Program Degrad.1.0

Auger cascade model for electron thermalisation in gas mixtures produced by photons or particles in electric and magnetic fields

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Outline:

- Aims: Calculate observables
- Physical processes
- Present status
- Some results
- Comparison to older simulations
- Upgrade path and schedule

Aims:

Update old Mip program with accurate auger cascade model to give:

1 Calculation of fano factors W , F1 ,F2 ,F3 for photons and electrons

W=ev/ion pair F1 = width F2=skew F3=kurtosis

2 Single or double beta decay calculation to give electron cloud size, structure and number of electrons and photons from excimers

3 Allow calculation of number of clusters/cm and cluster size for particle tracks.

TPC analysis uses Neff ~ number of clusters/cm * cluster size

Include new option of varying incident particle energy.

Physics

Atomic/molecular cascade :

- Auger and Coster-Kronig decay
- Fluorescence
- Outer shell electron shake off

Photon absorption:

- Photoelectric effect
- Compton Scattering

Electron scattering:

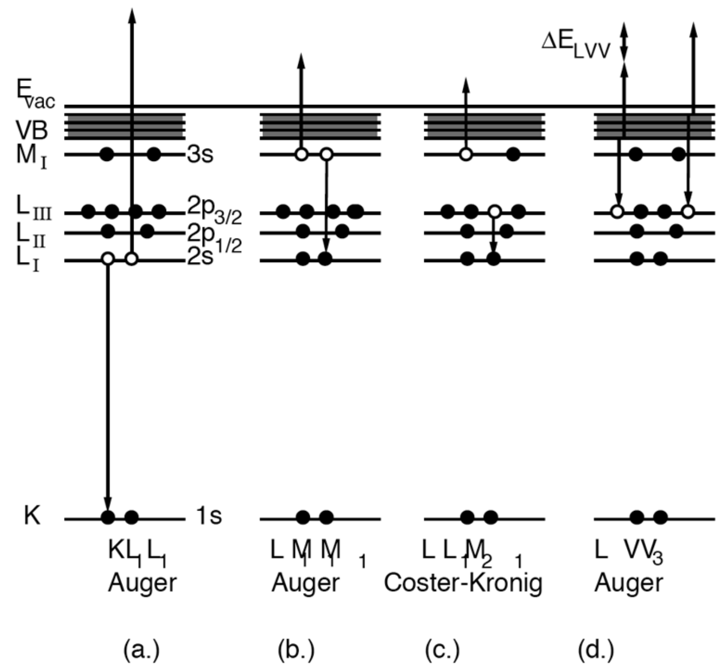
- Rotational, vibrational,excitation and ionisation scattering

Atomic de-excitation:

- Penning and Hornbeck-Molnar processes

Auger

Coster-Kronig



used first 17 atomic shells in Xenon

K,L1,L2,L3,M1,M2,M3,M4,M5,N1,N2,N3,N4,N5,O1,O2,O3

Fluorescence

emission of photon rather than electron

Shake off

outer shell electron emission from sudden change in potential

Photoelectric absorption

used cross-sections for each shell (17 in Xenon)

Bremsstrahlung

no effect on calculation below 2Mev

small cross-section , not included.

Compton Scattering

inelastic form factor needs to be split into atomic shells

(to be implemented)

Pair production

Not important below 2Mev

Electron scattering

INCLUDES CROSS-SECTIONS FOR ROTATIONAL VIBRATIONAL AND EXCITATION

FROM MAGBOLTZ

New ionisation model

NEW IONISATION MODEL : UPDATED MAGBOLTZ 10.1

SPLIT IONISATION CROSS-SECTION INTO INNER AND OUTER SHELLS.

e.g XENON INNER SHELLS - K,L1,L2,L3,M1,M2,M3,M4,M5

OUTER SHELLS - Charge States 1,2 and sum of 3,4,5,6

ARGON INNER SHELLS - K,L1,L2,L3

OUTER SHELLS - Charge states 1,2 and 3

Gases updated so far : Kr Ne He H2 N2 CH4 CF4 CO2 . The other gases will be updated

Model allows inner shell ionisations to emit fluorescence x-rays and auger electrons

To save computing time the model uses the average Auger and Fluorescence yield for each shell as given by the cascade calculation.

ATOMIC DE-EXCITATION

Penning effect

Transfer probabilities need to be entered in the gas subroutines

Probabilities depend energy difference between excitation
levels in gas1 and ionisation energy in gas 2

Hornbeck-Molnar

Associative ionisation can occur for high lying levels in the noble gases

e.g. Ar** +Ar --- Ar2+ + e-

Less than 2% in Argon but may be important in Xenon
(work continuing). Reduces yield of excimer formation.

Program Status

Program is fast: 6 Kev. 100k events in few minutes

1Mev 5k events in 1 hour

Good agreement with experimental W factors. ICRU Report 31

Icru : Xenon W= 22.1 +- 0.2ev. Argon W = 26.4 +- 0.2ev.

Calc: Xenon W= 22.50 +- 0.2ev. Argon W = 26.68 +- 0.2ev.

