Photon polarization treatment in Monte Carlo transport modelling

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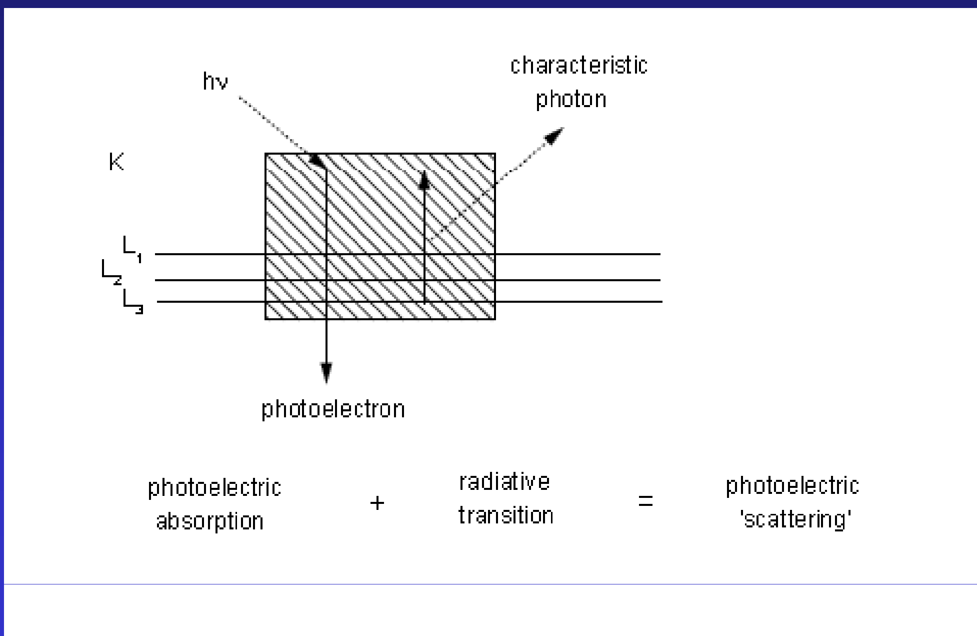
INTRODUCTION

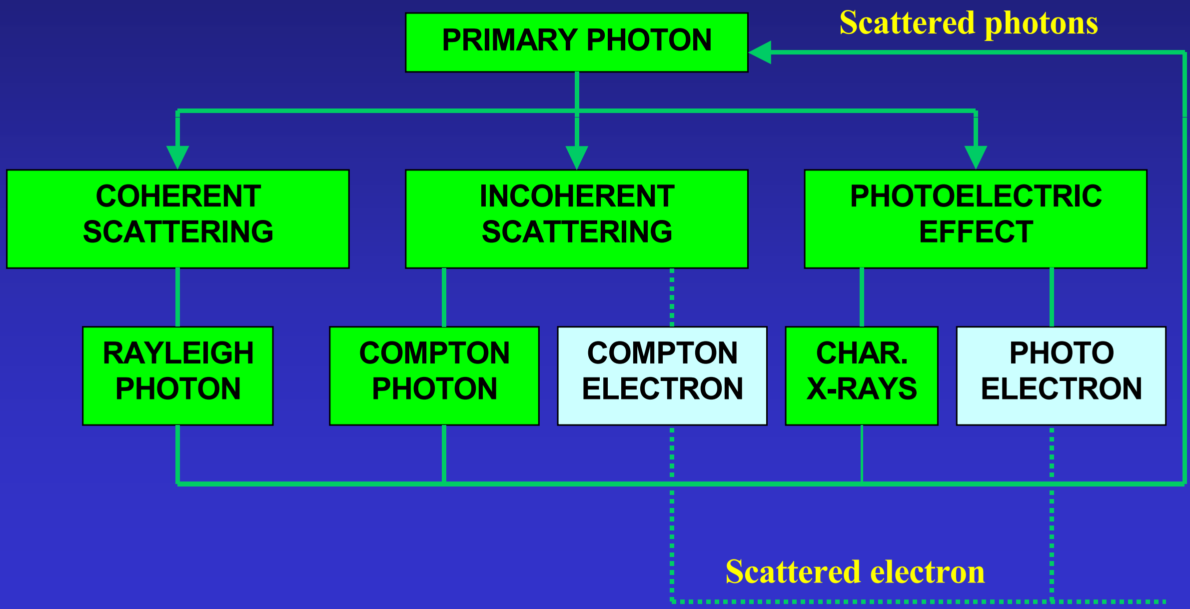
MULTIPLE SCATTERING

- 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 describe the influence of the prevailing interactions in the x-ray regime (**photoelectric effect**, **Compton scattering** and **Rayleigh scattering**)

Photoelectric effect as ‘scattering’



PREVAILING INTERACTIONS IN THE *X-RAY* REGIME



DESCRIPTION OF POLARIZATION

WHY POLARIZATION?

