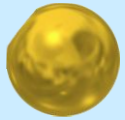
The WG6/WG7 gold nanoparticle exercise

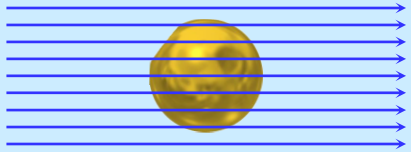
Hans Rabus

Nanoparticle exercise: simulation setup



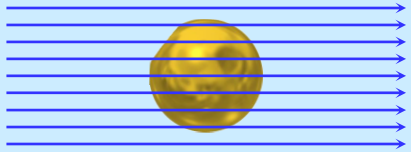
- a single gold nanoparticle in water

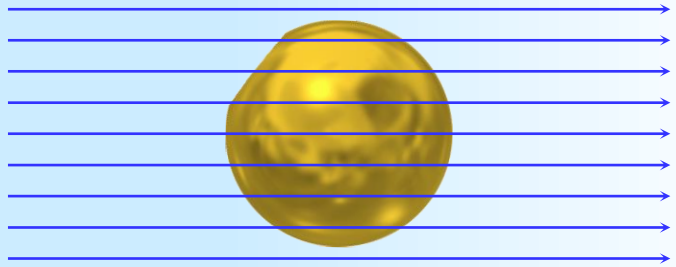
Nanoparticle exercise: simulation setup



- a single gold nanoparticle in water
- irradiated by a narrow photon beam

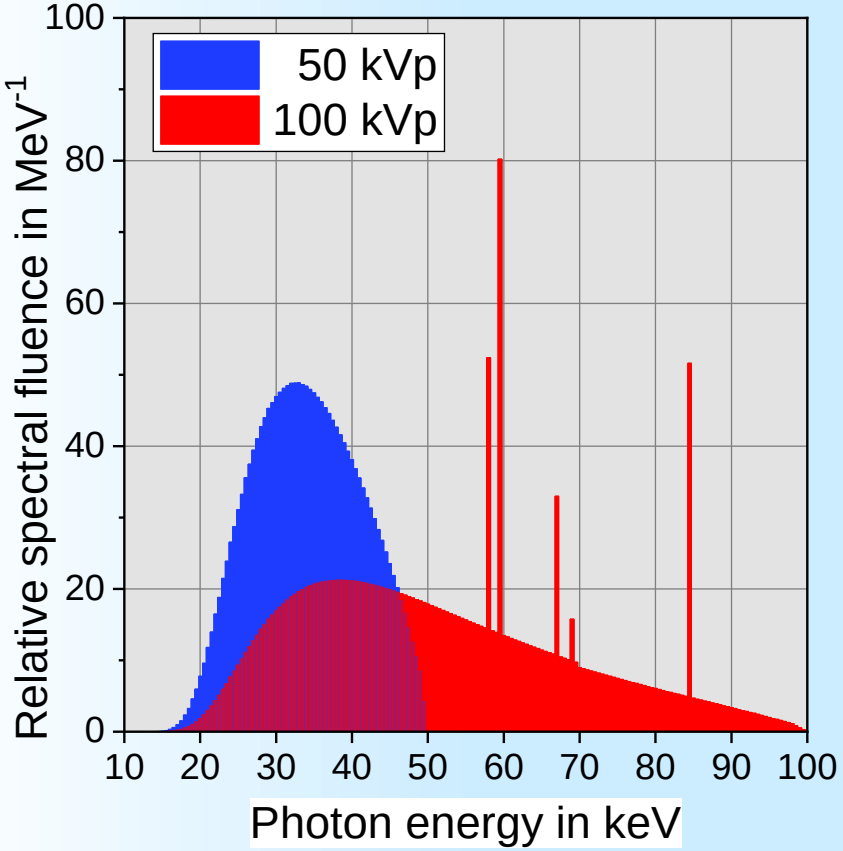
Nanoparticle exercise: simulation setup

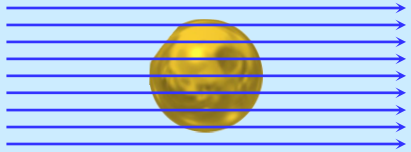


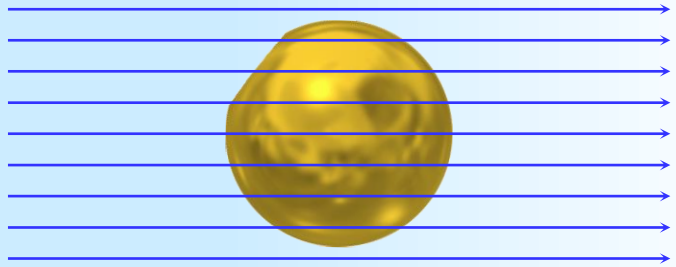


- a single gold nanoparticle in water
- irradiated by a narrow photon beam
- two different sizes (50 nm, 100 nm)

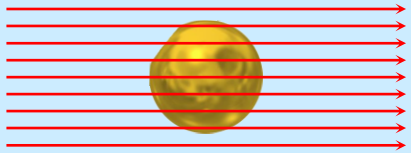
Nanoparticle exercise: simulation setup

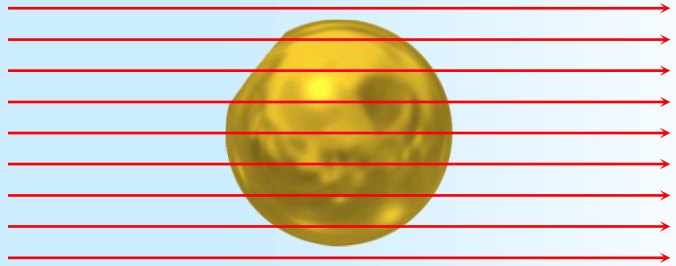




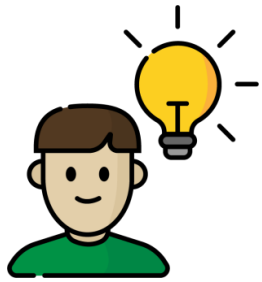


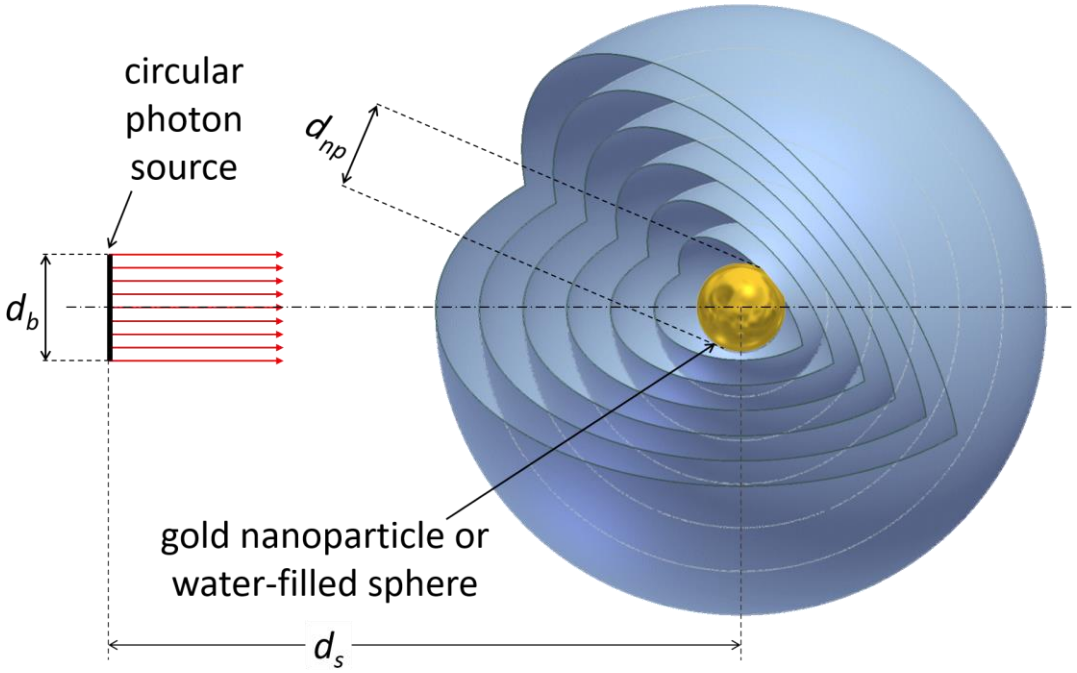
- a single gold nanoparticle in water
- irradiated by a narrow photon beam
- two different sizes (50 nm, 100 nm)
- two different photon spectra





Nanoparticle exercise: simulation tasks





Rabus et al., Phys Medica 84 (2021) 241-253

Task 1:

- Determine energy imparted in (thin) spherical shells around the nanoparticle

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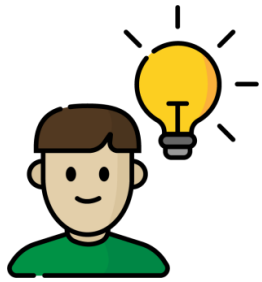
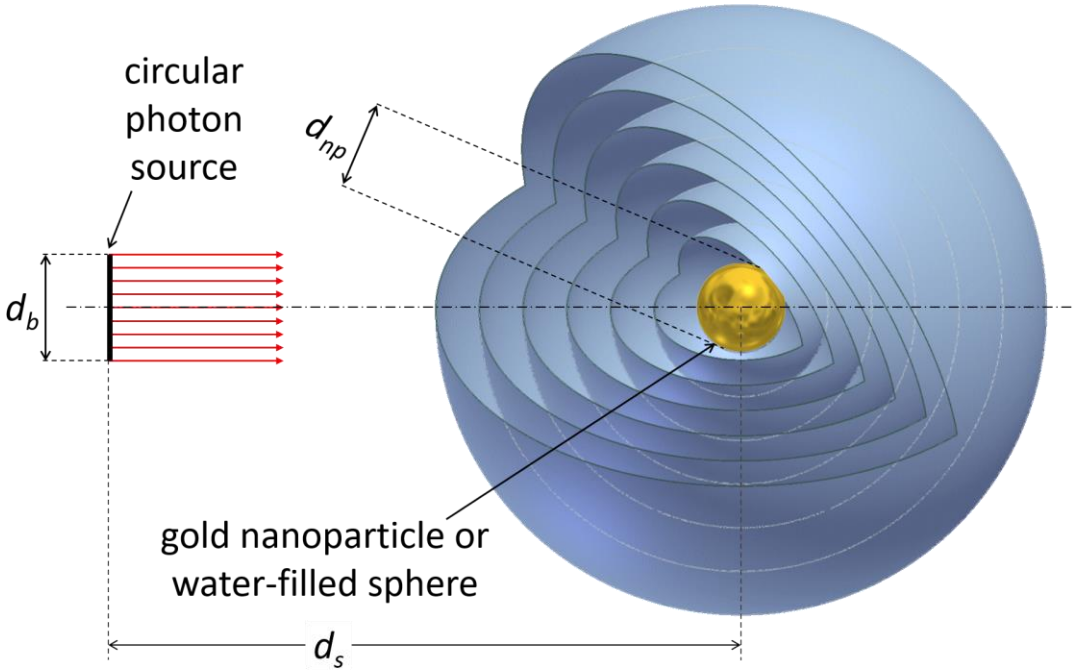
Nanoparticle exercise: simulation tasks





Rabus et al., Phys Medica 84 (2021) 241-253

Task 1:

- Determine energy imparted in (thin) spherical shells around the nanoparticle

Task 2:

- Determine the energy spectrum of electrons in (thick) spherical shells around the nanoparticle

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“Electron energy spectrum in a volume”

What would you score?

a. The energy distribution of electrons entering the volume.

b. The balance of electrons crossing the volume’s surface.

c. The step length distribution of electrons inside the volume.

d. Something different from the preceding three options.

e. Nothing / don’t know.

Poll

“Electron energy spectrum in a volume”

Q: “What shall I score?”

A: “Electrons leaving the nanoparticle”

“Electron energy spectrum in a volume”

Q: “What shall I score?”

A: “Electrons leaving the nanoparticle”

Well …

- … only electrons produced in the nanoparticle?
- … what about electrons going out twice after backscattering?
- … is there a unique tally in my code for this?