Published asymptotic Fano factors :

Xenon in range from 0.12 to 0.2 in Argon from 0.13 to 0.19

Calc: Xenon: gammas F = 0.175 electrons F= 0.170

Argon: gammas F= 0.145 electrons F= 0.142

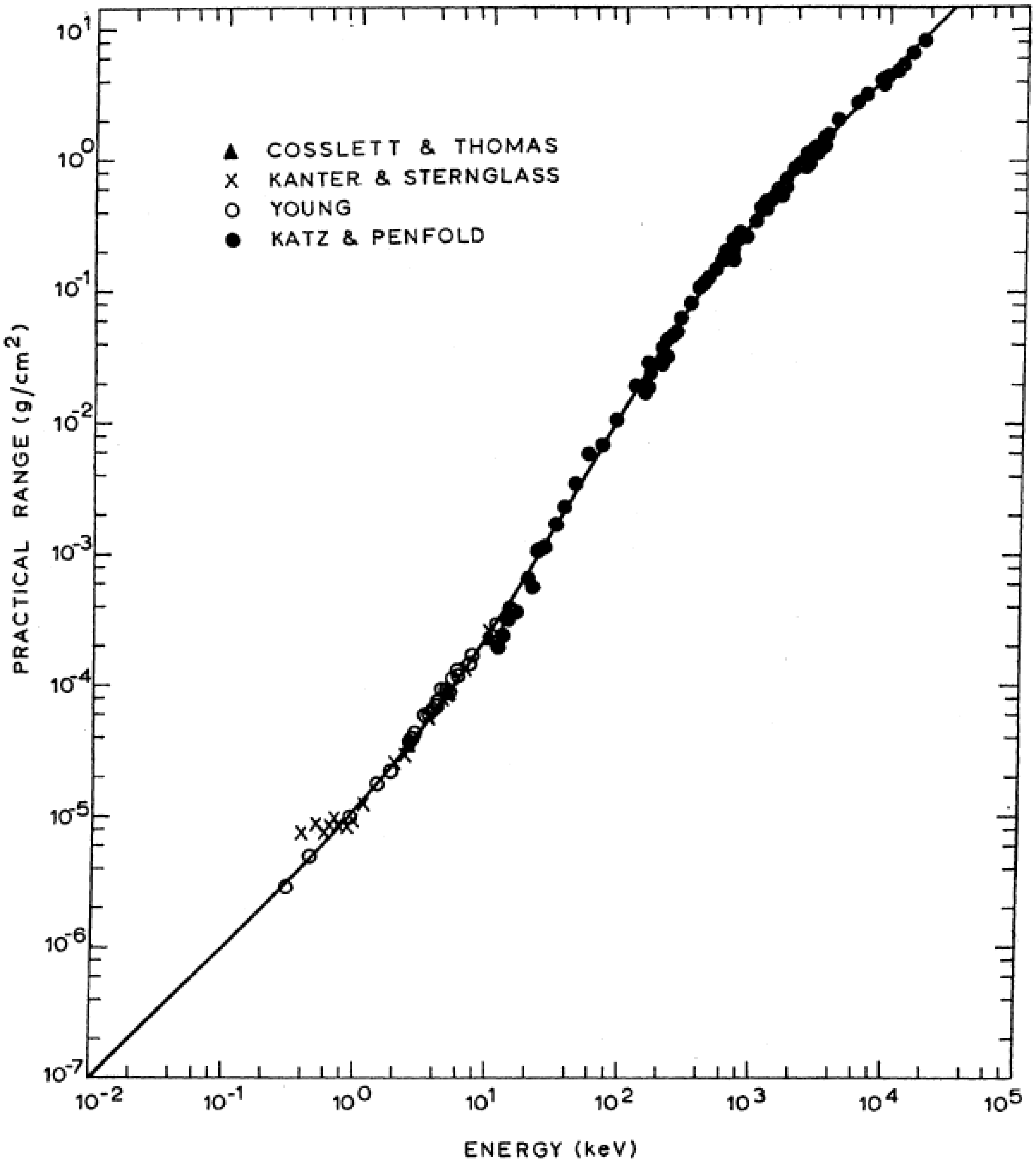
The range of electron thermalised cloud sizes for incident electrons and photons between 100 ev and 1Mev is in agreement with experiment.

Kobetich and Katz Phys Rev 170(1968)391

Beta decay option tested and gives similar ranges to electrons and gammas

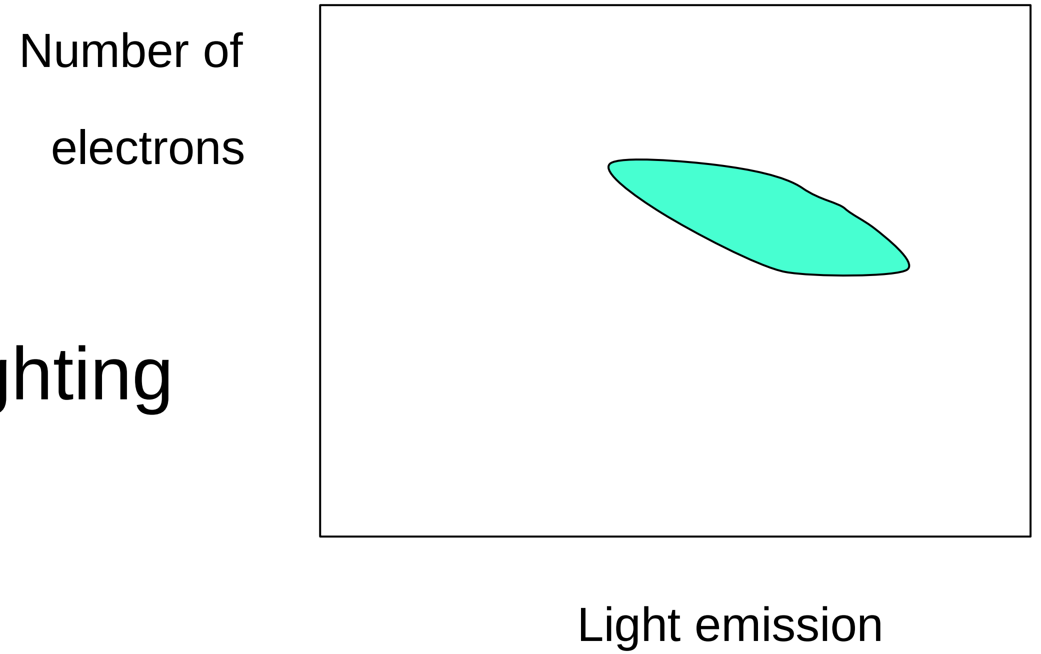
Mip simulation of track clusters gives same results as the MIP program

Next upgrade will include the full shell effects on the clusters and also allow variable incident particle energy .