Polarization state → wave nature of photons

By considering polarization we improve the model of photon diffusion

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Without polarization photons are considered only as a particles

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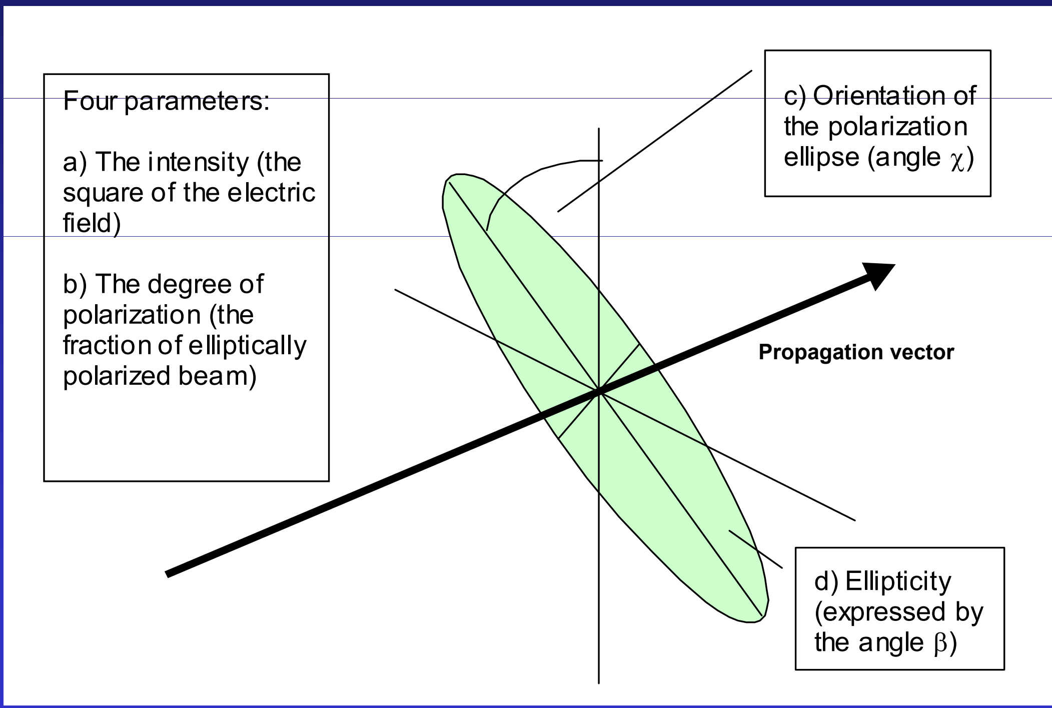
a good approximation in many cases, but not for phenomena that are influenced by their wave properties