Electron spectra – data of two participants

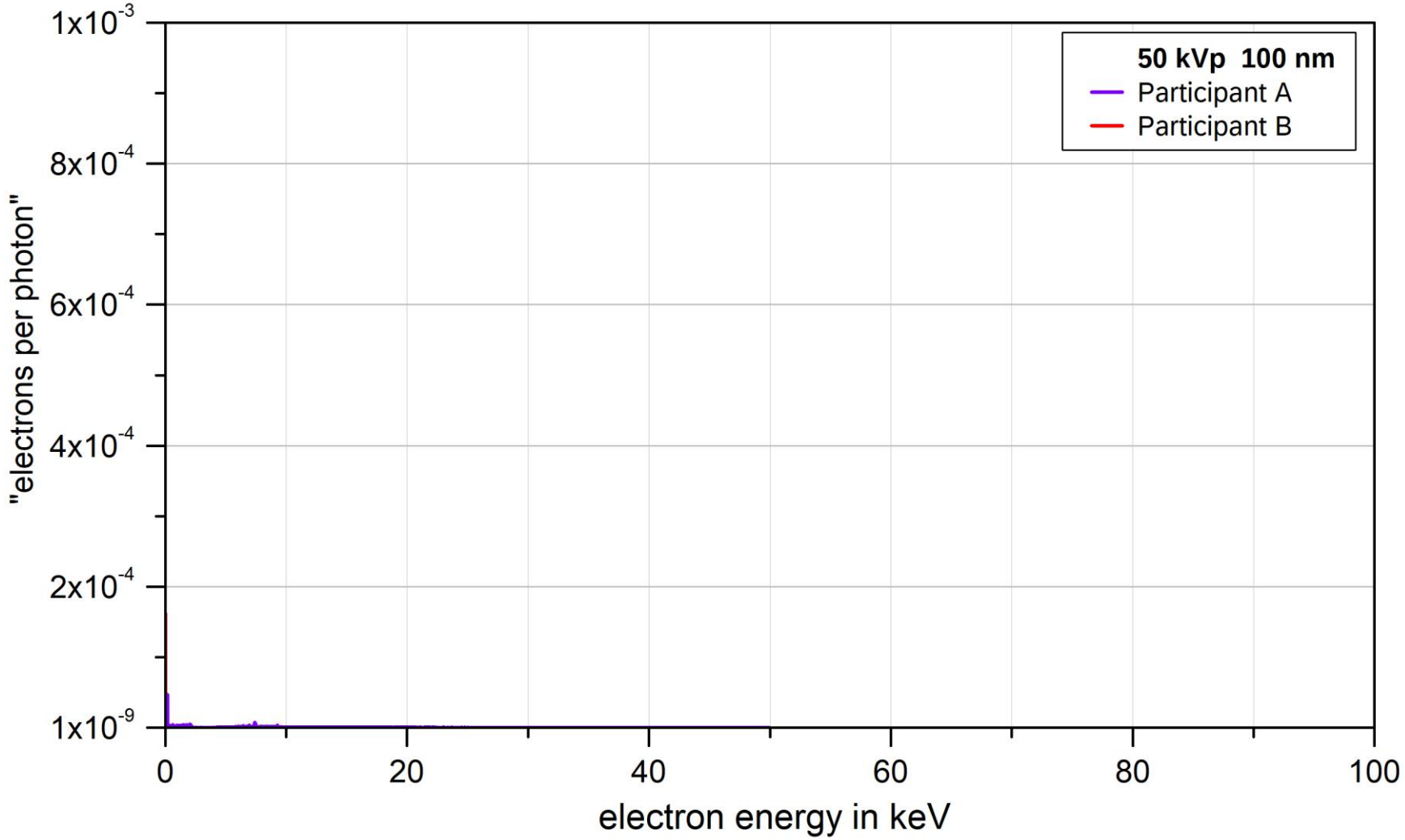
Data from Participant A

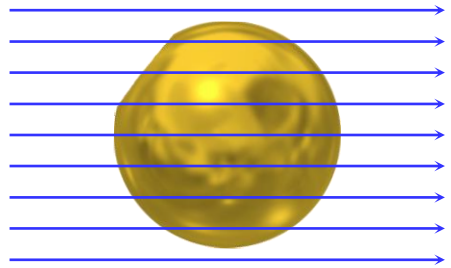
50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06
187.5	4.27E-06	187.5	5.82E-06
192.5	4.01E-06	192.5	5.73E-06

Data from participant B

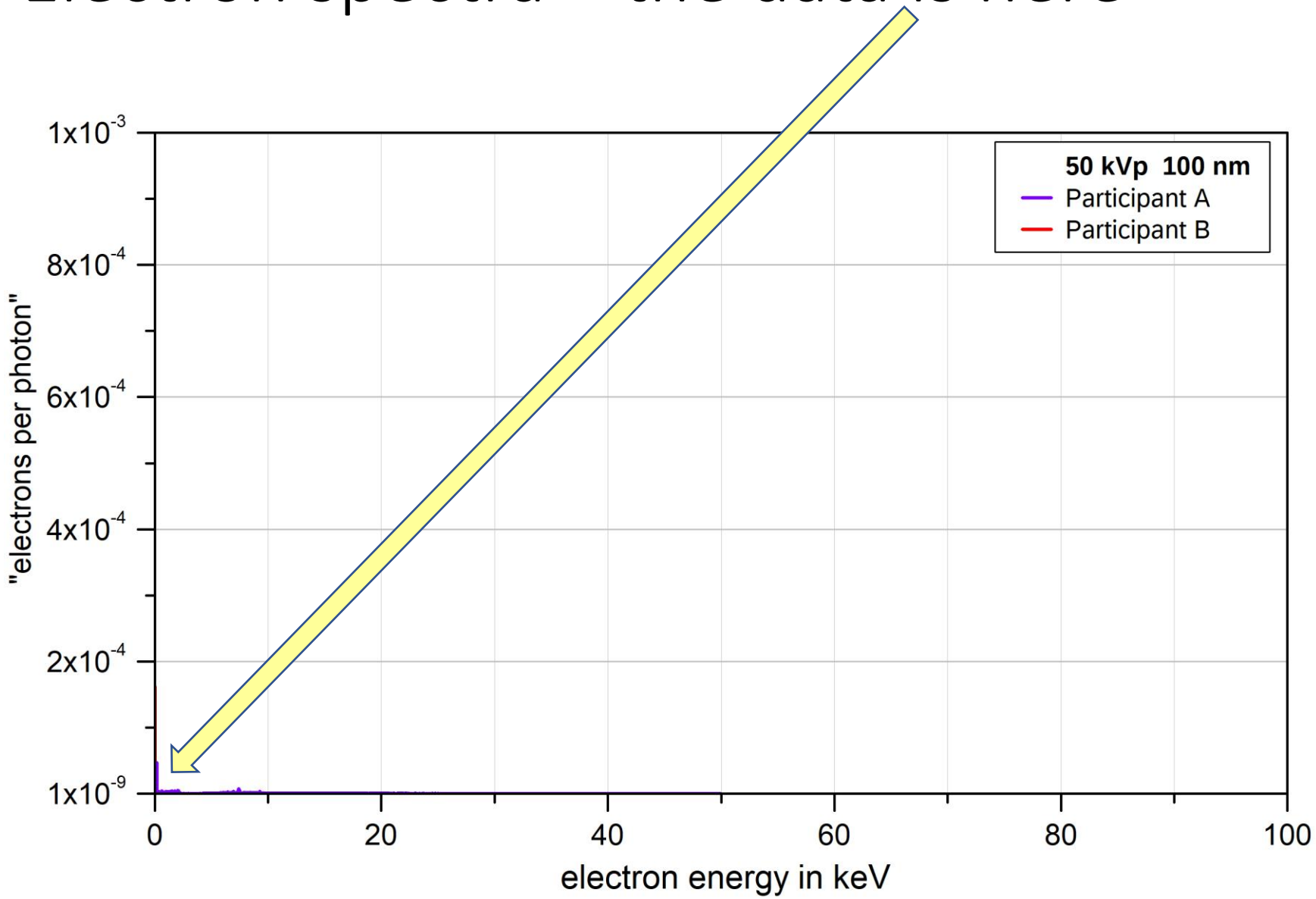
50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07
375	3.44E-07	375	5.16E-07
385	3.24E-07	385	5.94E-07

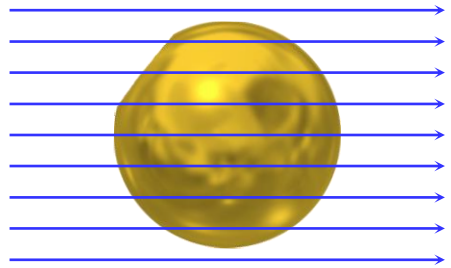
Electron spectra – where is the data?





Electron spectra – the data is here





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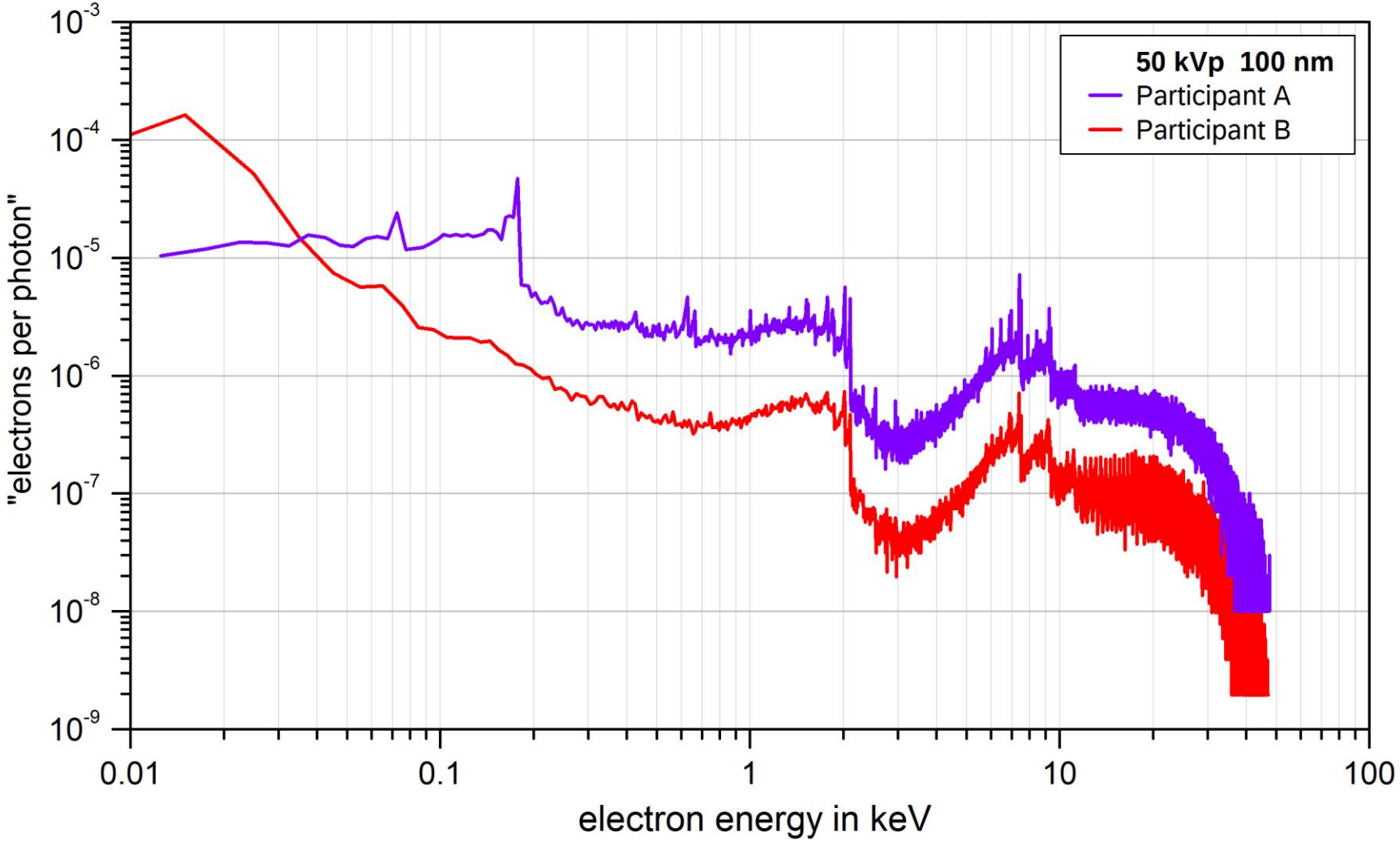
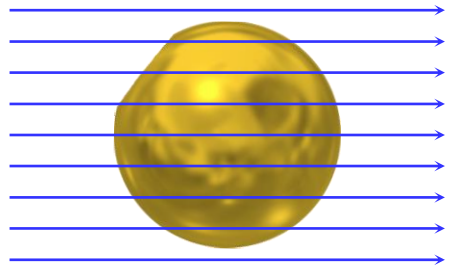
Electron spectra - from different participants

