Understanding the X-ray fluorescence spectrum: from theory to experiment

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Outline

- Description of x-ray emission

- Detector modification
  - Detector response function.
  - Detector resolution

MULTIPLE SCATTERING IN X-RAY SPECTROMETRY

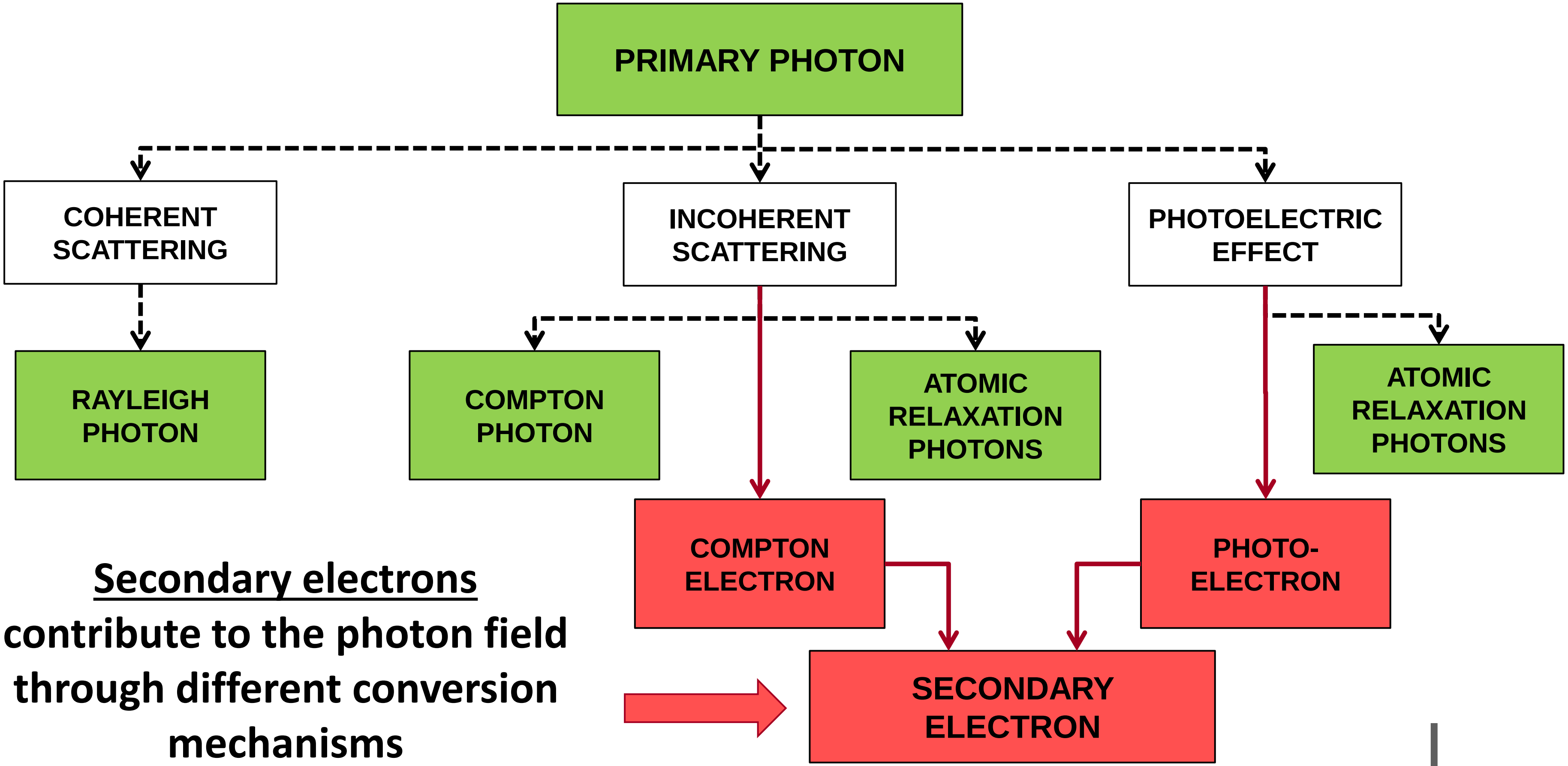
- X-rays penetrate deeply into the matter, and, in a thick medium, give place to a phenomenon known as multiple scattering (i.e, multiple collisions).

- Multiple scattering models use the prevailing interactions in the x-ray regime to describe the radiation field.

- Another important factor modifying the radiation field is the polarization.

Scheme of X-ray interaction mechanisms

The full description of the radiation field requires the modeling of coupled photon-electron transport



Secondary electrons contribute to the photon field through different conversion mechanisms

Multiple scattering is described using the Boltzmann transport model

The photon interactions are depicted with the interaction kernels k_i

$$\eta \frac{\partial}{\partial z} f(z,\vec{\omega},E) = -\mu(E) f(z,\vec{\omega},E)$$

$$+ \sum_{i}^{all\ interactions} \int_0^\infty \left(\int_{4\pi} \cup (z) k_i \left(\vec{\omega}', E', \vec{\omega}, E\right) f\left(z, \vec{\omega}', E'\right) d\omega' \right) dE'$$