Polarization state definition

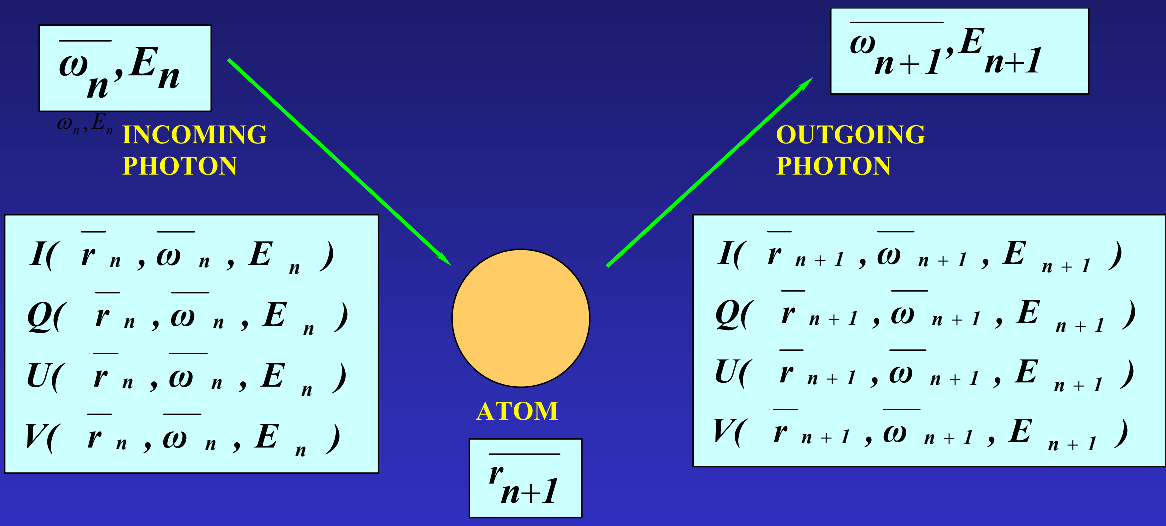


REPRESENTATION OF POLARIZED RADIATION

Stokes parameters I,Q,U,V (having the dimension of an intensity) can specify the physical magnitudes:

- **Intensity of the beam**
- **Degree of polarization**
- **Orientation of the ellipse of polarization**
- **Ellipticity**

COLLISION SCHEME



Modification of the polarization state due to a collision (Stokes representation)

TWO RELEVANT ASPECTS

- A collision always changes the polarization state
- The angular distribution for scattered unpolarized and polarized photons is different

PHOTON DIFFUSION IS DESCRIBED BY A "VECTOR" TRANSPORT EQUATION (THE 1-D EQUATION IS SHOWN HERE)

$$\eta \frac{\partial}{\partial z} \vec{f}^{(S)}(z, \vec{\varpi}, \lambda) = -\mu(\lambda) \vec{f}^{(S)}(z, \vec{\varpi}, \lambda) + \int_{4\pi} d\varpi' \int_0^\infty d\lambda' \mathrm{U}(z) \mathrm{H}^{(S)}(\vec{\varpi}, \lambda, \vec{\varpi}', \lambda') \vec{f}^{(S)}(z, \vec{\varpi}', \lambda') + \delta(z) \vec{S}^{(S)}(\vec{\varpi}, \lambda)$$

$$\bar{f} = \begin{bmatrix} I(z,\bar{\omega},\lambda) \\ Q(z,\bar{\omega},\lambda) \\ U(z,\bar{\omega},\lambda) \\ V(z,\bar{\omega},\lambda) \end{bmatrix}$$

VECTOR TRANSPORT EQUATION (CONT.)

where

$$\mathrm{H}^{(S)}(\vec{\varpi}, \lambda, \vec{\varpi}', \lambda') = \mathrm{L}^{(S)}(\pi - \Psi) \mathrm{K}^{(S)}(\vec{\varpi}, \lambda, \vec{\varpi}', \lambda') \mathrm{L}^{(S)}(-\Psi')$$

$H^{(S)}$ = kernel matrix in the meridian plane of reference

$K^{(S)}$ = scattering matrix in the scattering plane of reference

IMPORTANT PROPERTIES OF THE "VECTOR" TRANSPORT EQUATION

- Describes the evolution of the full polarization state (not only the intensity of the beam)
- Is linear (for the Stokes representation)
- Requires the simultaneous solution of the whole set of transport equations
- Cannot be transformed in a scalar equation !! (due to the coupling in the scattering term)