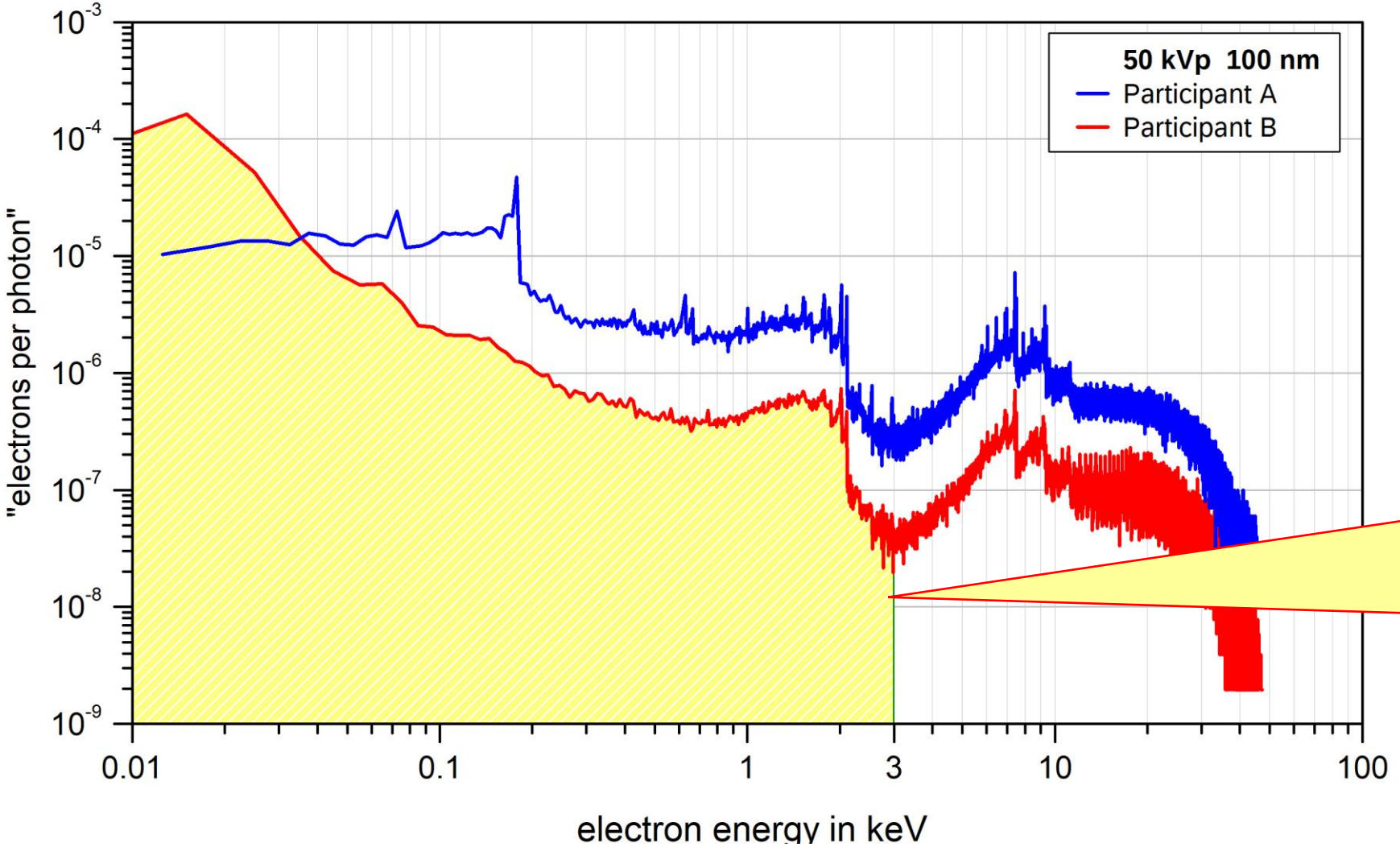


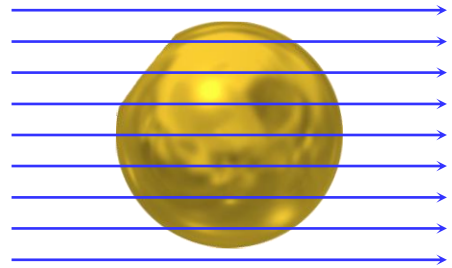


EURADOS

Electron spectra

Poll



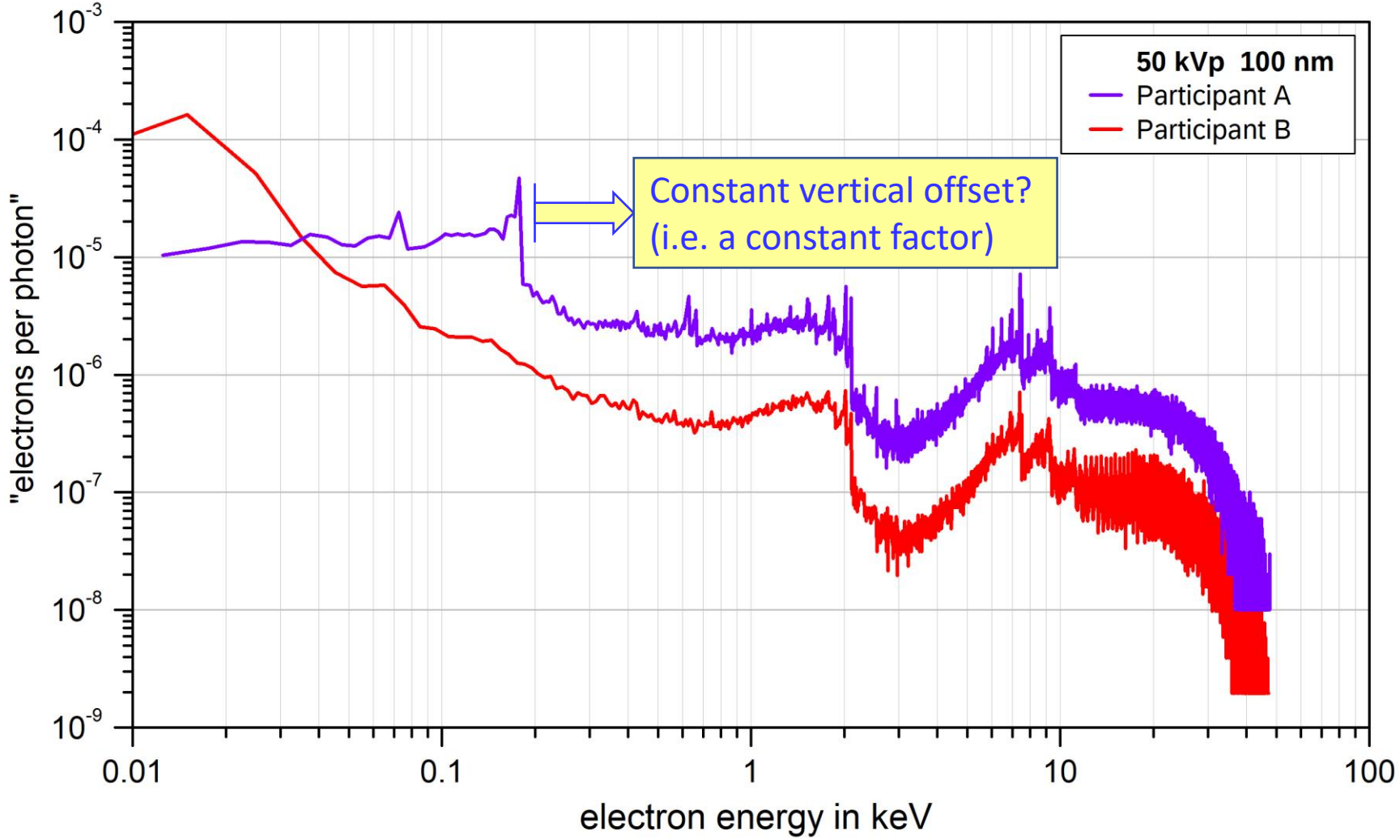


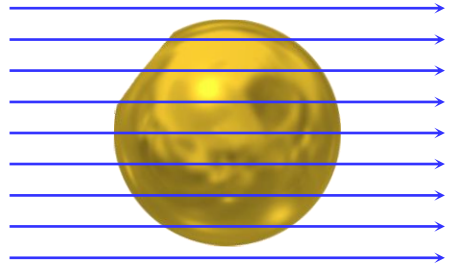
What is the proportion of electrons with energies < 3 keV?

a. **30 %**
b. **60 %**
c. **80 %**
d. **90 %**
e. **95 %**

EURADOS

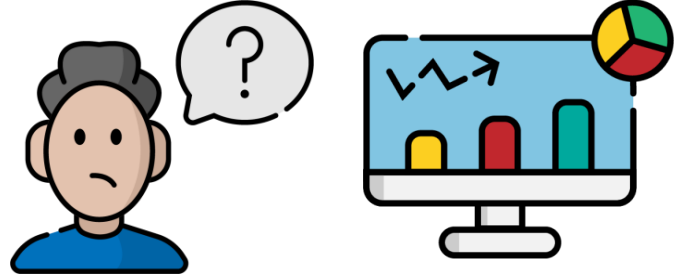
Electron spectra - from different participants





EURADOS

Electron spectrum – what is it?



Data from Participant A

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06

Data from participant B

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
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115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
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165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
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255	4.20E-07	255	7.30E-07
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295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

Meaning of the first column

- Linear or logarithmic bin size?
- Mean energy in the bin?
- Energy in the center of the bin?
- Start of the bin?
- End of the bin?

EURADOS

Electron spectrum – what is it?

Data from Participant A

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Data from participant B

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25	3.14E-05	25	5.15E-05
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45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

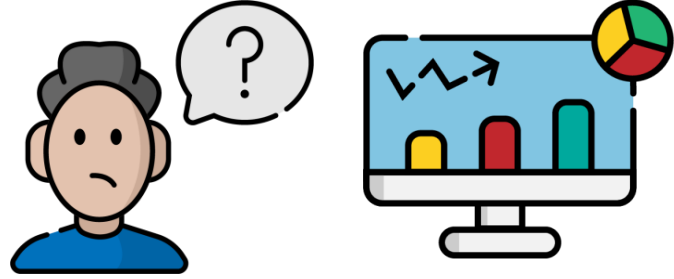
Meaning of the first column

- Linear or logarithmic bin size?
- Mean energy in the bin?
- Energy in the center of the bin?
- Start of the bin?
- End of the bin?

Different codes use different conventions!

EURADOS

Electron spectrum – what is it?



Data from Participant A

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06

Data from participant B

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.32E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	1.61E-07
235	5.08E-07	235	7.65E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

Meaning of the first column

- Linear or logarithmic bin size?
- Mean energy in the bin?
- Energy in the center of the bin?
- Start of the bin?
- End of the bin?

Different codes use different conventions!

- Both participants gave the mean energy
- Participant A used a bin size of 5 eV
- Participant B used a bin size of 10 eV

EURADOS

Electron spectrum – what is it?