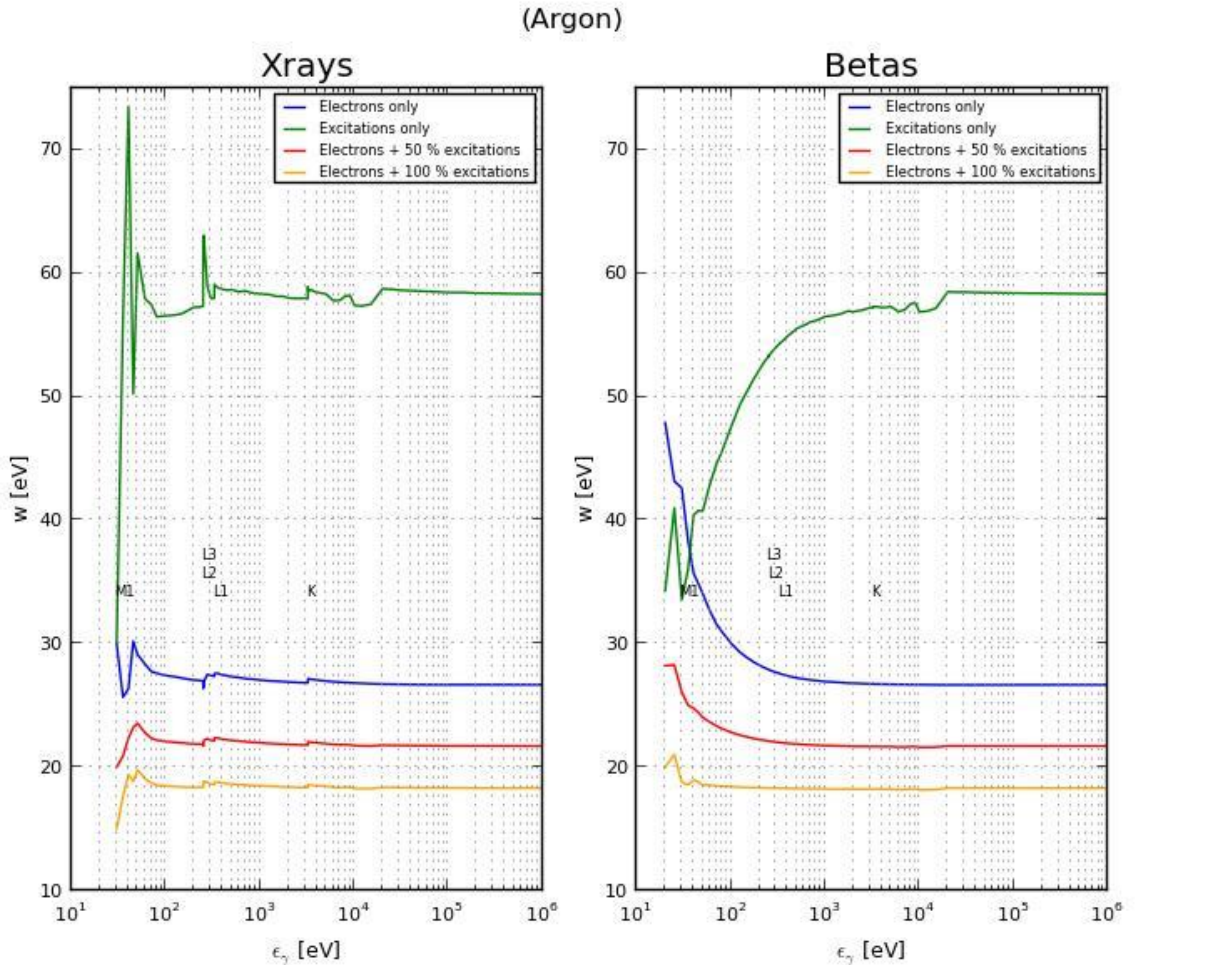

COSSLETT & THOMAS
KANTER & STERNGLASS
YOUNG
KATZ & PENFOLD
PRACTICAL RANGE (g/cm2)
ENERGY (keV)
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-2
10^-1
10^0
10^1
10^2
10^3
10^4
10^5