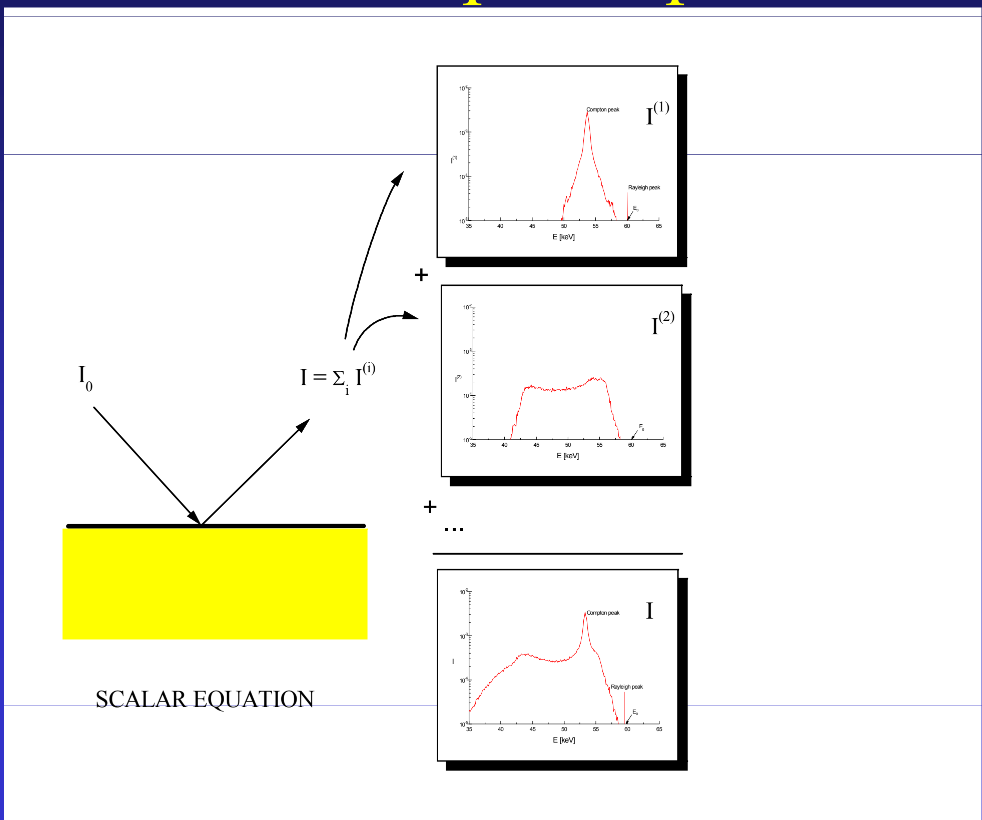
THEORETICAL MODELS

MODELS

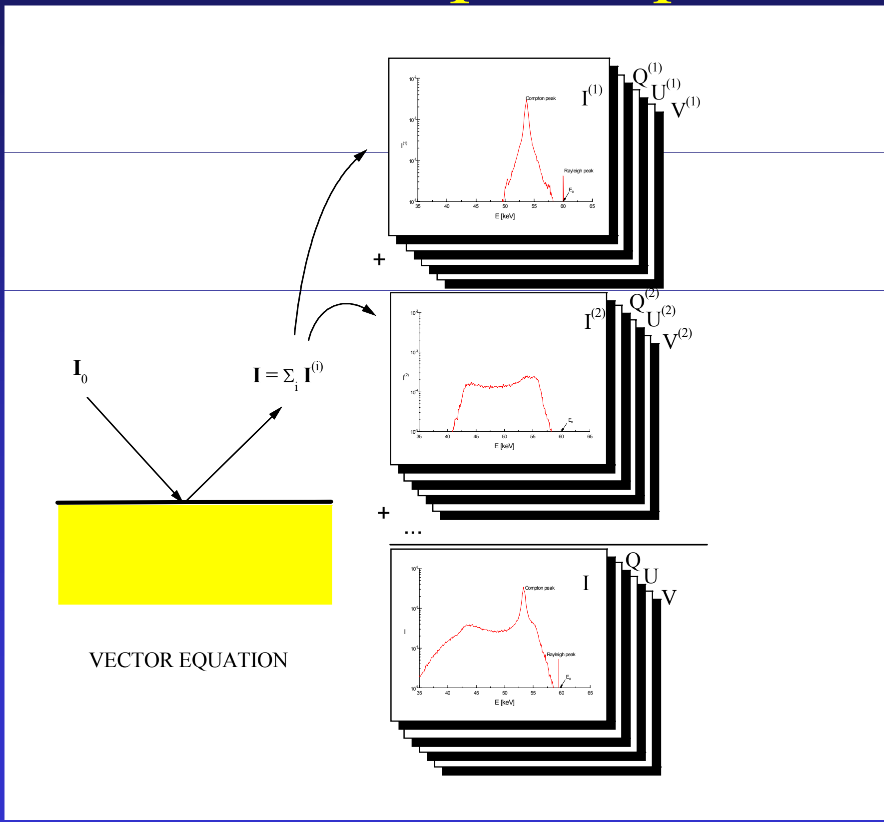
Different degrees of approximation to describe the diffusion photons:

- ***scalar model***: photons never modify an average polarization state
- ***vector model***: transport of photons starting with arbitrary polarization state

Scalar transport equation



Vector transport equation



THE CODES

SOLUTION TECHNIQUES

The transport equation is solved using an order-of-collisions scheme

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comparable results for deterministic and Monte Carlo solutions

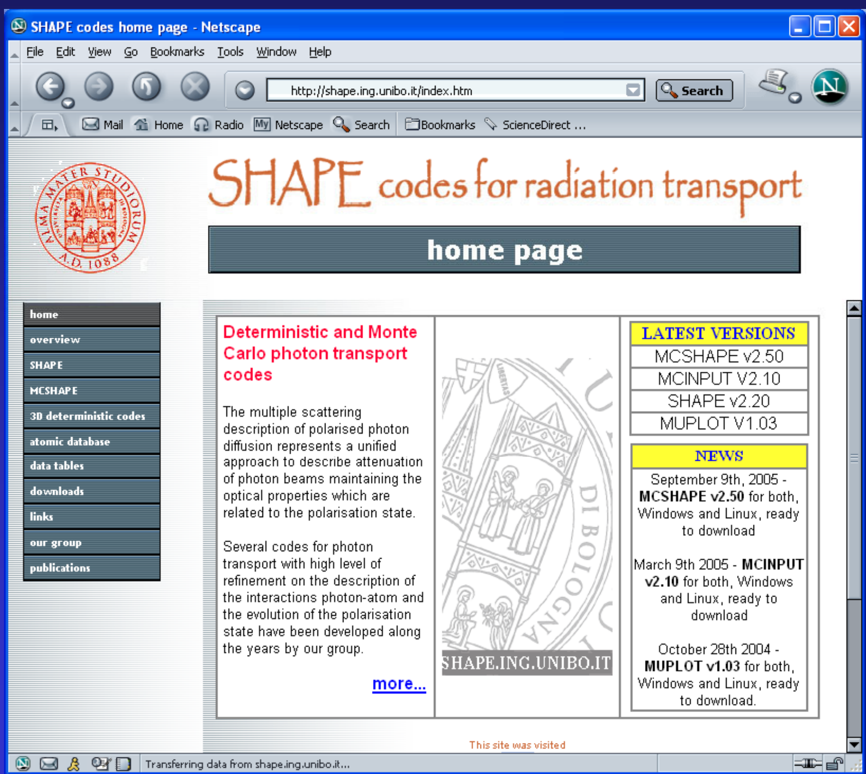
Deterministic vs. Monte Carlo

Solution	Deterministic	Monte Carlo (statistical)
Scope of the solution	Global	Local
Accuracy	↑	↓
Capability to describe the geometry	↓	↑
Number of collisions	↓	↑
Developed codes	SHAPE	MCSHAPE

CHARACTERISTICS OF THE CODE MCSHAPE

- Arbitrary polarization state of the source
- Multi-layer multi-component homogeneous targets
- Monochromatic or polychromatic source
- Doppler broadening (for Compton scattering)
- Full description of the polarization state
- N-collisions

WEB SITE http://shape.ing.unibo.it



These codes are going to be distributed by NEA Data Bank (OECD) and RSICC (US-DOE)

CODES COMPARISON (part 1: Physics)

Features	Details	SHAPE v2.20	D3DSHAPE v1.0	MCSHAPE v2.61
Physics	photoelectric effect	☒	☒	☒
	~1000 characteristic lines	☒	☒	☒
	line width	☒		☒
	atomic Rayleigh scattering	☒	☒	☒
	atomic Compton scattering	☒	☒	☒
	Compton profile	first collision only	☒	☒
	electron bremsstrahlung	foreseen in v3	☒	foreseen in v3
	open data bases	☒	☒	☒
	user defined elements			foreseen in v3
	infinite thickness targets	☒	☒	☒
	finite thickness targets		☒	☒
	multilayer targets			☒
	polarization representation	Stokes		Stokes
	source polarization state	**linear/ unpolarised**	unpolarised	**arbitrary**
	calculated spectrum	intensity component only		**full polarization state**
	monochromatic source	☒	☒	☒
	polychromatic source	postprocessor		☒
	external detector	solid state Si/Ge		foreseen in v3
	reflection geometry	☒	☒	☒
	transmission geometry			☒

UNIQUE FEATURES!