Data from Participant A

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06

Data from participant B

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

Meaning of the second column

- Absolute frequency (“counts”) in bin?
- Frequency per primary particle?
- Relative frequency?
- Frequency density per primary particle?

EURADOS

Electron spectrum – what is it?

Data from Participant A

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06

Data from participant B

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

Meaning of the second column

- Absolute frequency (“counts”) in bin?
- Frequency per primary particle?
- Relative frequency?
- Frequency density per primary particle?

Stipulated tallies of codes, mostly give the frequency density per primary particle

EURADOS

Electron spectrum – what is it?

Data from Participant A

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06

Data from participant B

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

Meaning of the second column

- Absolute frequency (“counts”) in bin?
- Frequency per primary particle?
- Relative frequency?
- Frequency density per primary particle?

Stipulated tallies of codes, mostly give the frequency density per primary particle

If you code the tallying yourself, make sure to understand and report how you did it.

EURADOS

Electron spectrum – what is it?

Data from Participant A

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
2.5	0	2.5	0
7.5	0	7.5	0
12.5	8.53E-06	12.5	1.03E-05
17.5	9.15E-06	17.5	1.18E-05
22.5	1.02E-05	22.5	1.35E-05
27.5	9.98E-06	27.5	1.34E-05
32.5	1.01E-05	32.5	1.26E-05
37.5	1.27E-05	37.5	1.56E-05
42.5	1.08E-05	42.5	1.48E-05
47.5	8.83E-06	47.5	1.27E-05
52.5	9.07E-06	52.5	1.24E-05
57.5	1.06E-05	57.5	1.45E-05
62.5	1.03E-05	62.5	1.51E-05
67.5	9.99E-06	67.5	1.45E-05
72.5	1.82E-05	72.5	2.41E-05
77.5	7.91E-06	77.5	1.17E-05
82.5	7.29E-06	82.5	1.20E-05
87.5	8.12E-06	87.5	1.23E-05
92.5	8.71E-06	92.5	1.30E-05
97.5	8.43E-06	97.5	1.41E-05
102.5	9.42E-06	102.5	1.57E-05
107.5	9.49E-06	107.5	1.53E-05
112.5	9.55E-06	112.5	1.57E-05
117.5	9.41E-06	117.5	1.53E-05
122.5	9.86E-06	122.5	1.58E-05
127.5	9.59E-06	127.5	1.52E-05
132.5	1.01E-05	132.5	1.55E-05
137.5	9.93E-06	137.5	1.60E-05
142.5	1.11E-05	142.5	1.73E-05
147.5	1.05E-05	147.5	1.72E-05
152.5	9.72E-06	152.5	1.64E-05
157.5	8.66E-06	157.5	1.43E-05
162.5	1.25E-05	162.5	2.19E-05
167.5	1.27E-05	167.5	2.26E-05
172.5	1.22E-05	172.5	2.19E-05
177.5	2.60E-05	177.5	4.73E-05
182.5	3.84E-06	182.5	5.90E-06

Data from participant B

50 kVp, 50 nm		50 kVp, 100 nm	
E (eV)	f(E)	E (eV)	f(E)
5	3.64E-05	5	5.77E-05
15	9.67E-05	15	1.63E-04
25	3.14E-05	25	5.15E-05
35	9.04E-06	35	1.49E-05
45	4.66E-06	45	7.43E-06
55	3.47E-06	55	5.67E-06
65	3.82E-06	65	5.77E-06
75	2.69E-06	75	4.01E-06
85	1.64E-06	85	2.54E-06
95	1.47E-06	95	2.46E-06
105	1.42E-06	105	2.11E-06
115	1.33E-06	115	2.09E-06
125	1.19E-06	125	2.09E-06
135	1.28E-06	135	1.93E-06
145	1.22E-06	145	1.97E-06
155	1.05E-06	155	1.64E-06
165	9.34E-07	165	1.48E-06
175	8.44E-07	175	1.26E-06
185	7.93E-07	185	1.23E-06
195	6.86E-07	195	1.15E-06
205	6.05E-07	205	1.01E-06
215	5.25E-07	215	9.47E-07
225	6.02E-07	225	9.61E-07
235	5.08E-07	235	7.66E-07
245	5.25E-07	245	7.85E-07
255	4.20E-07	255	7.30E-07
265	4.36E-07	265	6.19E-07
275	3.77E-07	275	7.07E-07
285	3.69E-07	285	6.70E-07
295	3.57E-07	295	6.64E-07
305	3.83E-07	305	5.68E-07
315	4.45E-07	315	5.94E-07
325	3.07E-07	325	6.62E-07
335	3.57E-07	335	6.60E-07
345	3.16E-07	345	5.80E-07
355	3.73E-07	355	5.43E-07
365	3.71E-07	365	5.78E-07

Meaning of the second column

- Absolute frequency (“counts”) in bin?
- Frequency per primary particle?
- Relative frequency?
- Frequency density per primary particle?

Stipulated tallies of codes, mostly give the frequency density per primary particle

If you code the tallying yourself, make sure to understand and report how you did it.

It is relevant for comparisons and, e.g., for rebinning and calculating integral values.

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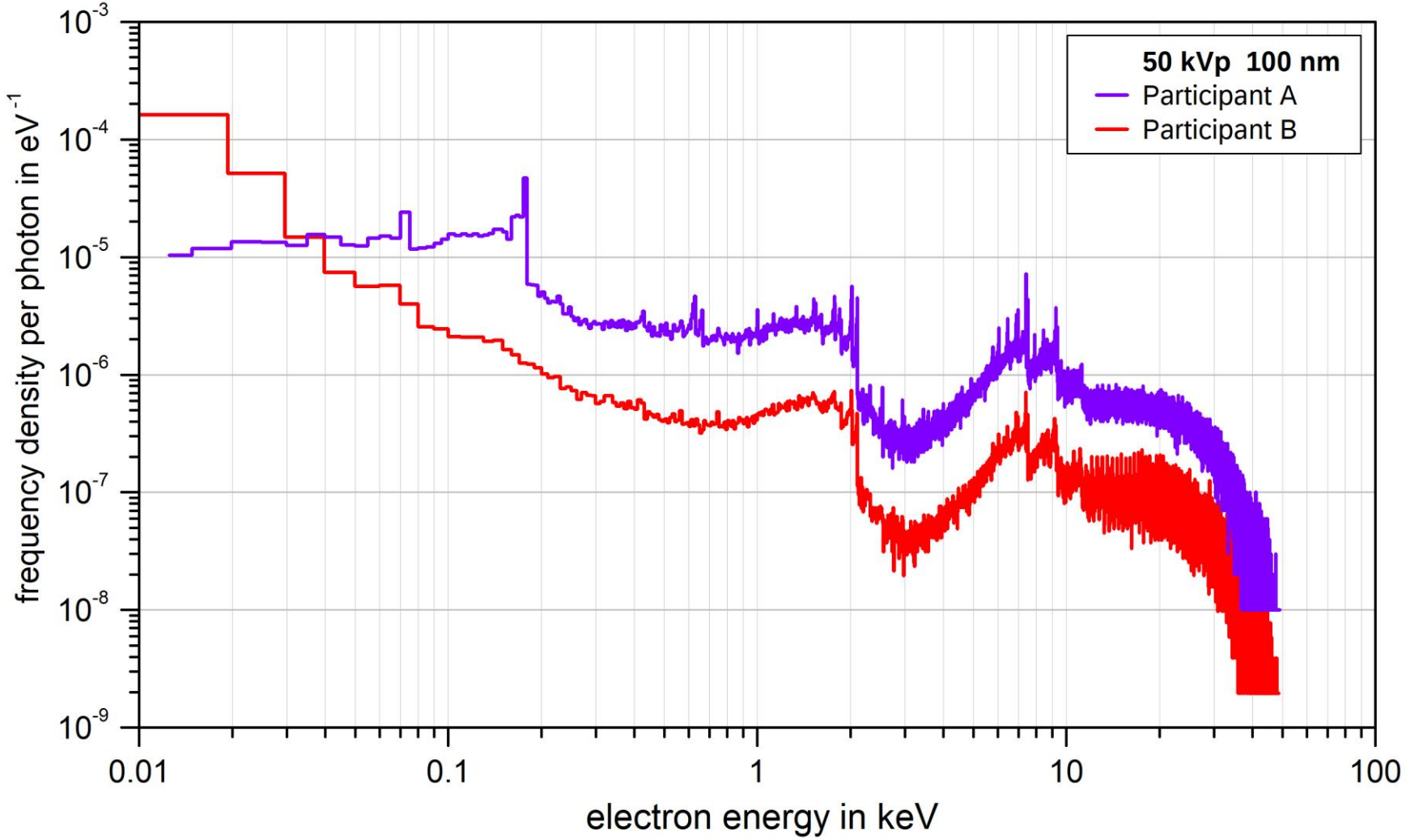
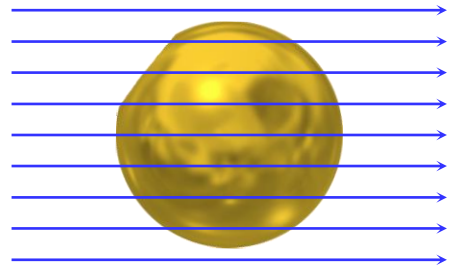
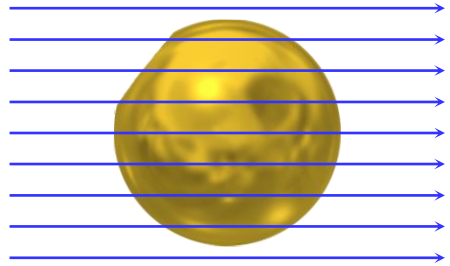
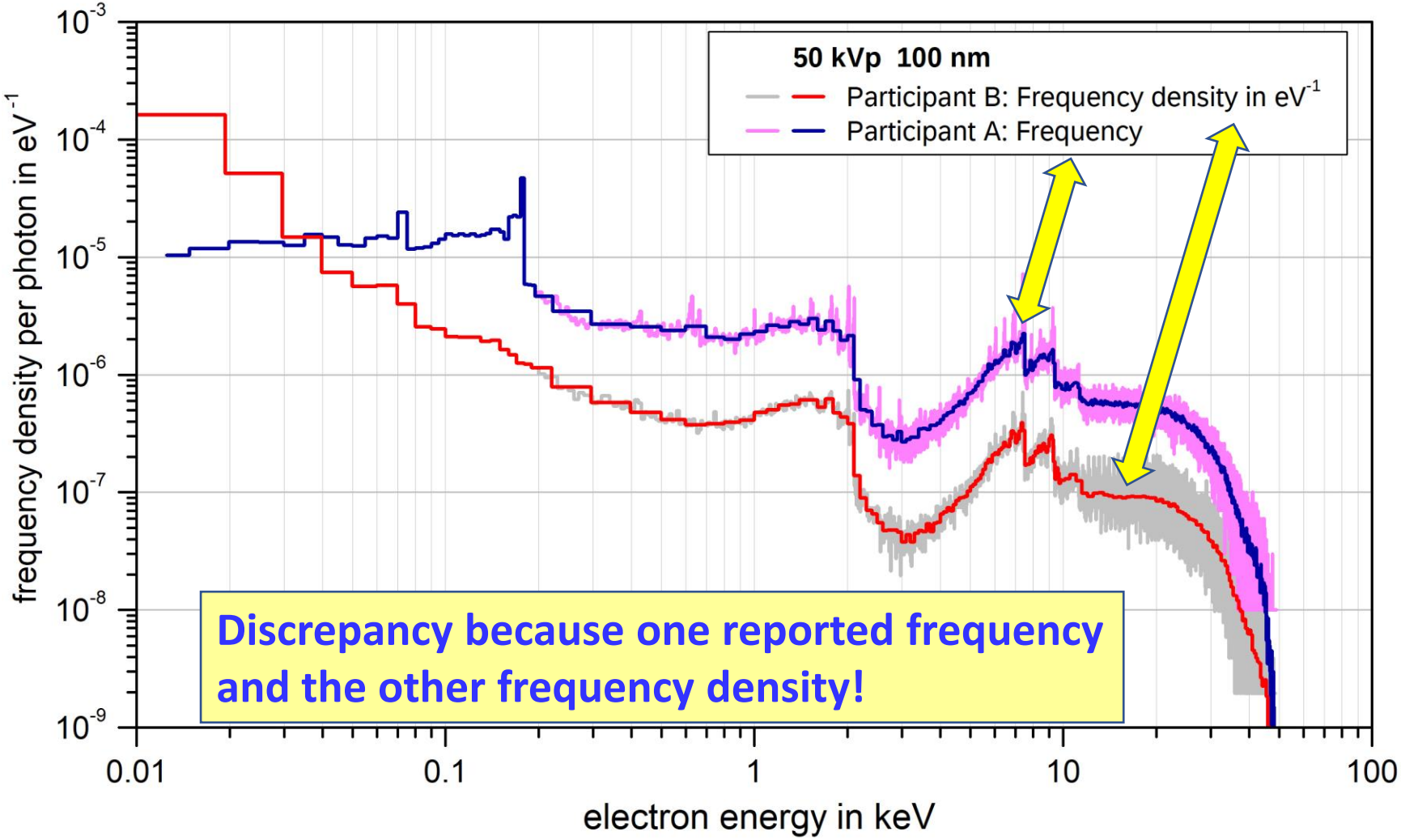
Electron spectra - from different participants