$$+ S(z,\vec{\omega},E)$$

MCSHAPE

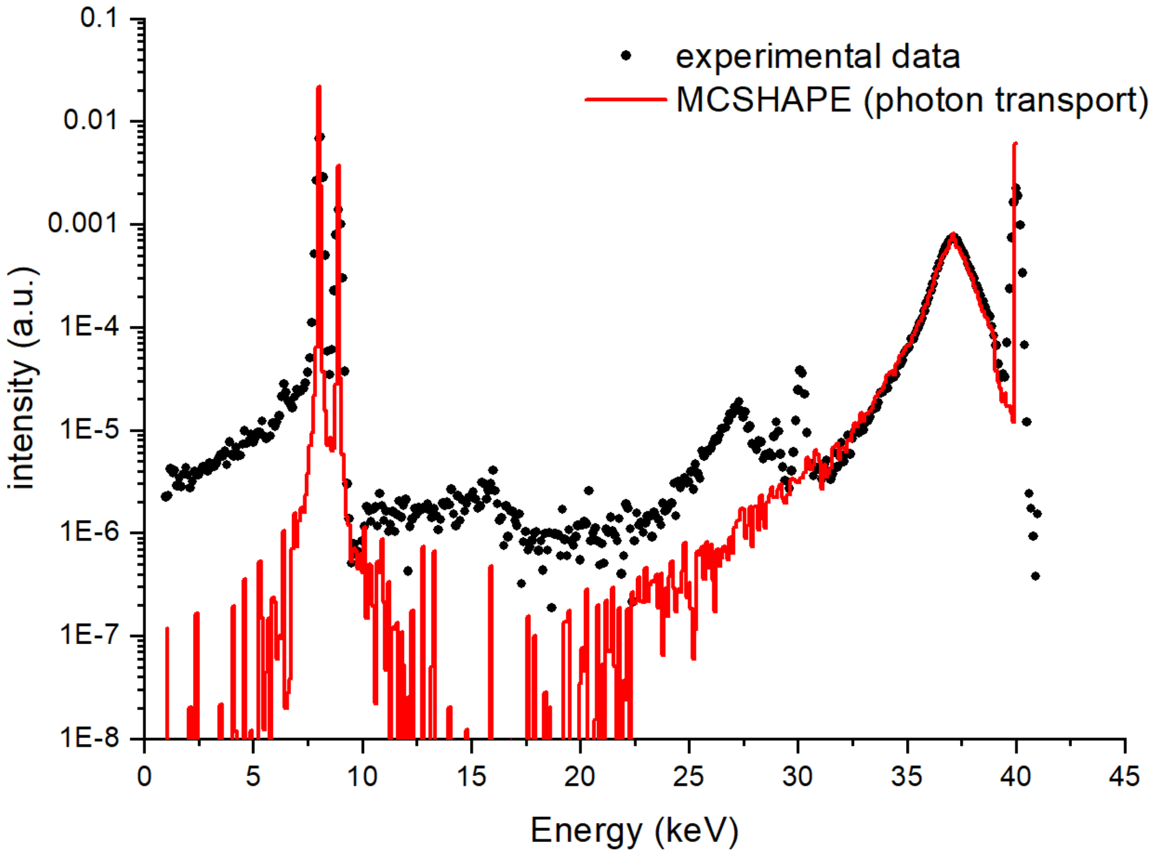
MCSHAPE is a Monte Carlo code developed at the University of Bologna which can simulate the diffusion of photons with arbitrary polarization state and has the unique feature of describing the evolution of the polarization state along the interactions with the atoms.

The adopted transport model is derived from the so called Boltzmann-Chandrasekhar 'vector' transport equation. The polarization state of the photons is described by using the Stokes parameters I, Q, U and V, having the dimension of intensities and containing the physical information about the polarization state.

This code simulates the propagation in heterogeneous media of photons injected by either polarized (i.e., synchrotron) or unpolarized sources (x-ray tubes).