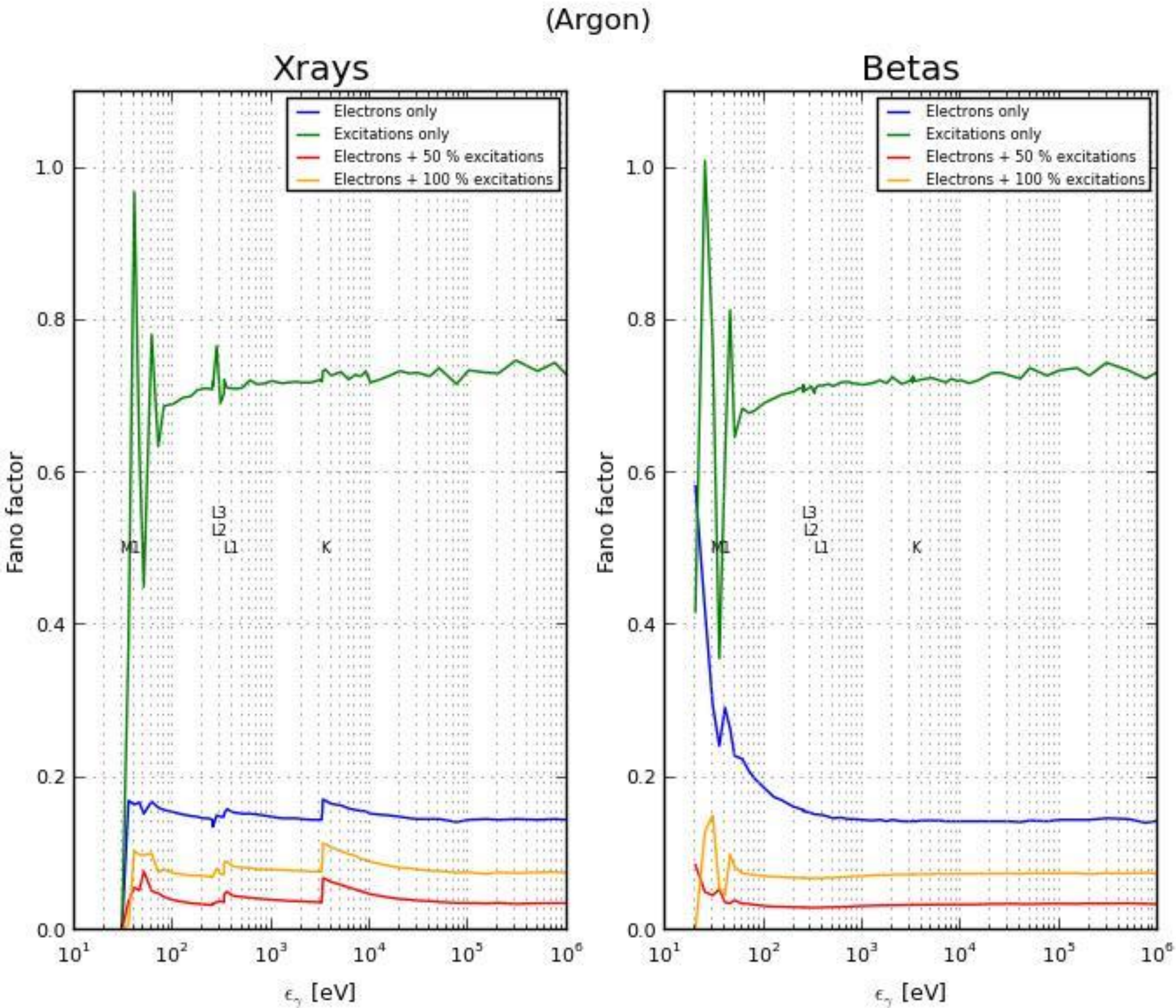
All following plots of W and fano factors are for the limit of zero electric field. The fano factor can increase by 30% for quite low values of the electric field

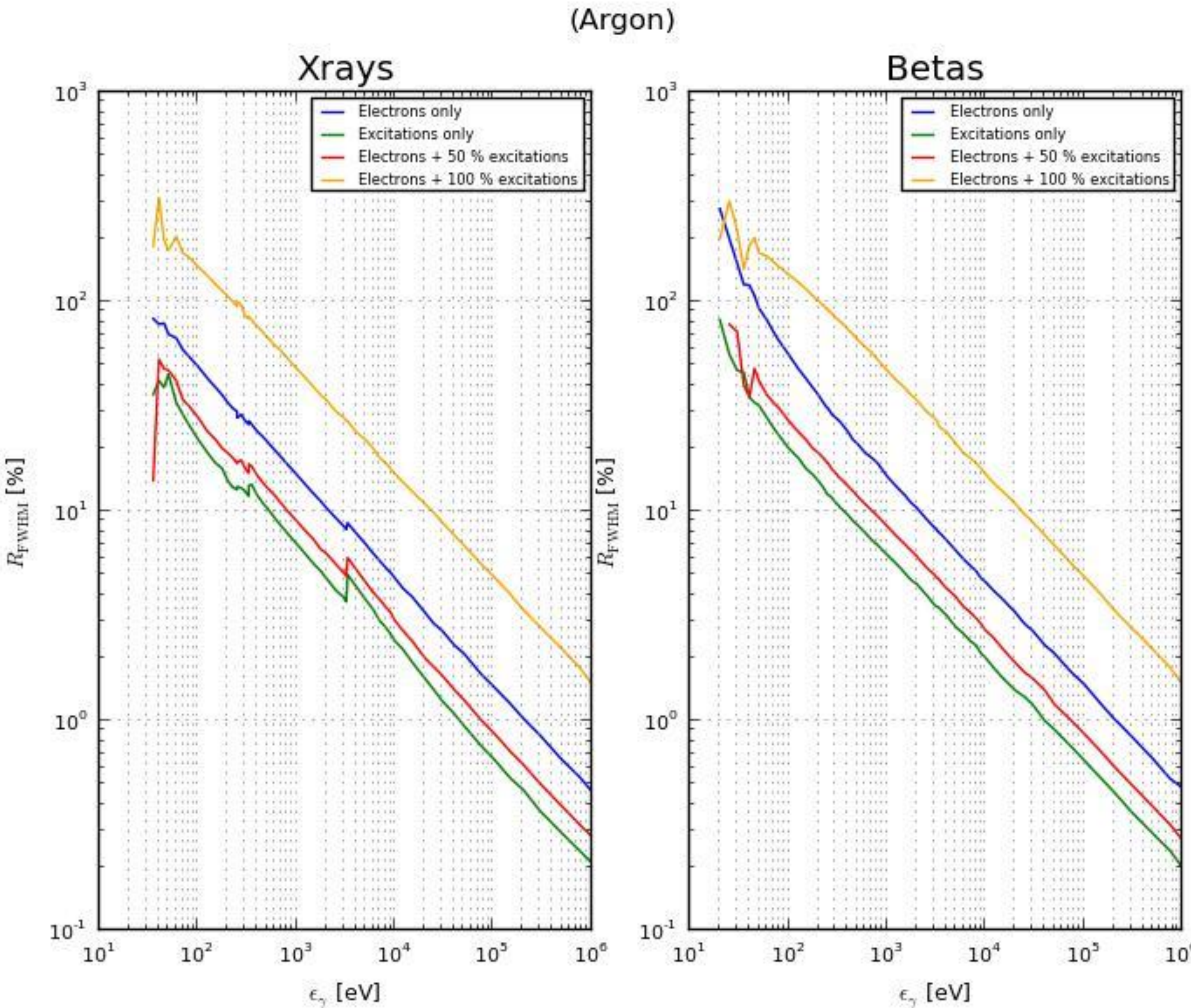
To correct for anti-correlation used equal weighting of electrons and light emission in following plots.