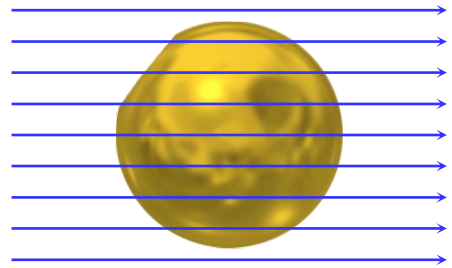


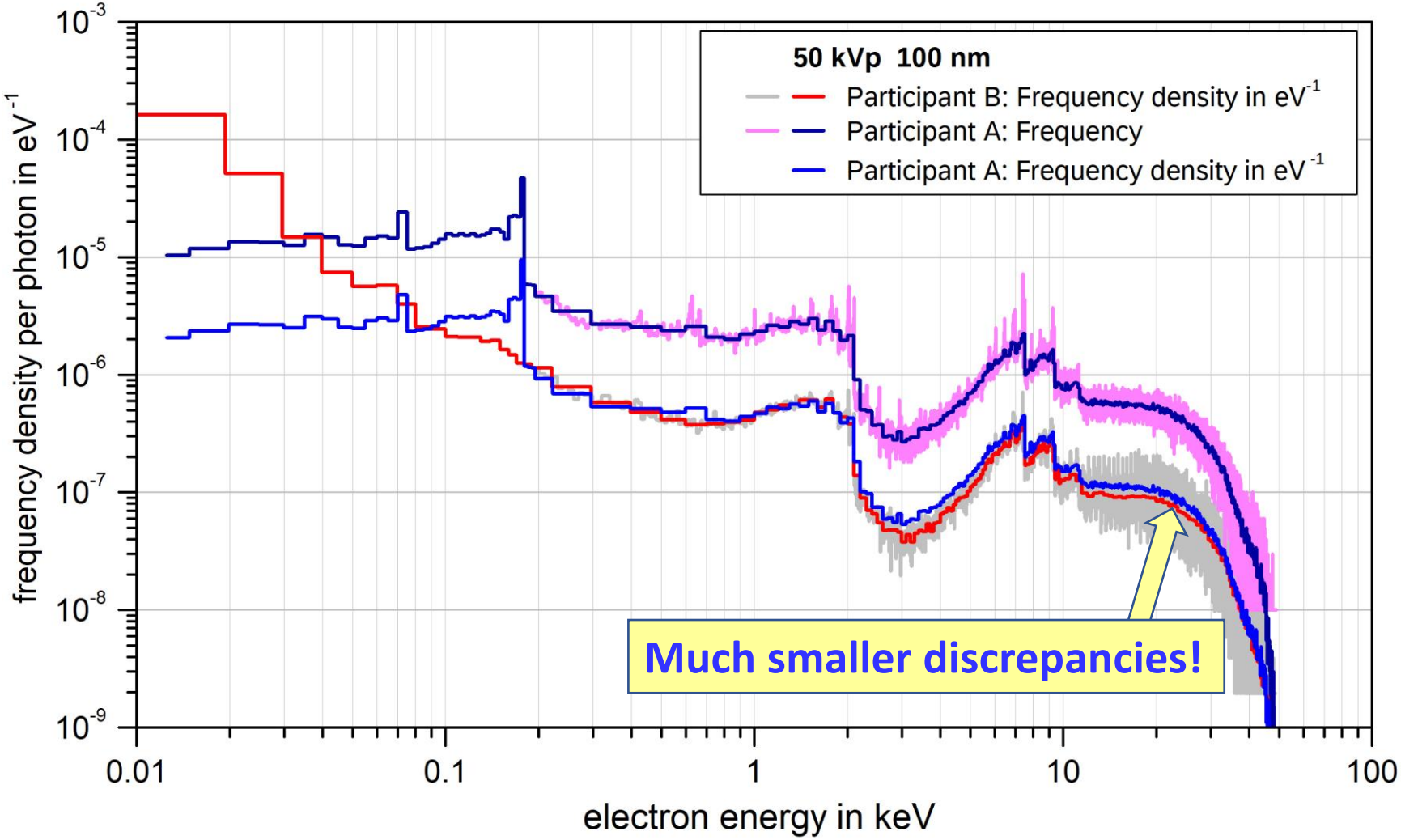
Electron spectra - from different participants



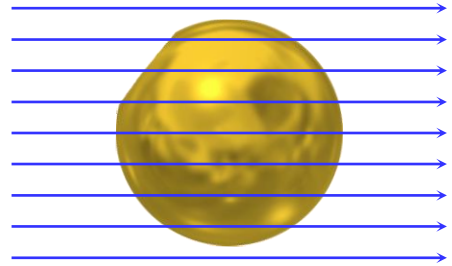


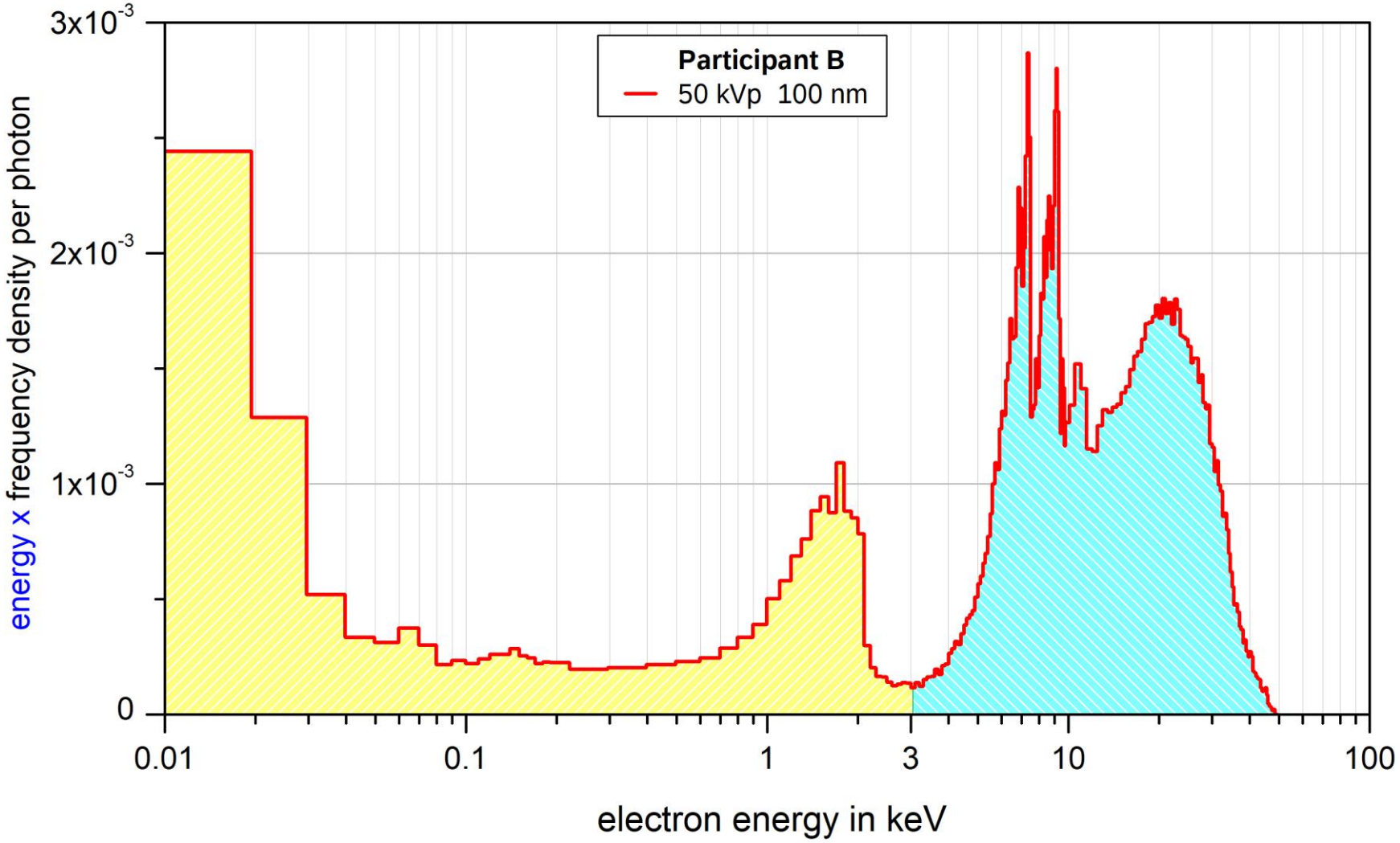
Electron spectra - from different participants