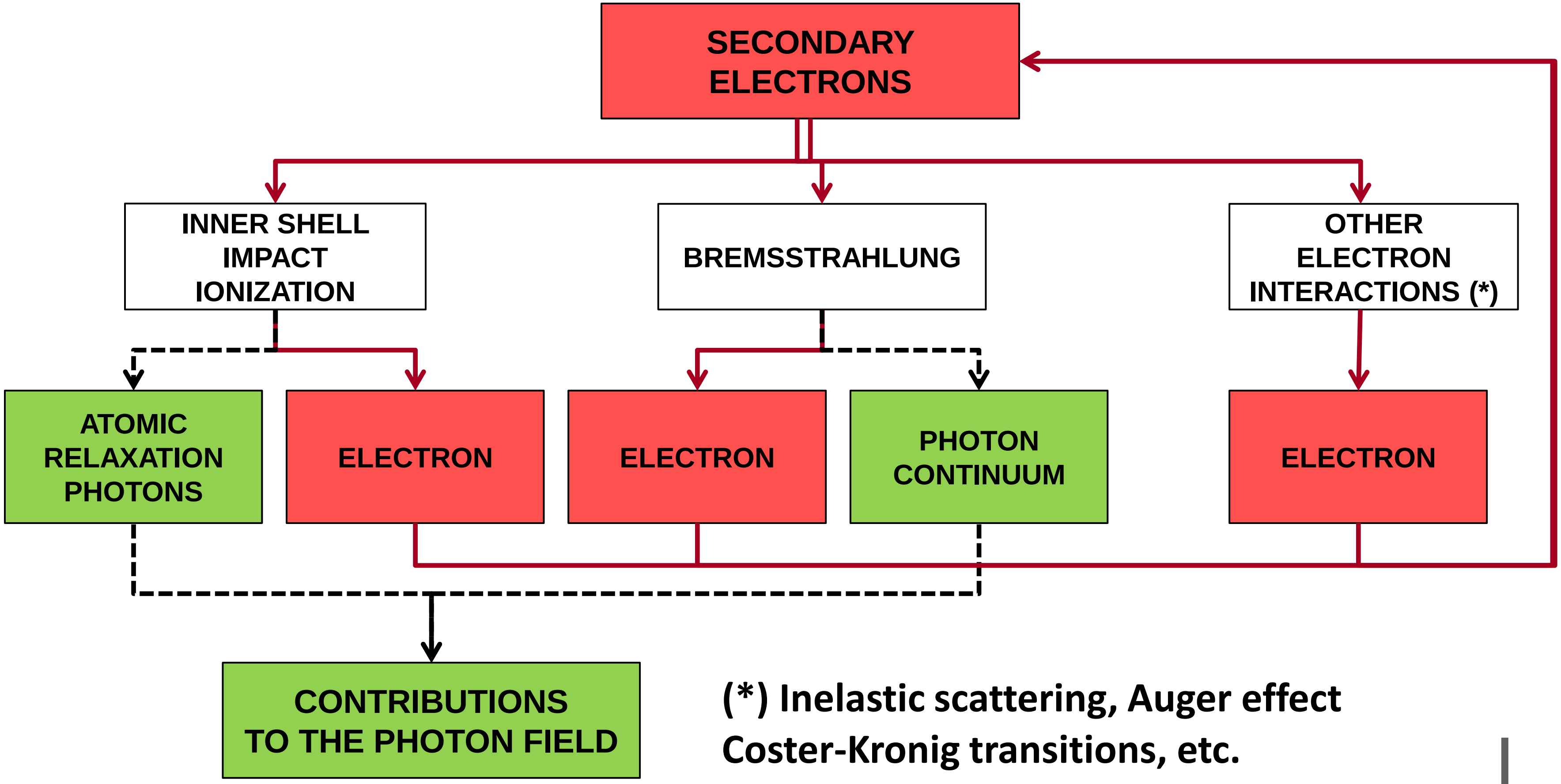
- Website: http://shape.ing.unibo.it

Simulation with MCSHAPE (only photon transport)



X-ray production mechanisms from coupling terms

The full description of the radiation field requires the modeling of coupled photon-electron transport



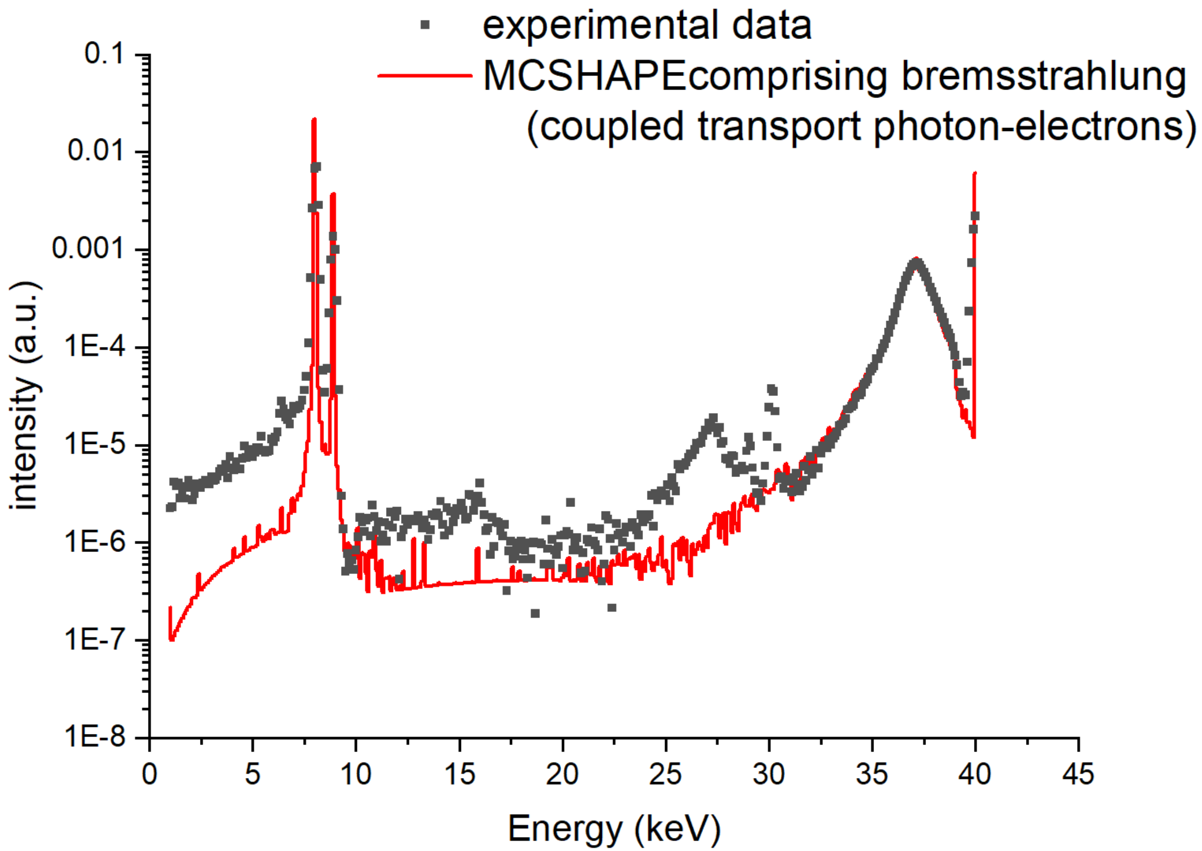
(*) Inelastic scattering, Auger effect
Coster-Kronig transitions, etc.