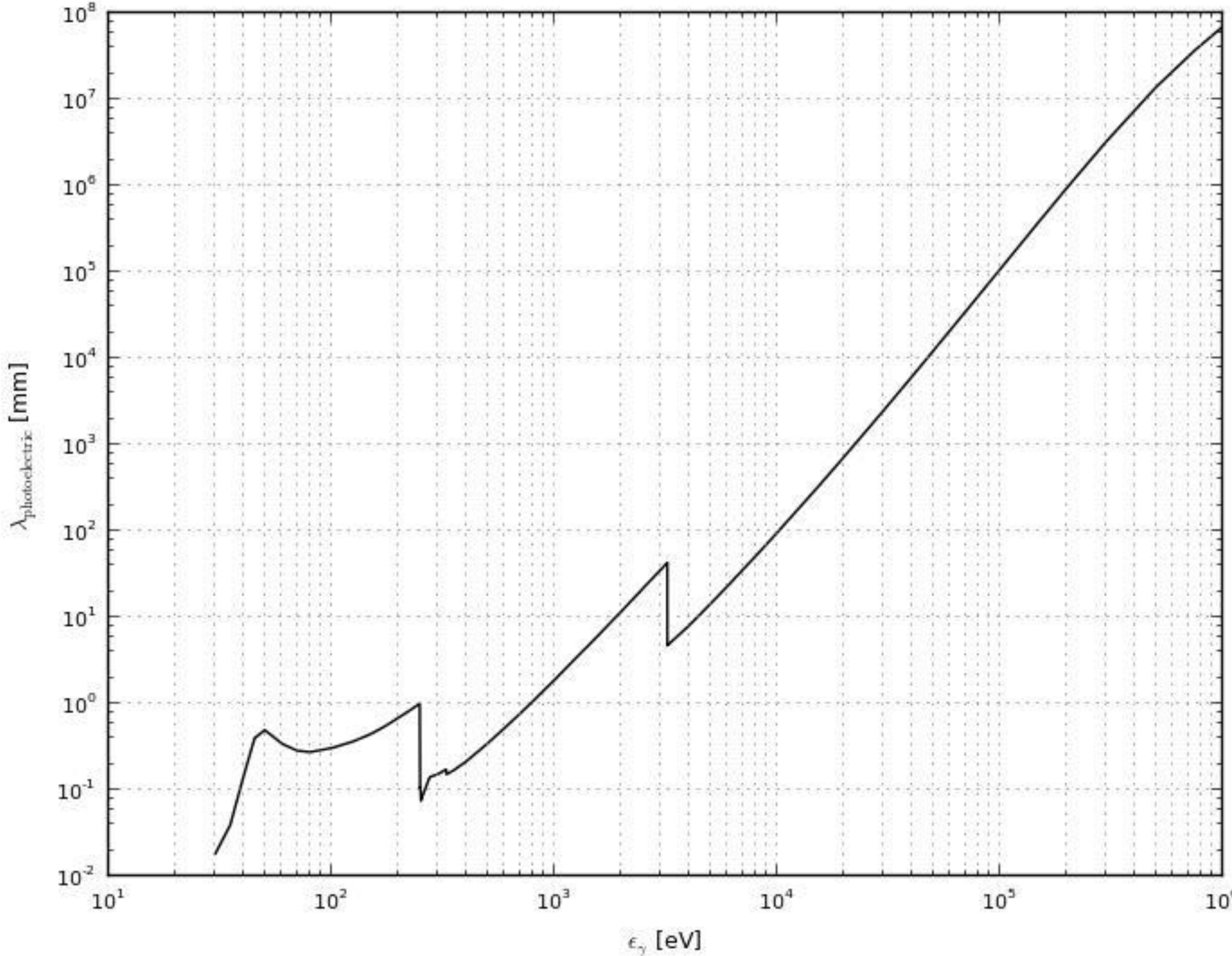
However optimum not 1/1 weighting


(Argon)
Xrays
Betas
Electrons only
Excitations only
Electrons + 50 % excitations
Electrons + 100 % excitations
w [eV]
ϵ_γ [eV]
M1
L3
L2
L1
K


(Argon)
Xrays
Betas
Electrons only
Excitations only
Electrons + 50 % excitations
Electrons + 100 % excitations
Fano factor
M1
L3
L2
L1
K
1.0
0.8
0.6
0.4
0.2
0.0
10^1
10^2
10^3
10^4
10^5
10^6
ϵ_γ [eV]