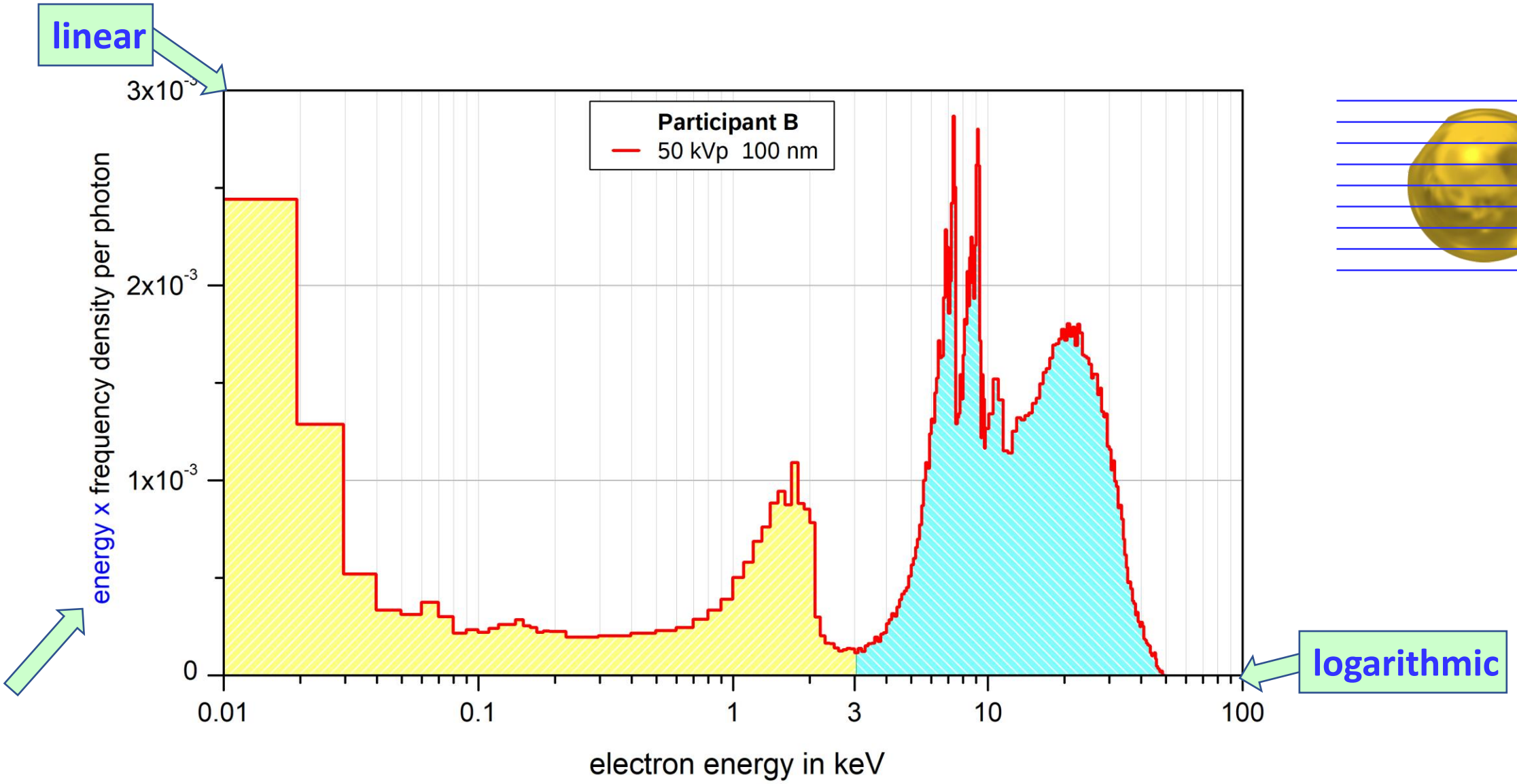


Electron spectra – microdosimetry style

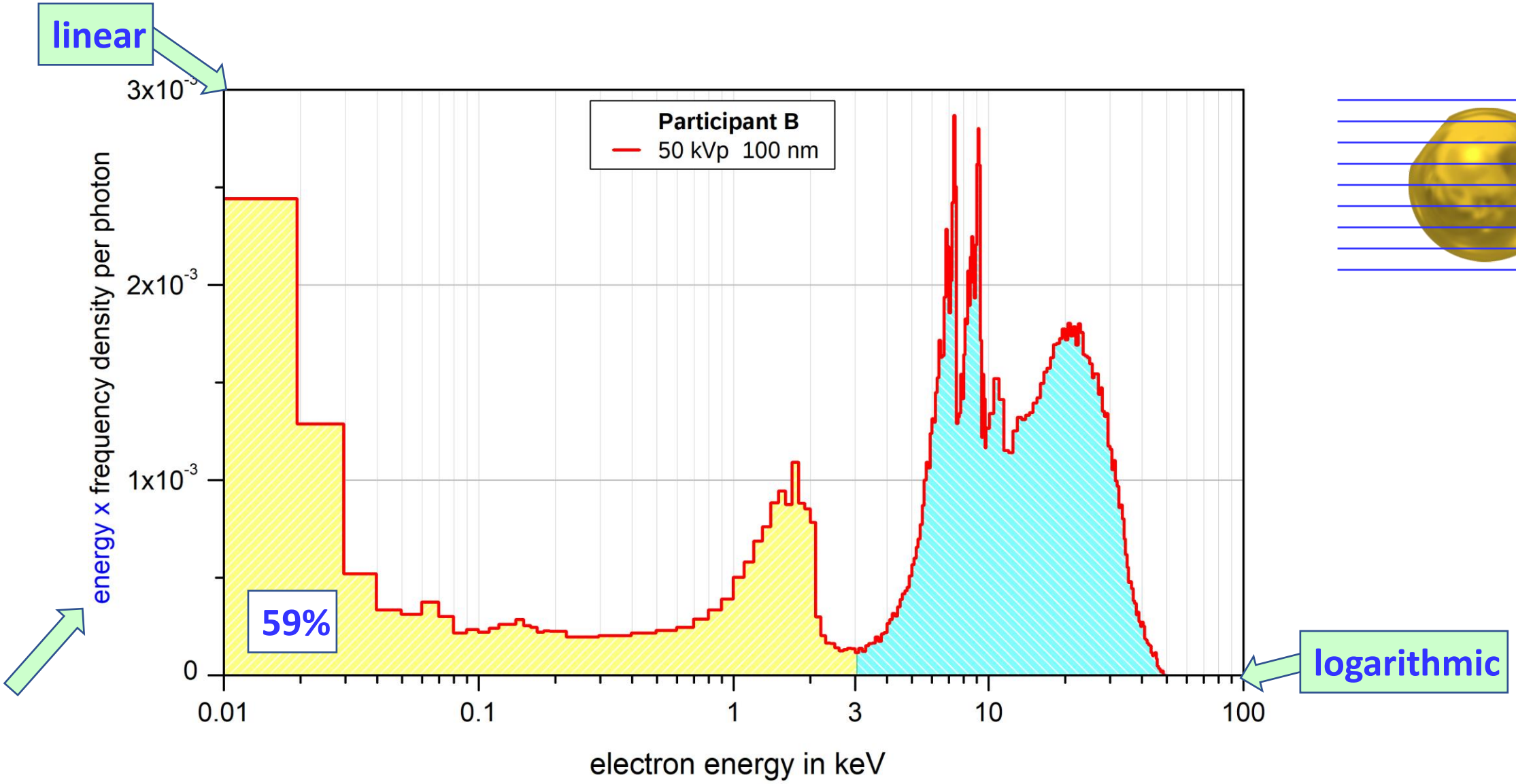




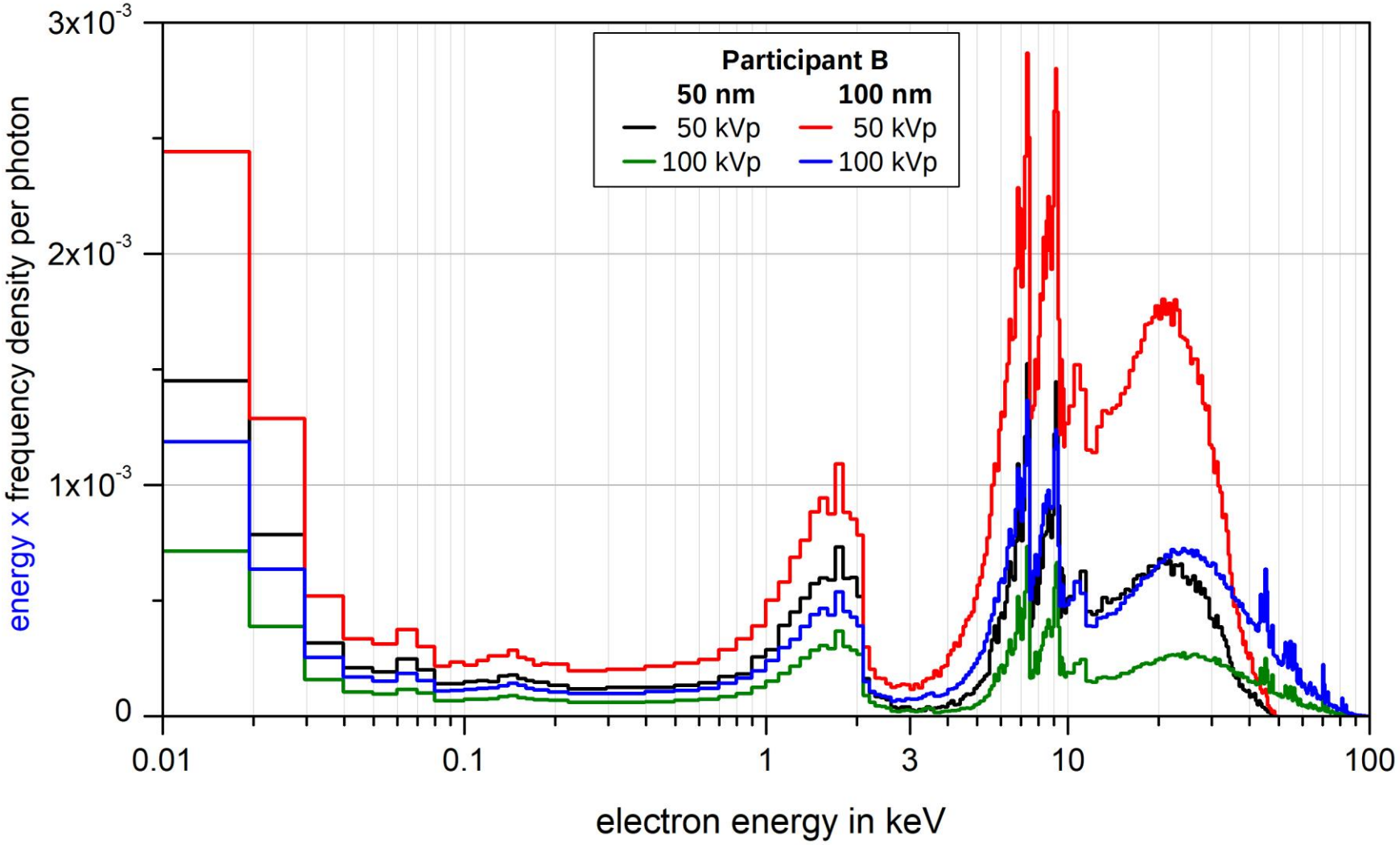
Electron spectra – microdosimetry style

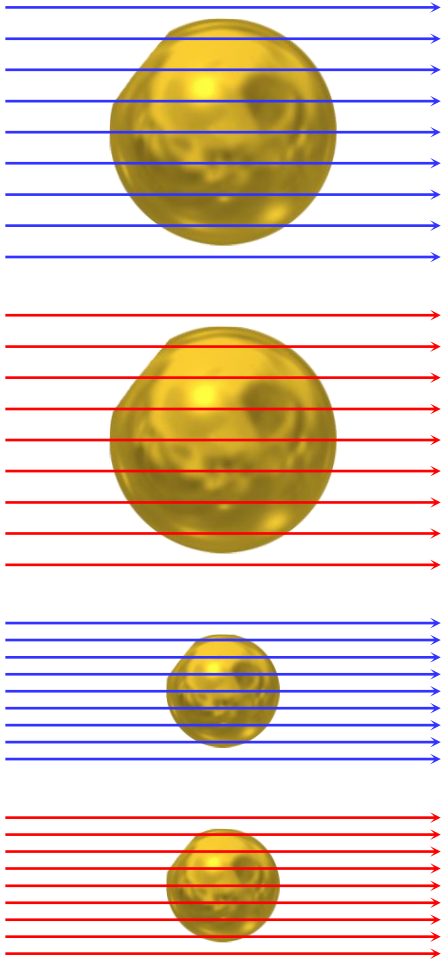


Electron spectra – microdosimetry style



How to know: is this plausible or meaningful?