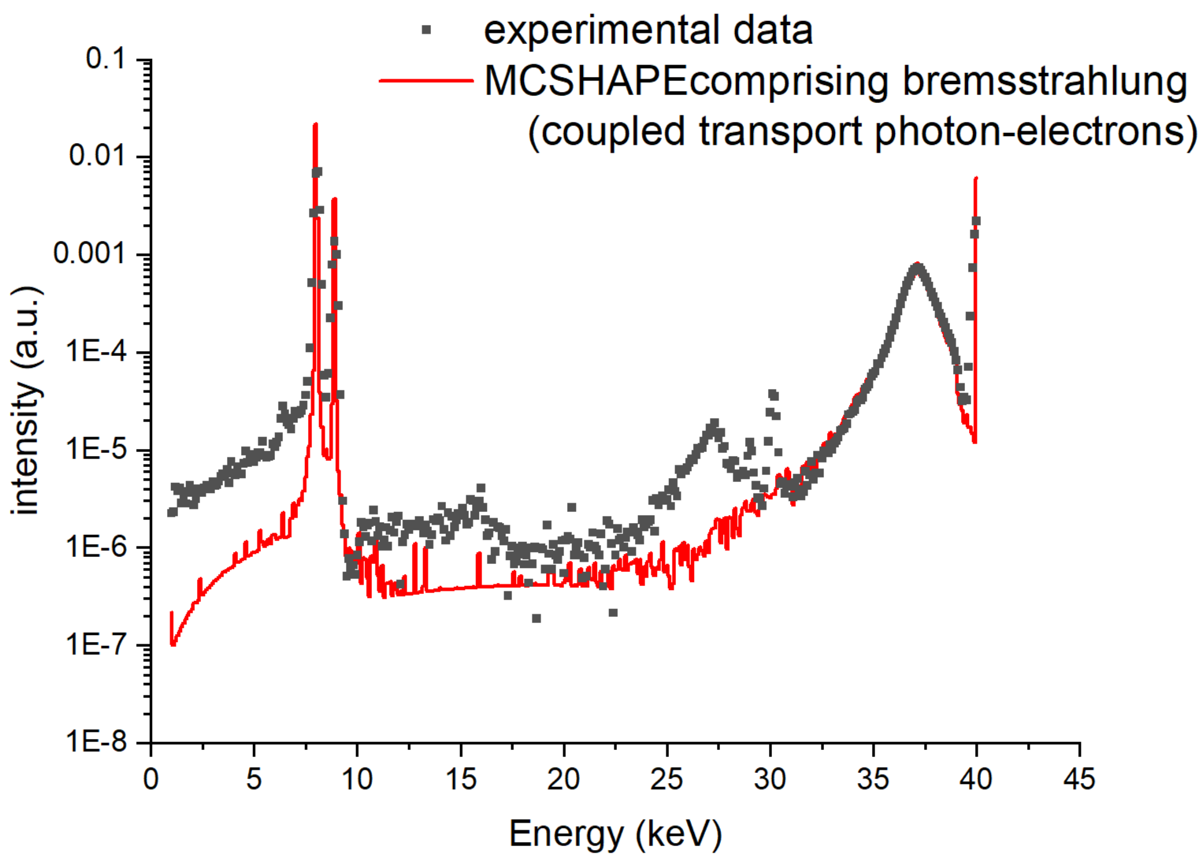
MS is better described using the modified Boltzmann transport model

The Boltzmann transport model needs to be modified to include the electron-photon contributions

$$\begin{cases} \eta \dfrac{\partial}{\partial z} f^p(z,\vec{\omega},E) = -\mu^p(E) f^p(z,\vec{\omega},E) \\ + \displaystyle\sum_{i}^{all\ photon\ interactions} \int_0^\infty \left(\int_{4\pi} \cup\,(z) k_i^{\,p\to p}(\vec{\omega}', E', \vec{\omega}, E) f^p(z,\vec{\omega}',E') d\omega' \right) dE' \\ \boxed{+ \displaystyle\sum_{j}^{all\ coupling\ terms} \int_0^\infty \left(\int_{4\pi} \cup\,(z) k_j^{\,e\to p}(\vec{\omega}', E', \vec{\omega}, E) f^p(z,\vec{\omega}',E') d\omega' \right) dE'} \\ + S^p(z,\vec{\omega},E) \end{cases}$$

Simulation with MCSHAPE (comprising electron-photon coupling terms)





experimental data
MCSHAPEcomprising bremsstrahlung
(coupled transport photon-electrons)
0.1
0.01
0.001
1E-4
1E-5
1E-6
1E-7
1E-8
intensity (a.u.)
0
5
10
15
20
25
30
35
40
45
Energy (keV)

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  - Detector response function.
  - Detector resolution.

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Simulation of the detector response function with the code MCSHAPE

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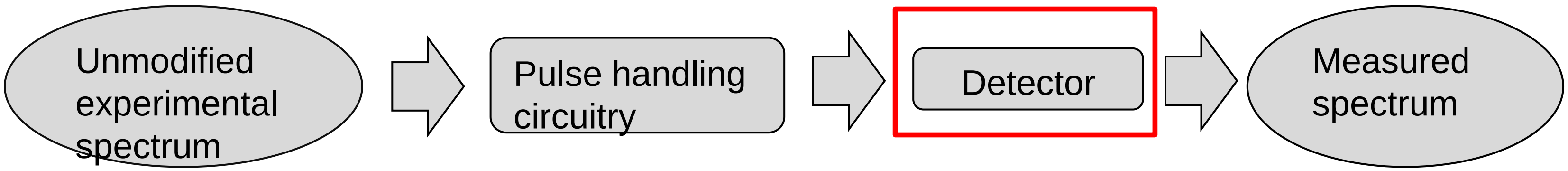
A modeling tool for detector resolution and incomplete charge collection†