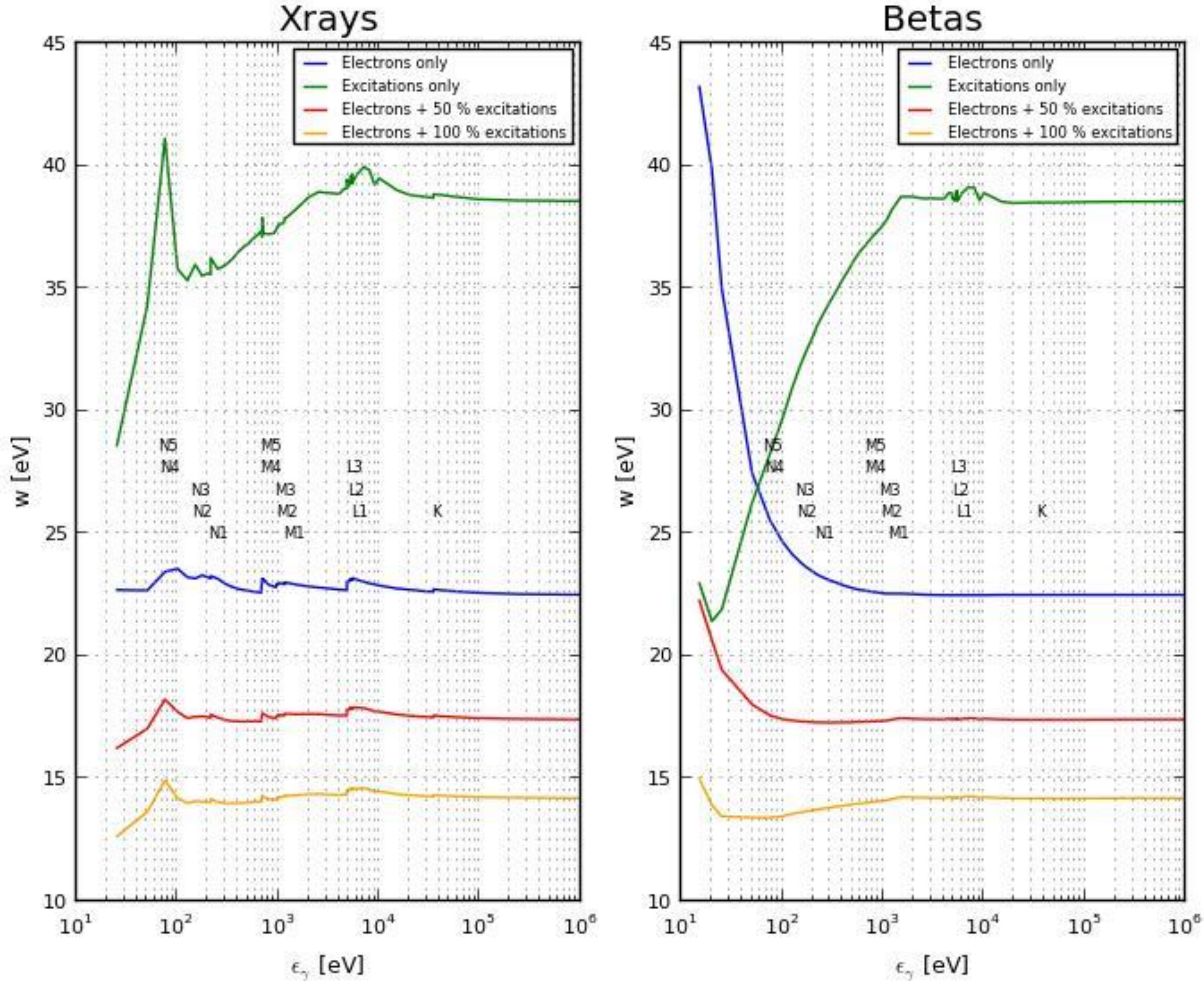

(Argon)
Xrays
Betas
Electrons only
Excitations only
Electrons + 50 % excitations
Electrons + 100 % excitations
R_{FWHM} [%]
ϵ_γ [eV]
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}

(Argon)