CODES COMPARISON (part 2: model and programming)

Features	Details	SHAPE v2.20	D3DSHAPE v1.0	MCSHAPE v2.61
Miscellaneous	selective computation of single interaction chains	☒	partial	partial
Transport model	particle	photons	photons / electrons	photons
	scalar equation	☒	☒	
	vector equation	☒		☒
	solution	deterministic	deterministic	Monte Carlo
	collisions	3	3	100
	1-D spatial geometry	☒		☒
	3-D spatial geometry		☒	**using MCSHAPE3D**
Code	language	DELPHI	FORTRAN 77	FORTRAN 90
	additional libraries	graphics		WINTERACTER
	platform	WINDOWS	LINUX	WINDOWS / LINUX
	distribution	web site	alpha testing	web site
	parallelization			MPICH v1.0 (only Linux)
Applications	spectroscopy	☒	☒	☒
	analytical chemistry	☒	☒	☒
	radiation metrology	☒	☒	☒
	x-ray optics			with MCSHAPE3D
	dosimetry		foreseen in v2	with MCSHAPE3D
	radiation transport teaching	☒	☒	☒

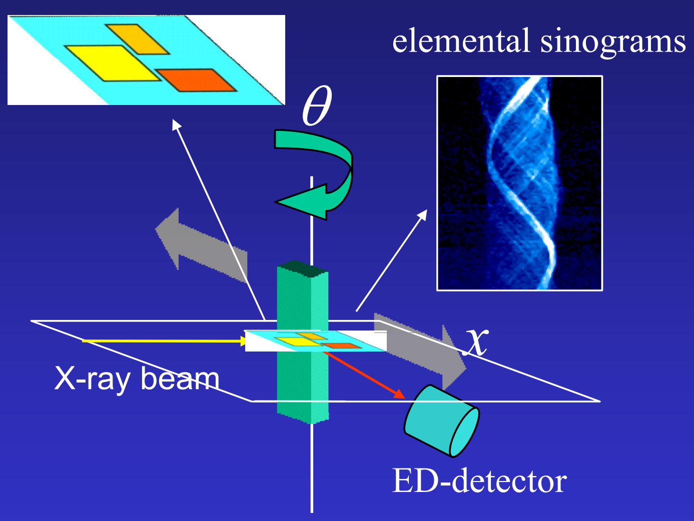
NEW!!
3D version
of MCSHAPE

3D - MCSHAPE

- TARGET:
  - heterogeneus target -> *VOXEL MODEL*
  - interfaced with GAMBIT (FLUENT environment)
- SOURCE:
  - uniform source on a disk
  - uniform source on a rectangle
  - point source
- DETECTOR:
  - disk detector
  - rectangular detector
  - plane infinite detector
  - Collimator in front of the detector