Jorge E. Fernández, Viviana Scot and Lorenzo Sabbatucci*

J.E. Fernandez, Viviana Scot, L. Sabbatucci: A modeling tool for detector resolution and incomplete charge collection. X-ray Spectrometry 44 (2015) 177-182

Detector Response



(Detector influence on radiation measures)

The measured spectrum is given by the following convolution product:

$$I_{measured}(E) = \int R(E', E)\, \phi(E')\, I(E')\, dE'$$

Where

$R(E', E)$ is the response function

$\phi(E')$ is the detector efficiency

$I(E')$ is the original spectrum

Model of detector response

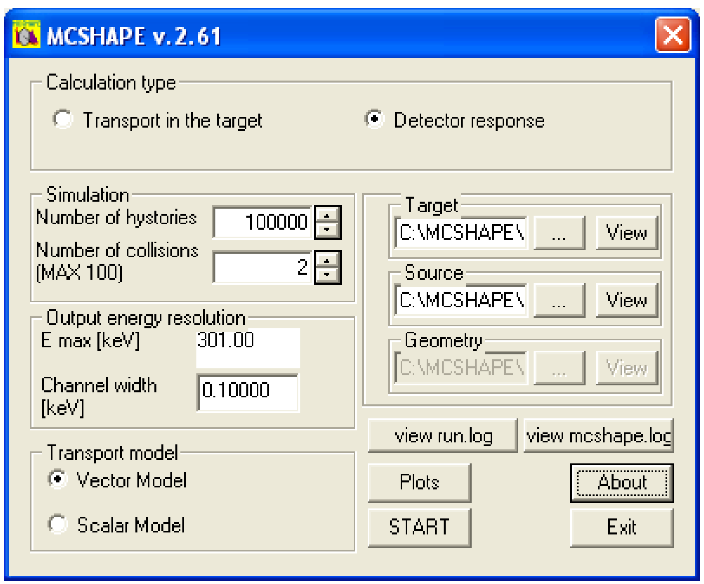
$$R(E_0, E) = \int Q(E'', E_0)\, G(E'', E)\, dE''$$

$Q(E'', E_0)$ is the energy deposition spectrum

$G(E'', E)$ is the detector resolution

Energy deposition spectrum

- It is built by computing the escape spectrum distribution
- In a first approximation its integral is normalized (really is not because of the Rayleigh scattering)
- It can be calculated by using a MC code



MCSHAPE Computes the energy deposition spectrum

What is computed with MCSHAPE?

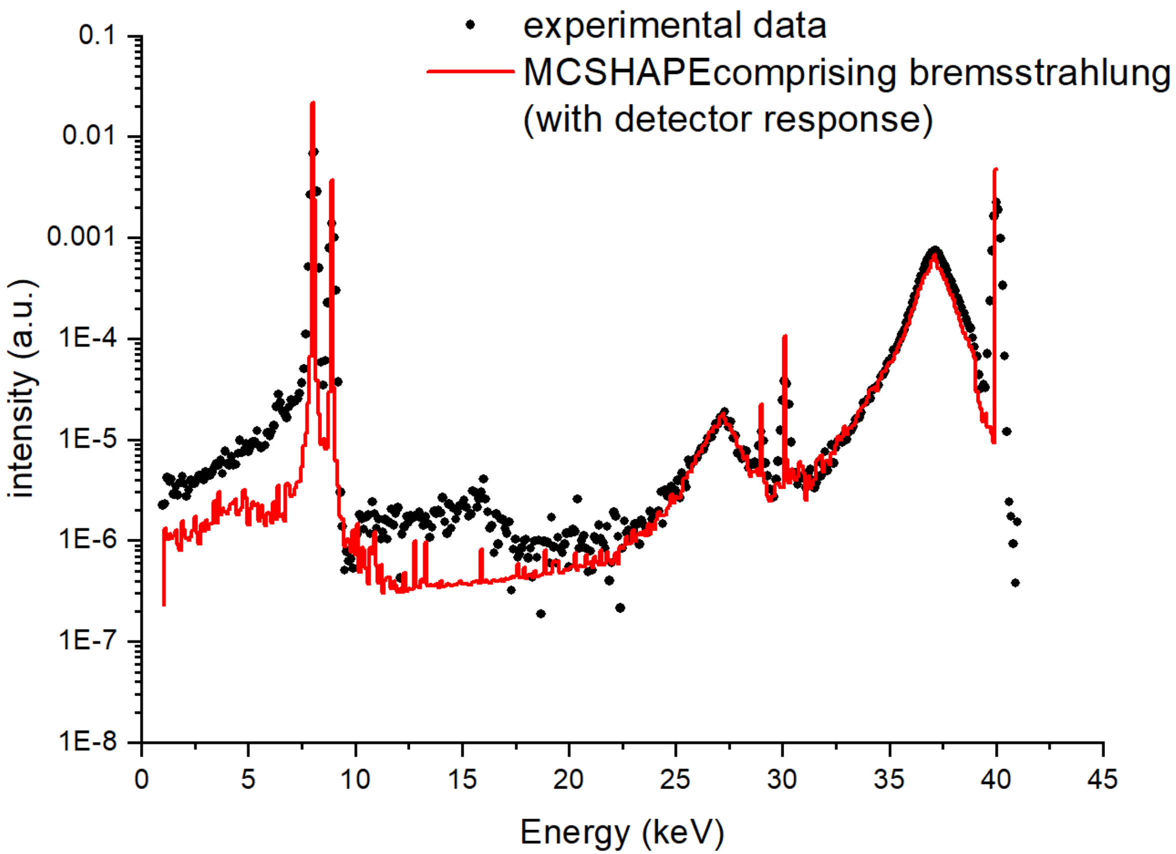
$$I_{measured}(E) = \int R(E',E)\,\varphi(E')\,I(E')\,dE'$$