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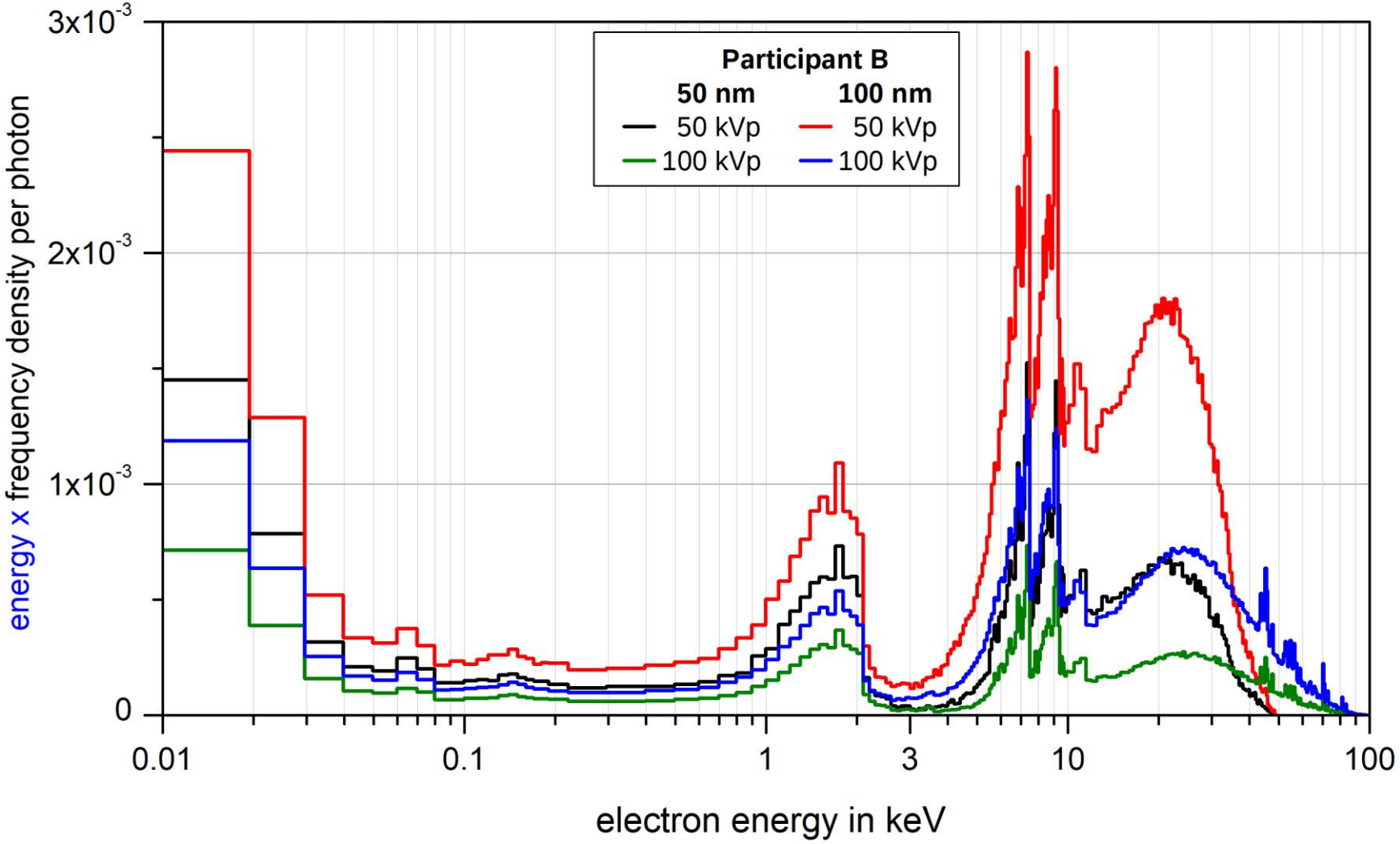

Integral: Number of electrons per photon

	50 nm	100 nm
50 kVp	**5.2×10^{-3}**	**8.8×10^{-3}**
100 kVp	**2.5×10^{-3}**	**4.3×10^{-3}**

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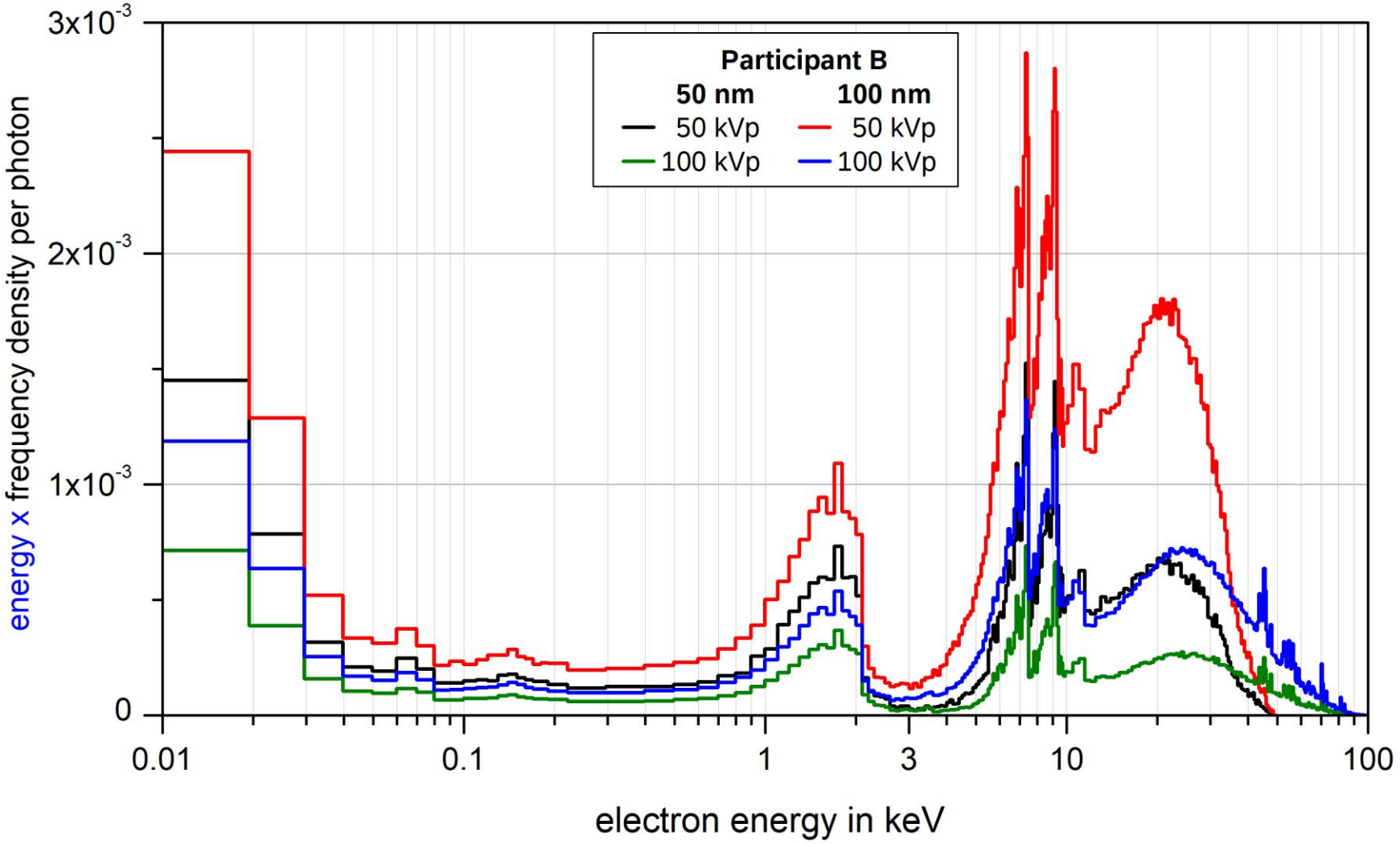

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Number of interactions in GNP per photon

	50 nm	100 nm
50 kVp	**1.1×10^{-3}**	**2.6×10^{-3}**
100 kVp	**0.5×10^{-3}**	**1.3×10^{-3}**

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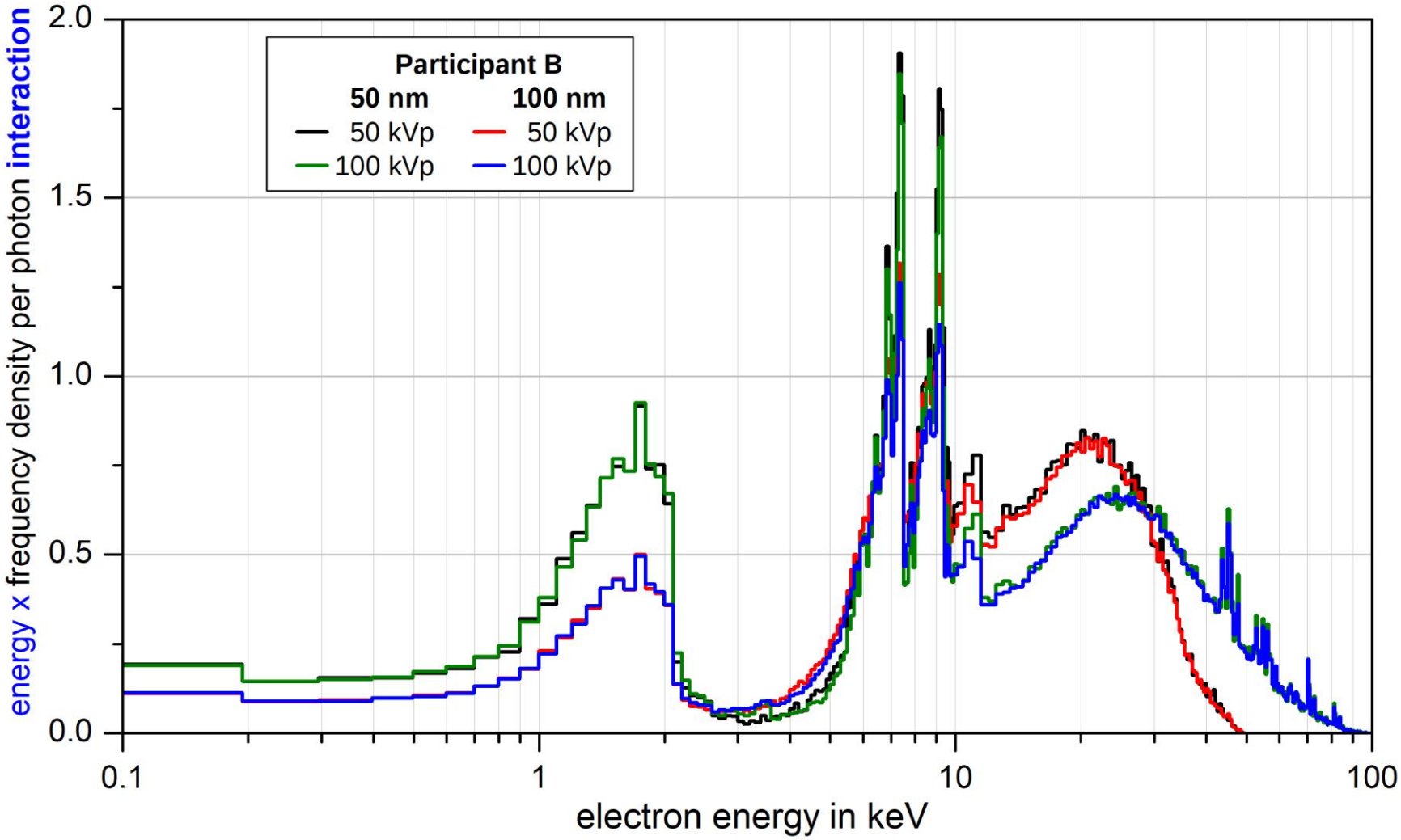
How to know: is this plausible or meaningful?