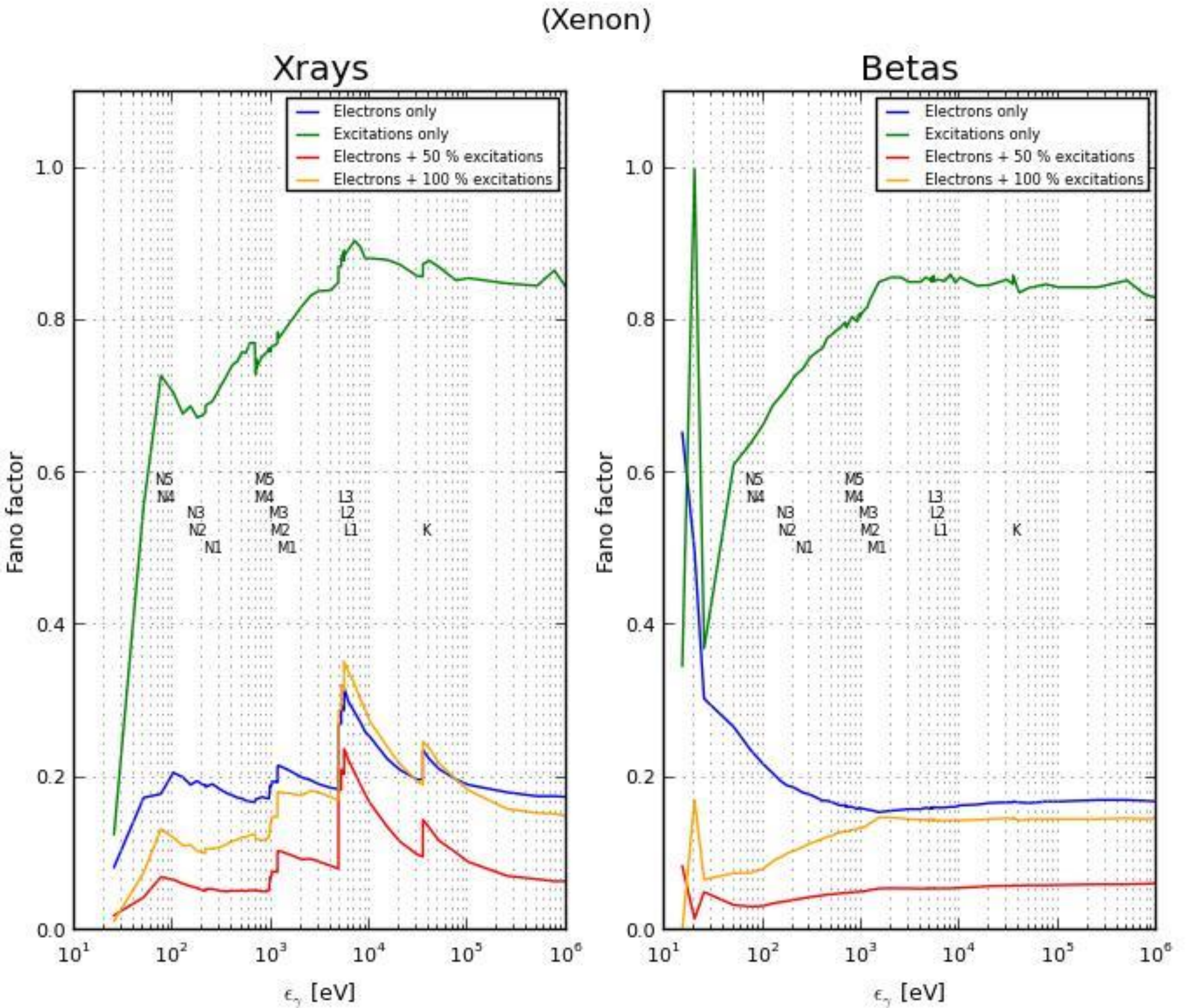


10^8
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
$\lambda_{\mathrm{photoelectric}}$ [mm]
10^1
10^2
10^3
10^4
10^5
10^6
ϵ_γ [eV]

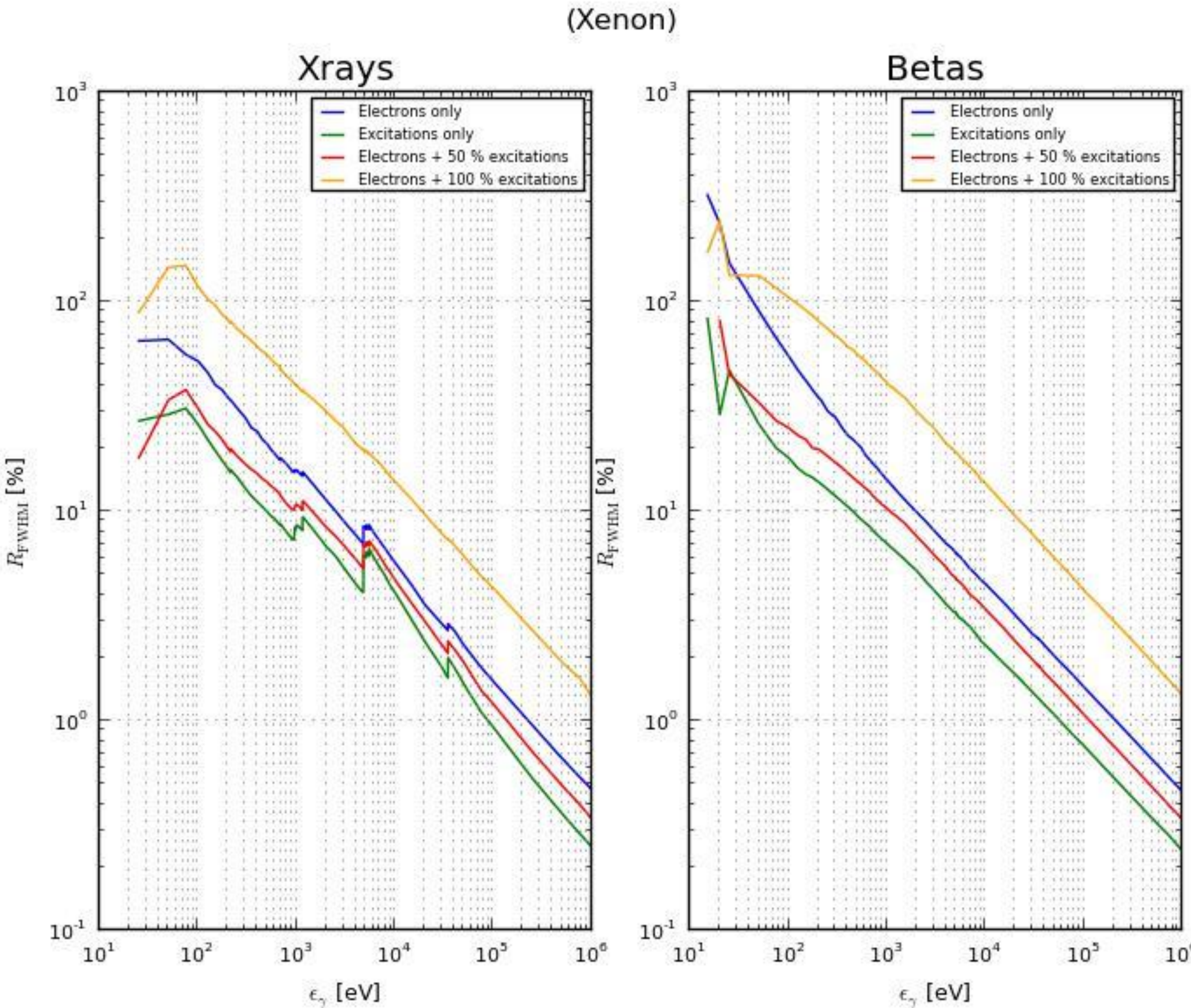
(Xenon)