$$= \int \left(\int Q(E'',E')\,G(E'',E)\,dE'' \right) \varphi(E')\,I(E')\,dE'$$

$$= \underbrace{\int \underbrace{\left(\int Q(E'',E')\,\varphi(E')\,I(E')\,dE' \right)}_{computed\ by\ MCSHAPE\ v2.71} G(E'',E)\,dE''}_{computed\ by\ the\ postprocessor\ code\ RESOLUTION}$$

J..E. Fernandez, V. Scot : Simulation of the detector response function with the code MCSHAPE, Radiation Physics and Chemistry 78 (2009) 882–887.

Complete simulation comprising detector response (no resolution)



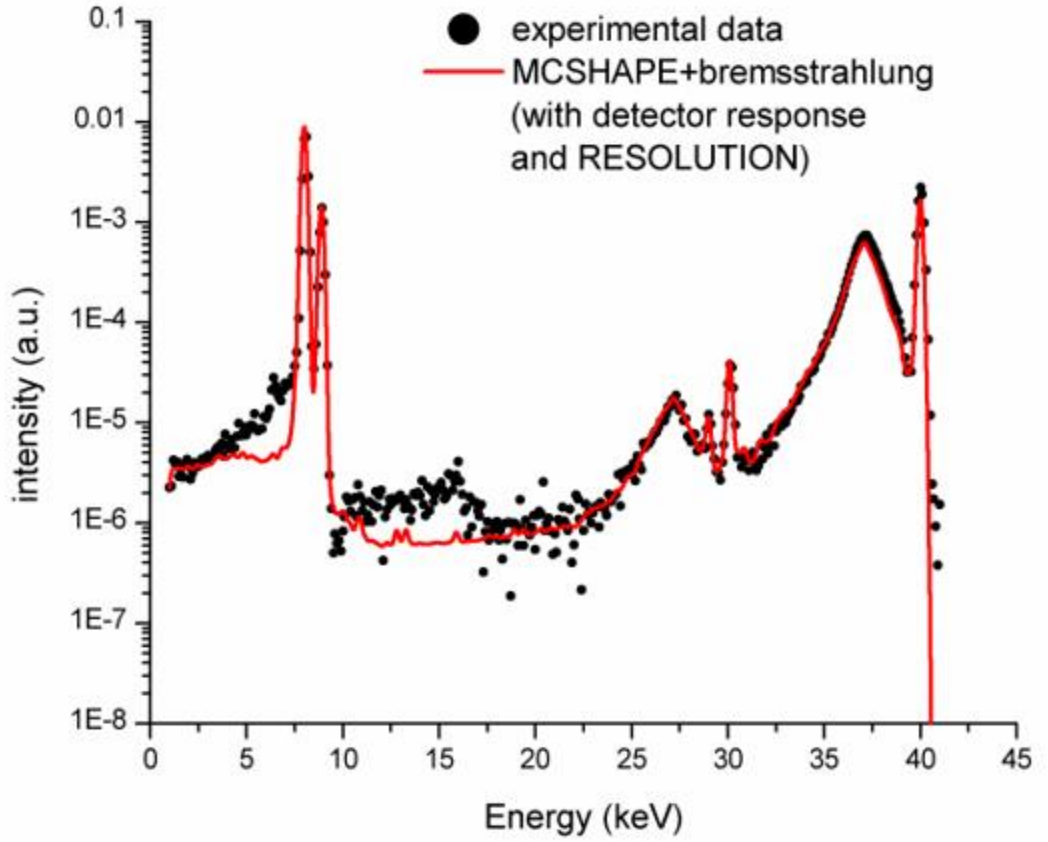
Detector resolution

In a first approximation it can be described by a normalized Gaussian

$$G(E_0, E) = \frac{0.9395}{FWHM(E_0)} \exp\left\{ -2.773 \frac{(E_0 - E)^2}{FWHM^2(E_0)} \right\}$$