Integral: Electrons per photon interaction

	50 nm	100 nm
50 kVp	**4.77**	**3.40**
100 kVp	**4.72**	**3.35**

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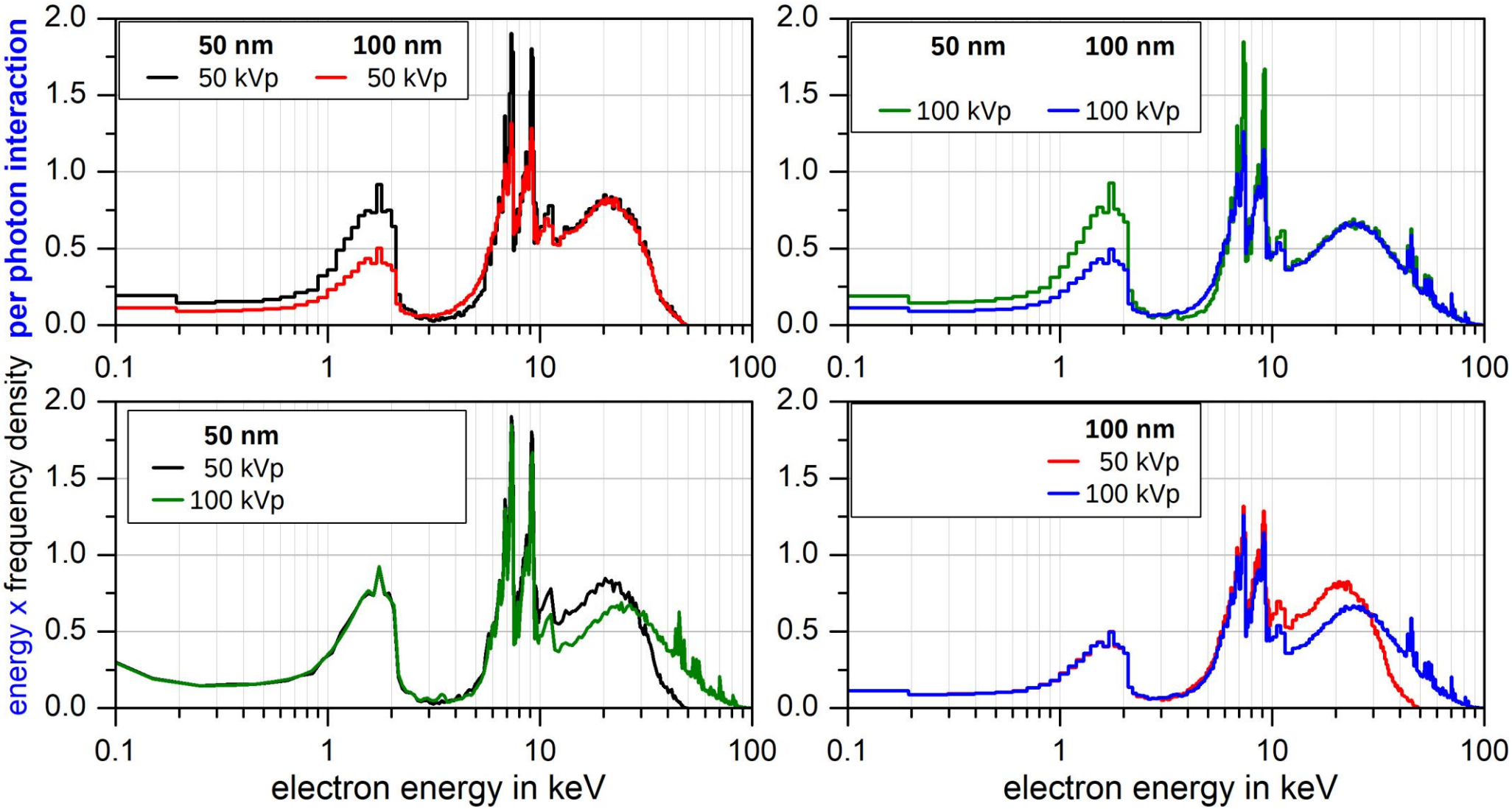
Normalize to probability of photon interaction



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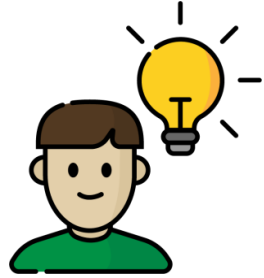
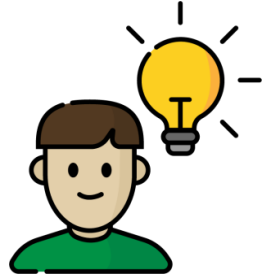
- If not: Read the paper from the Special Issue (Rabus et al., Radiat. Meas. 147, 106637 (2021), doi: 10.1016/j.radmeas.2021.106637)
- There will be a EURADOS Report on the exercise with templates

Take home messages



- Be sure you understand the problem you want to simulate

Take home messages



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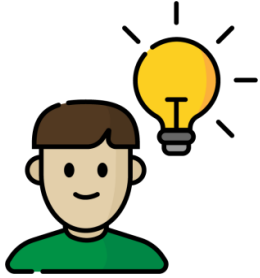

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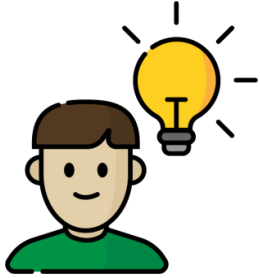

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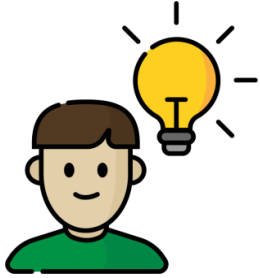
Take home messages



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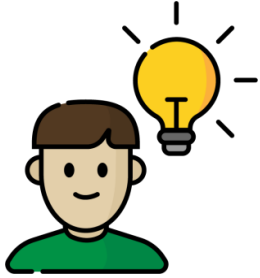

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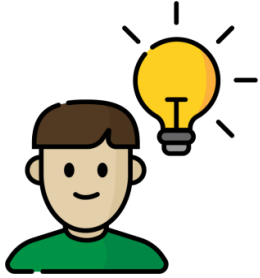

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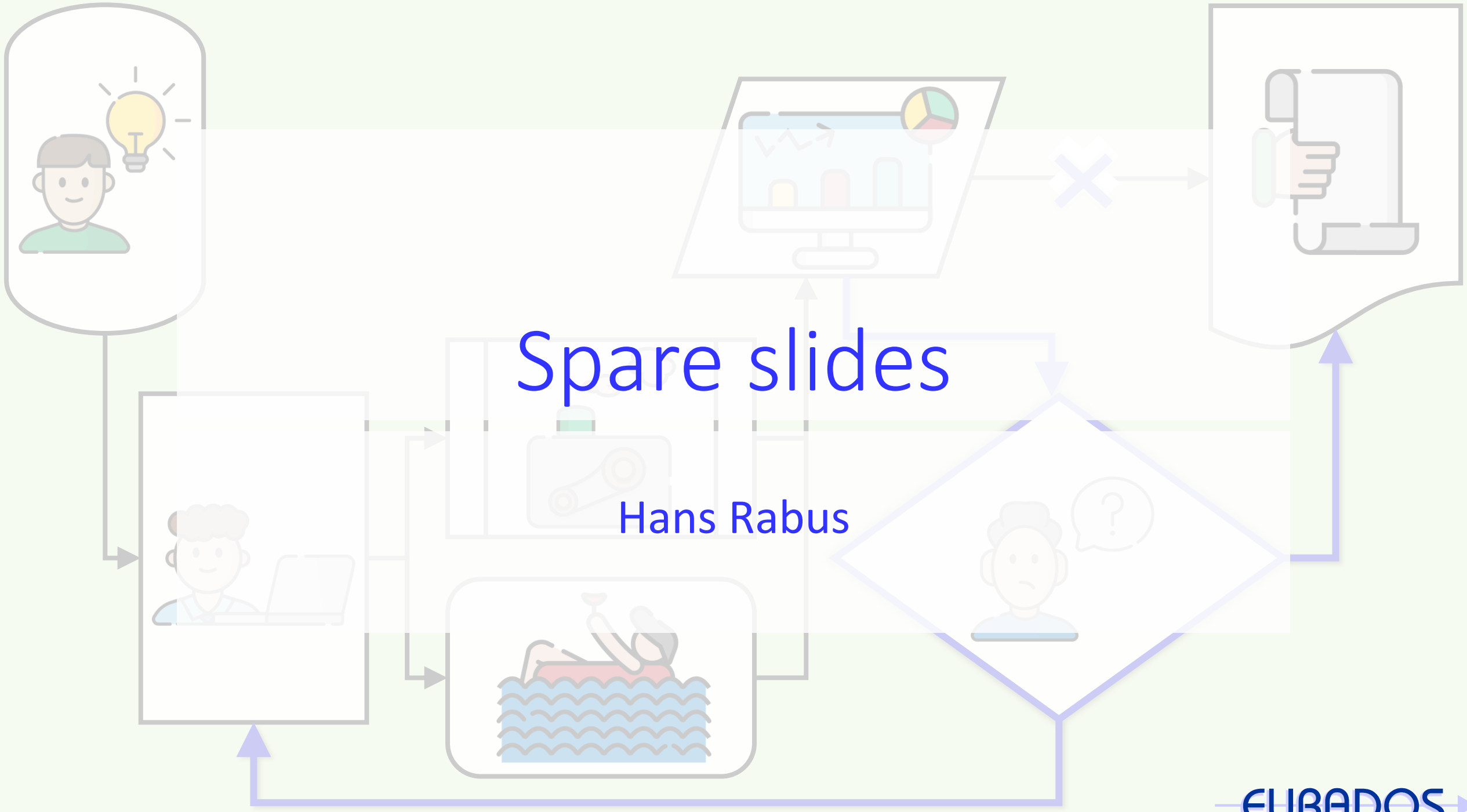
Spare slides

Hans Rabus



Electron spectrum – what is it?

Quantity	Meaning or formula	Notes
Absolute frequency	Number of electrons, N_i, with energies E in the i[th] energy bin, i.e., between $E_{i,min}$ and $E_{i,max}$	Integer number
Frequency per primary particle	Ratio of number of electrons in the i[th] energy bin, N_i to the number of primary photons, N_p.	Number
Relative frequency	Proportion of electrons in the i[th] energy bin, $f_i^{(r)} = \frac{N_i}{\sum_i N_i}$	Number, $\sum_i f_i^{(r)} = 1$
Frequency density per primary particle	$\bar{f}_1(E_i) = \frac{1}{\Delta E_i} \int_{E_{i,min}}^{E_{i,max}} f_1(E) dE = \frac{N_i \,/\, N_p}{\Delta E_i}$	Unit: eV^{-1} $\Delta E_i = E_{i,max} - E_{i,min}$

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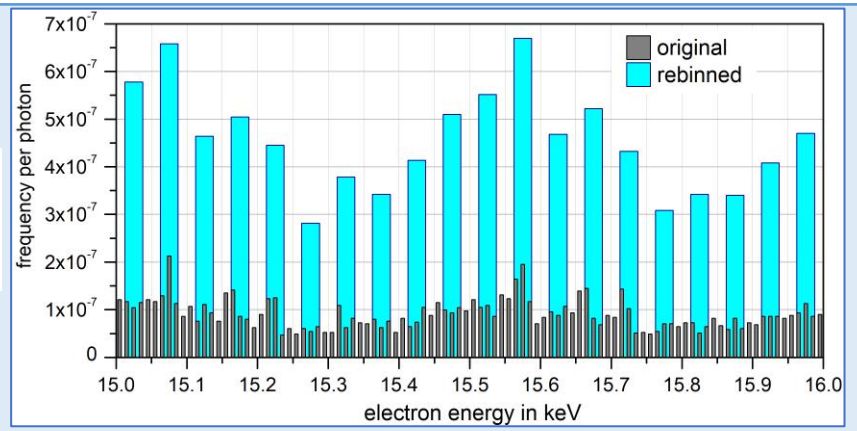
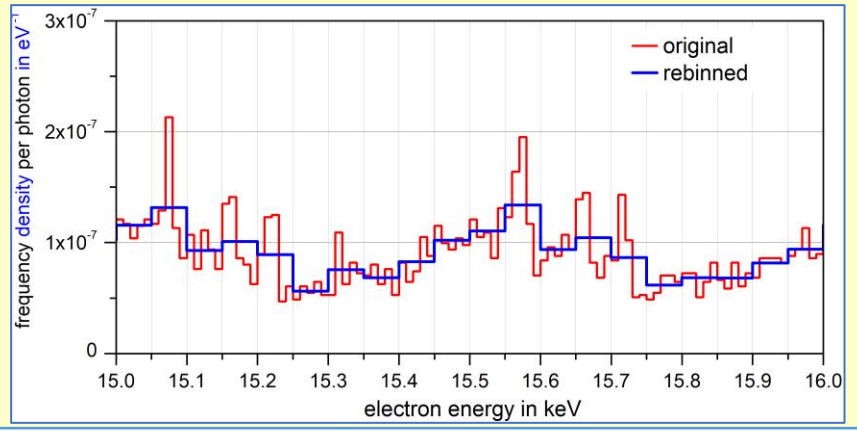
For spectra, the frequency density is the most suitable quantity (for reporting).

Electron spectra – plotting & rebinning

Quantity	Rebinning	Plotting
Absolute frequency	$N_i = \sum_{j \in i} N_j$	
Frequency per primary particle	$N_i \,/\, N_p = \sum_{j \in i} N_j \,/\, N_p$	
Relative frequency	$f_i^{(r)} = \sum_{j \in i} f_j^{(r)}$	
Mean frequency density per primary particle	$\bar{f}(E_i) = \frac{1}{\Delta E_i} \sum_{j \in i} \bar{f}(E_i) \Delta E_j$ $\Delta E_i = \sum_{j \in i} \Delta E_j$	





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