқылы қайта бөлінеді. *1s*-бос орны ыдыраған кезде энергияның көп бөлігі каскадты фотондармен, негізінен *K, L* арқылы тасымалданады. Қатерлі ісіктің фотонды активтендіру терапиясында радиосенсибилизатор ретінде платина негізіндегі препараттарды қолдану перспективалары талқыланды.

Кілт сөздер: платина, жұмыс каскады, ыдырау ағашы, ион өнімділігі, каскадтан энергияны қайта шығару, радиосенсибилизация, Оже терапиясы, фотонды белсендіру терапиясы.

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Образование конечных ионов и переизлучение энергии при каскадном распаде одиночных вакансий в *K* и *L* электронных оболочках атома платины

Методом построения и анализа деревьев каскадного распада проведено моделирование каскадных распадов одиночных вакансий в 1s, 2s, $2p_{1/2}$ и $2p_{3/2}$ подоболочках изолированного атома платины. Рассчитаны выходы конечных ионов и спектры каскадных электронов и фотонов. Средние заряды конечных ионов, образующихся в результате каскадных распадов 1s, 2s, $2p_{1/2}$ и $2p_{3/2}$ вакансий в атоме Pt, равны 7,75; 9,82; 7,80 и 7,95 соответственно. Для распадов каждой исходной внутренней вакансии рассчитаны энергии, запасенные в конечных каскадных ионах, и энергии, переизлученные с каскадными электронами и фотонами. В случае распада вакансий в подоболочках 2s, $2p_{1/2}$ и $2p_{3/2}$ большая часть энергии, первоначально полученной атомом при создании начальной внутренней вакансии, переизлучается каскадными Оже и Костер-Крониговскими электронами. При распаде *1s*-вакансии большая часть энергии уносится каскадными фотонами, преимущественно *K, L*. Обсуждены перспективы использования препаратов на основе платины в качестве радиосенсибилизаторов в фотонно-активационной терапии рака.

Ключевые слова: платина, каскад вакансий, дерево распада, выходы ионов, каскадное переизлучение энергии, радиосенсибилизация, Оже терапия, фотонно-активационная терапия.

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