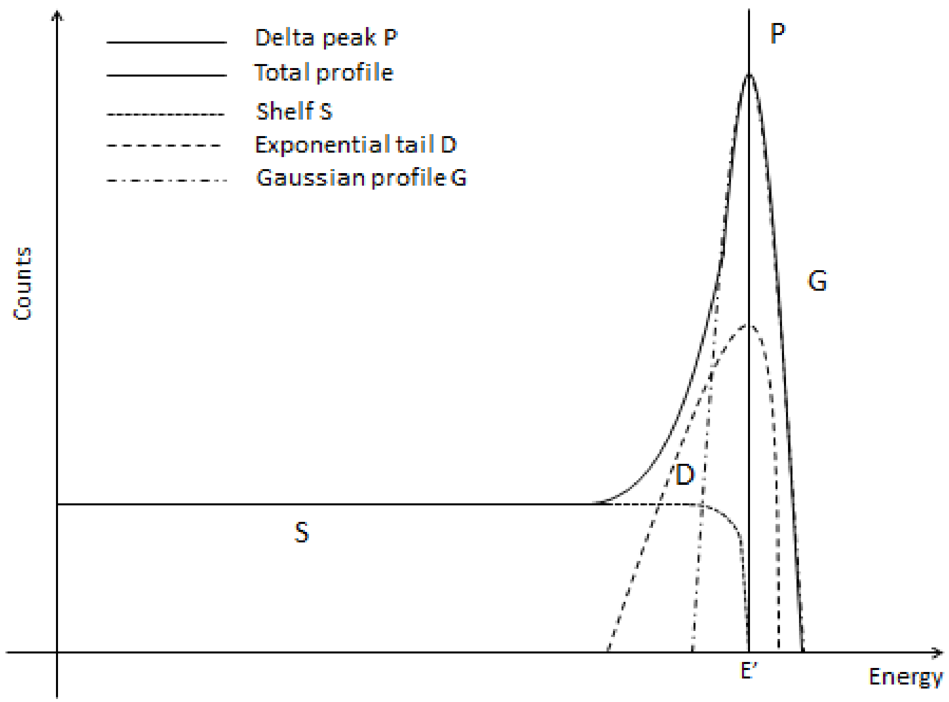
the FWHM is a function of energy

Complete simulation comprising detector response (Gaussian resolution)



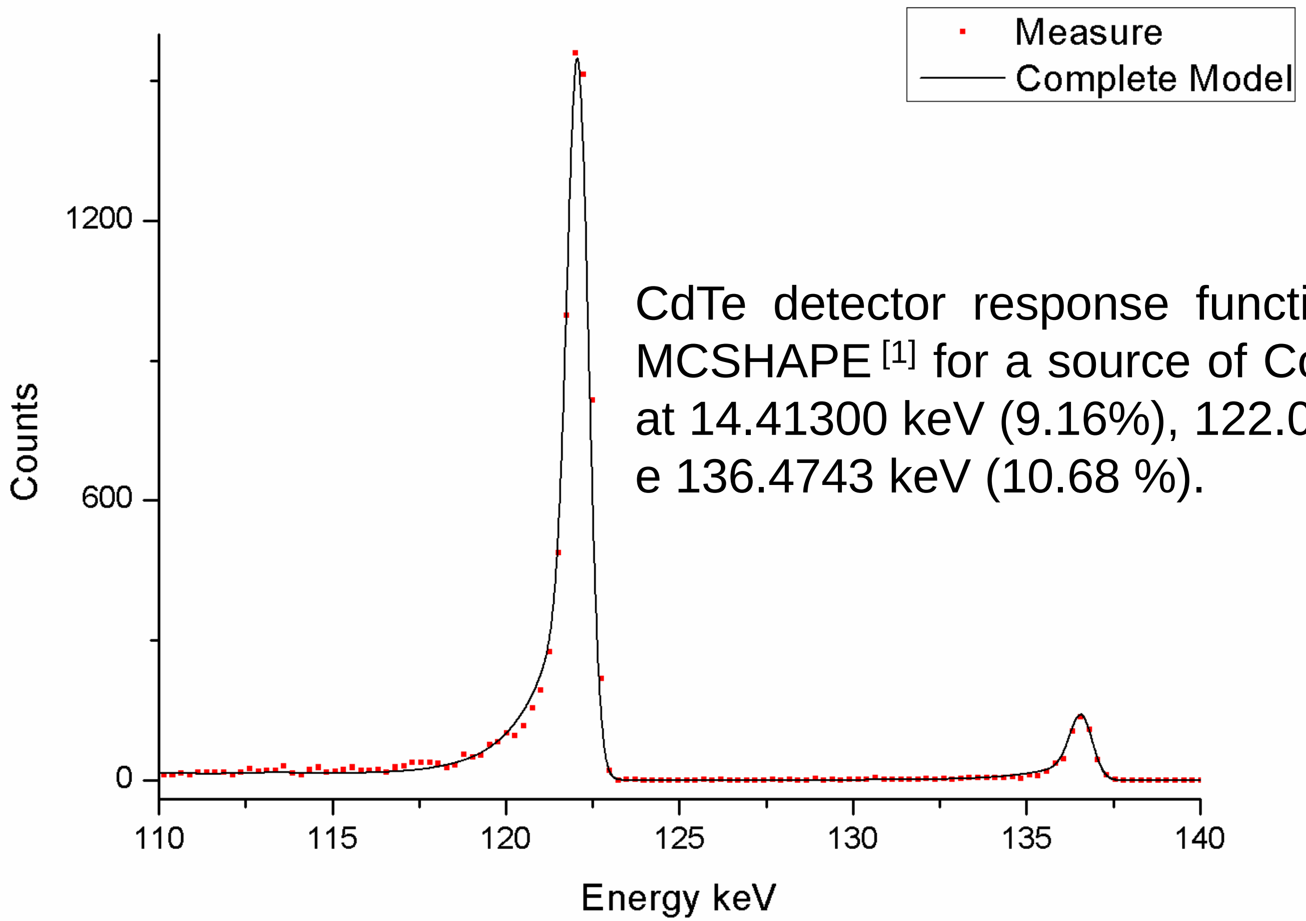
Resolution including incomplete charge collection

A more refined version of RESOLUTION includes, for a solid state detector, the effect of incomplete charge collection.