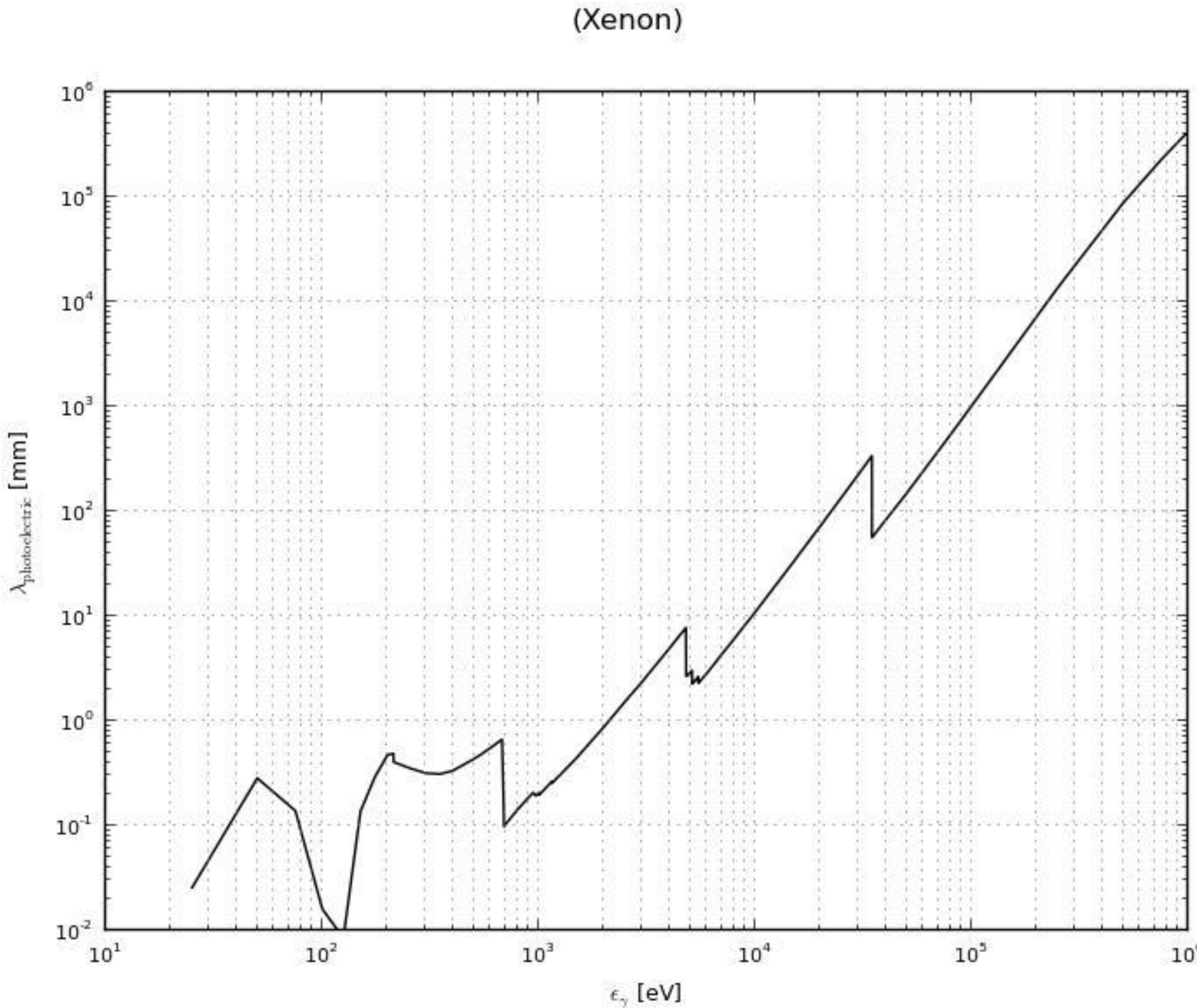
Xrays
Betas
Electrons only
Excitations only
Electrons + 50 % excitations
Electrons + 100 % excitations
w [eV]
ϵ_γ [eV]
N5
N4
N3
N2
N1
M5
M4
M3
M2
M1
L3
L2
L1
K



(Xenon)
Xrays
Betas
Electrons only
Excitations only
Electrons + 50 % excitations
Electrons + 100 % excitations
Fano factor
N5
N4
N3
N2
N1
M5
M4
M3
M2
M1
L3
L2
L1
K
ϵ_γ [eV]



(Xenon)
Xrays
Betas
Electrons only
Excitations only
Electrons + 50 % excitations
Electrons + 100 % excitations
R_{FWHM} [%]
ϵ_γ [eV]



(Xenon)
$\lambda_{\mathrm{photoelectric}}$ [mm]
ϵ_γ [eV]
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}

Comparison to previous calculations and some experiments:

Dias et al J. Appl. Phys. 82(1997)2742

Non-linearity at shell edges: only comparison in Xenon possible

Discontinuity from linearity: all in ev.

Kshell : Calc. : 157

Dias : 206

Exp. : 165 + -10

	L1 shell	L2 shell	L3 shell	Total L1-L3
Calc. :	19	18	76	113
Dias :	20	15	90	135
Exp. 1 :	16+-2	26 +-2	55 +-2	96 +-6
Exp. 2 :				128+-15

Light yield from S1 signal : calculation : Xenon 38.5 ev/photon

Experiment: range from 78 to 140 ev/photon

Effect of Drift field at High electron energy

For Beta decay in Xenon :

electric field in range 25 to 100v/cm/atmosphere

Electric Field	Resolution % FWHM at 1Mev
0.01	0.46
25	0.48
50	0.52
100	0.66

May be possible to correct the events by correlation with electron cloud size along electric-field direction .

Effect of approximations:

1) no Compton scattering

2) non relativistic

3) no Hornbeck-Molnar

1) +-1% on Fano factor and W above K shell energy.

Missing multi-site events with gammas

2) +-1% on W : increase in energy loss to elastics from use of relativistic electron mass.

Decrease in Range above 100Kev (few %??)

3) No effect in Argon need to check Xenon.

Cross-section data may be missing in Xenon.

Upgrade schedule

1) Compton effect with shell form factors Oct 2013

2) Relativistic electron kinematics for energies above 100kev Oct 2013

3) Allow simulation of Particle tracks with variable energy and include shell effects on clusters xxx 2014