Electronic Supplementary Material (ESI) for Nanoscale.

Modelling energy deposition in nanoscintillators to predict the efficiency of the X-ray-induced photodynamic effect

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1 Supplementary Informations

1.1 SI1: Optimization of the tumour's model geometry

The scheme of our tumour's model geometry is presented figure 1. We divided the tumour volume into two zones. There is a near zone having a radius of 1 μm, which contains a random distribution of NPs. To take into account the NPs at distance larger than 1 μm from the primary absorber, we introduced in the model as spherically symmetric shells of Gd_2O_3 with a thicknesses corresponding to the NP diameter and an appropriate spacing in agreement with the NP concentration. d is the distance between the 1 μm water sphere which contains all the NPs, and the first Gd_2O_3 layer. To limit the influence of the distance d on the energy deposited value, we performed several calculations varying this distance d from 0 to h. The results obtained for 100 nm diameter NPs and 100 nm thick shells are presented in the figure 1 for an occupation ratio equal to 7.10^{-3}. The observed bump or dip depending on the d value around 10 keV is due to edge effects and have no physical meaning. The value limiting the amplitude of this oscillation around 10 keV - when electrons start depositing energy in the Gd_2O_3 layers - is $d = h/2$. To optimize the geometry we chose a distance $h/2$ and we shifted the center of the shells of $h/2$ in one random direction to average the influence of d. Note that the edge effect has a limited impact on the total energy deposition since it slightly deviates from the real behavior only in a weak energy range.

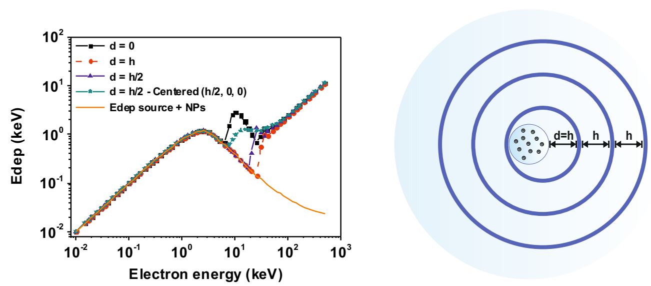

Fig. 1 Left: Energy deposited (in keV) in Gd_2O_3 (NPs + shells) for 100 nm diameter NP, with a ratio $C = 7.10^{-3}$. The distance d corresponds to the distance between V_{inner} and the inner bound of the first shell of Gd_2O_3 . The orange curve represents the deposited energy in all the NPs of Gd_2O_3 to clearly distinguish the effect of layers. Right: a scheme of the used geometry

1.2 SI2: Intermediate results: Contribution of secondary electrons and photons

The energy deposition in the matter is due to the secondary electrons and photons interactions. In the main contribution, we present the energy deposition in Gd_2O_3 without any information on the contribution of the different parts of the model, which is the useful results for the PDT application, nevertheless the reader might be interested to have the information on these respective contributions in order to estimate the tendency in the case of larger tumour volumes, other NP diameters or concentrations.

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Table 1 Energy deposited (in keV) by primary electrons in Gd_2O_3 and in water when the interaction with the primary γ-ray occurs in a Gd_2O_3 NP or in water. The NP diameter is equal to 10 nm and the ratio $C = 7 \cdot 10^{-3}$.

	NP source: Gd_2O_3			NP source: water		
	Gd_2O_3	Water	Out	Gd_2O_3	Water	Out
100 keV	1.25	59.50	0.01	0.26	14.97	0
200 keV	2.87	134.58	0.09	0.79	42.79	0.01
300 keV	3.96	183.08	0.19	1.56	79.41	0.04
400 keV	4.76	218.12	0.29	2.49	121.35	0.09
500 keV	5.58	253.99	0.41	3.53	167.03	0.18

Table 2 Energy deposited (in keV) by primary photons in Gd_2O_3 and in water when the primary interaction with the γ-ray occurs in a Gd_2O_3 NP or in water. The NP diameter is equal to 10 nm and the ratio $C = 7 \cdot 10^{-3}$.

	NP source: Gd_2O_3			NP source: water		
	Gd_2O_3	Water	Out	Gd_2O_3	Water	Out
100 keV	0.31	3.37	33.84	0.19	3.20	81.34
200 keV	0.26	3.21	57.56	0.07	2.45	153.84
300 keV	0.21	3.10	108.37	0.06	2.57	216.30
400 keV	0.17	3.11	172.75	0.06	2.98	272.97
500 keV	0.14	3.24	236.03	0.07	3.42	325.73

Table 3 Energy deposited (in keV) by primary electrons in Gd_2O_3 and in water depending on the material of the source NP. The NP diameter is equal to 100 nm and the ratio $C = 7 \cdot 10^{-3}$.

	NP source: Gd_2O_3			NP source: water		
	Gd_2O_3	Water	Out	Gd_2O_3	Water	Out
100 keV	2.76	57.99	0.01	0.73	14.50	0
200 keV	4.17	133.27	0.09	1.31	42.26	0.01
300 keV	5.08	181.95	0.19	2.09	78.89	0.04
400 keV	5.71	217.16	0.31	3.02	120.82	0.09
500 keV	6.41	253.14	0.43	4.06	166.49	0.18

Table 4 Energy deposited (in keV) by primary photons in Gd_2O_3 and in water depending on the material of the source NP. The NP diameter is equal to 100 nm and the ratio $C = 7 \cdot 10^{-3}$.

	NP source: Gd_2O_3			NP source: water		
	Gd_2O_3	Water	Out	Gd_2O_3	Water	Out
100 keV	0.63	3.23	33.65	0.32	2.98	81.42
200 keV	0.54	3.11	57.38	0.12	2.58	153.63
300 keV	0.42	3.06	108.20	0.09	2.73	216.00
400 keV	0.33	3.21	172.49	0.09	3.08	272.58
500 keV	0.26	3.37	235.79	0.09	3.32	325.32

Table 5 Values of the η_{nano} parameter (in %) for Gd_2O_3 NPs of 10 and 100 nm diameter distributed in the tumour volume with an occupation ratio equal to $2 \cdot 10^{-3}$ and $7 \cdot 10^{-3}$.

	$C = 2 \cdot 10^{-3}$		$C = 7 \cdot 10^{-3}$	
E_γ (keV)	10 nm	100 nm	10 nm	100 nm
100 keV	0.23	0.91	0.95	2.12
200 keV	0.15	0.40	0.61	0.97
300 keV	0.17	0.31	0.61	0.82
400 keV	0.20	0.28	0.67	0.82
500 keV	0.22	0.28	0.74	0.86

1.3 SI3: Estimation of the η_{nano} coefficient

η_{nano} is defined as the fraction of energy deposited in the nanoscintillators after the interaction of a high energy photon with the tumoural volume. In the case of Gd_2O_3 NPs of 10 and 100 nm diameter, we deduced this ratios by dividing the total energy deposited in nanoscintillators (table 3 of the paper) by the energy of the interacting γ-photon. These results are also presented in the table 5 for the two considered occupation ratios as well as for two used diameters (10 and 100 nm), in order to evaluate the effect of the concentration and NP size.

2 Aknowledgement

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