Tail and shelf below a Gaussian line.
Functional parameters are specific to a single detector

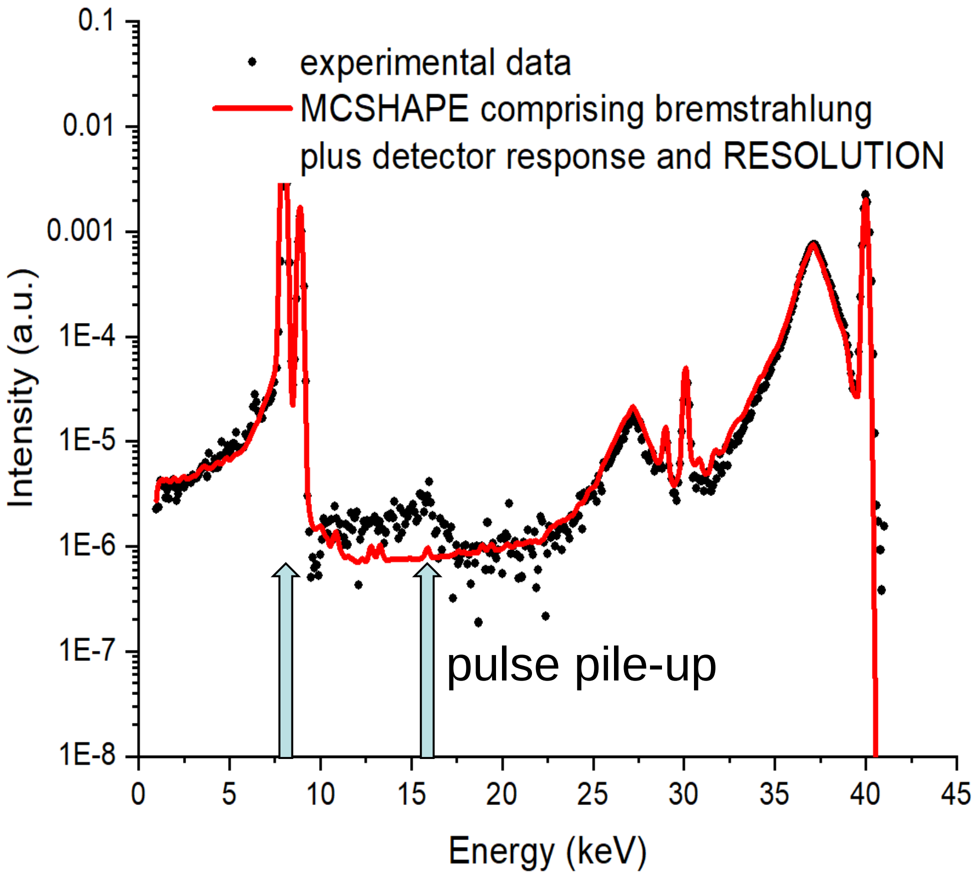
RESOLUTION Example: CdTe response function



CdTe detector response function computed with MCSHAPE [1] for a source of Co57, with emission at 14.41300 keV (9.16%), 122.0614 keV (85.60 %) e 136.4743 keV (10.68 %).

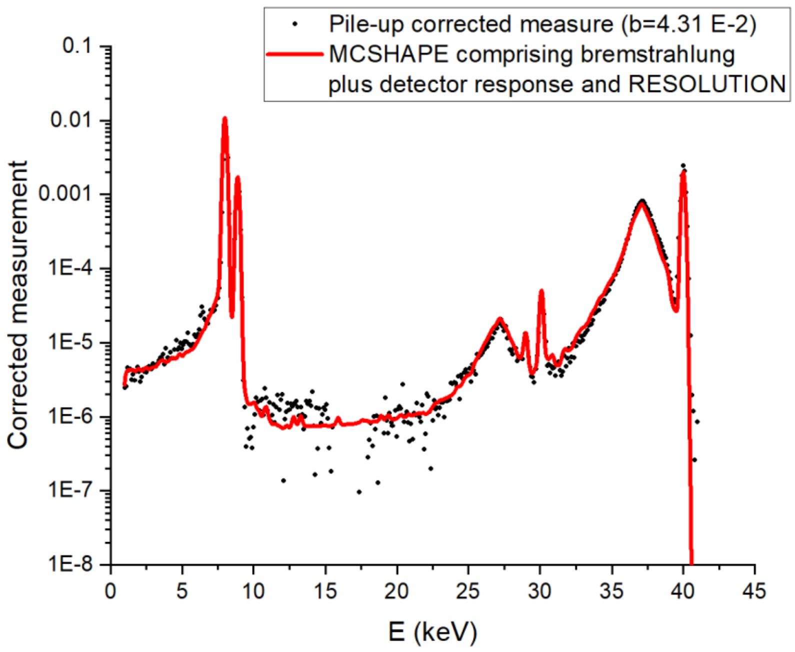
J. E. Fernández, V. Scot, L. Sabbatucci: A modeling tool for detector resolution and incomplete charge collection, X-ray Spectrom. 44 (2015)177-182.

Complete simulation comprising detector response (modified Gaussian resolution)



Detector parameters
2
2.9600001E-04
5.9999999E-02
1.0000000E-06
2.000000
0.2500000
7.000000
0.0000000E+00
0.0000000E+00
0.0000000E+00
1.5000000E-02
9.9999997E-06
0.0000000E+00
3.0000001E-06
4.9999999E-03
0.0000000E+00
0.0000000E+00

Pile-up correction vs complete simulation



The measure has been post corrected with the code DRPPU to reduce the pile-up effect.

L. Sabbatucci, J.E. Fernández, First principles pulse pile-up balance equation and fast deterministic solution. Rad. Phys. Chem. 137 (2017) 12-17.
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Conclusions

The complete explanation of an X-ray spectrum requires several steps:

1) To use an adequate simulation tool capable of describing the physics to a higher extent
2) To perform an adequate simulation of the detector response
3) To describe well the resolution of the detector
4) Sometimes you discover that pulse pile-up is still present and measurements need to be corrected

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Thank you for your attention!

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