V. Scot, J.E. Fernandez, L. Vincze, K. Janssens, submitted to NIM-B (2005)

3D – MCSHAPE: XRF Tomography

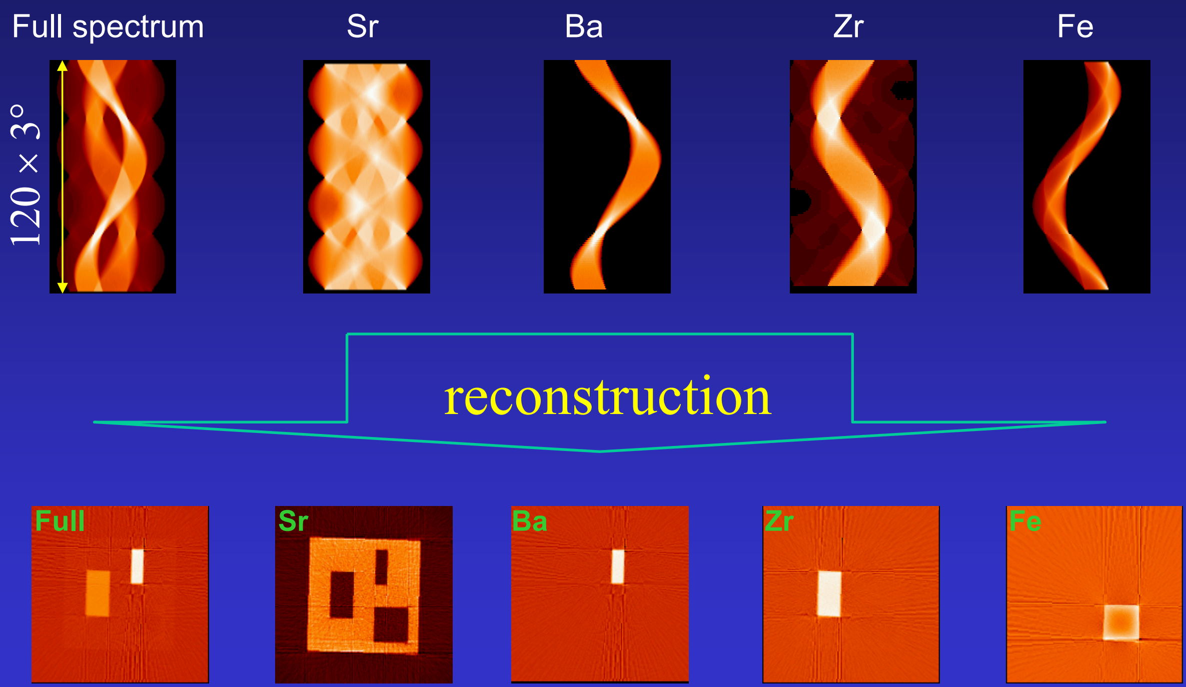


- **Total dimension**: 0.1 x 0.1 x 0.01 cm
- **Composition**:
  Region **A**: **C** + **0.1%Sr**, ρ = 1.0 g/cm^3
  Other elements:
  Region **B**: **SiO_2** + **1%Fe**, ρ = 2.23 g/cm^3
  Region **C**: **SiO_2** + **1%Ba**, ρ = 2.23 g/cm^3
  Region **D**: **SiO_2** + **1%Zr**, ρ = 2.23 g/cm^3

- **Source**:
  energy: 59.54 keV
  type: point source
  unpolarized
- **Detector**:
  type: disk with 30 mm^2 of total area
  no collimator

V. Scot, J.E. Fernandez, L. Vincze, K. Janssens, submitted to NIM-B (2005)

3D – MCSHAPE: XRF Tomography



V. Scot, J.E. Fernandez, L. Vincze, K. Janssens, submitted to NIM-B (2005)

CONCLUSIONS

CONCLUSIONS

- The vector MC code MCSHAPE give:

  (for infinite or finite, and single or multi-layer multi-component targets and recently 3D targets)

  - a detailed description of multiple scattering of the prevailing interactions in the x-ray regime

  - a full analysis of the final state of polarization at each collision number

CONCLUSIONS (cont.)

- Good agreement with experimental data has been obtained for both, unpolarized and polarized sources
- Foreseen applications in several fields, specially for x- or γ-ray dosimetry

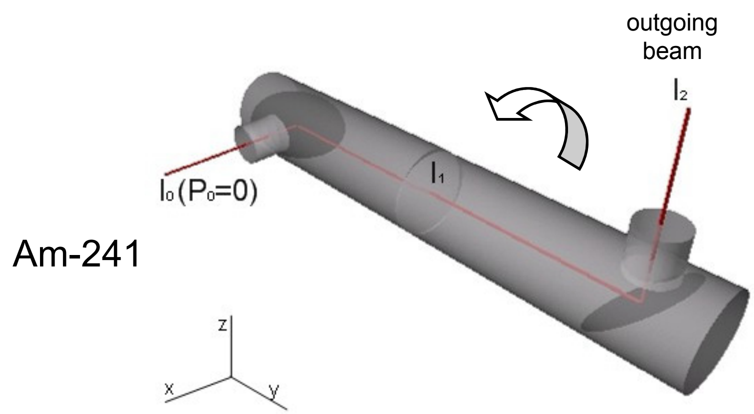
Example 1: polarised source vs unpolarised source

First target (polariser): water target

Second target (specimen): Water (99 %) – Ho (1 %)

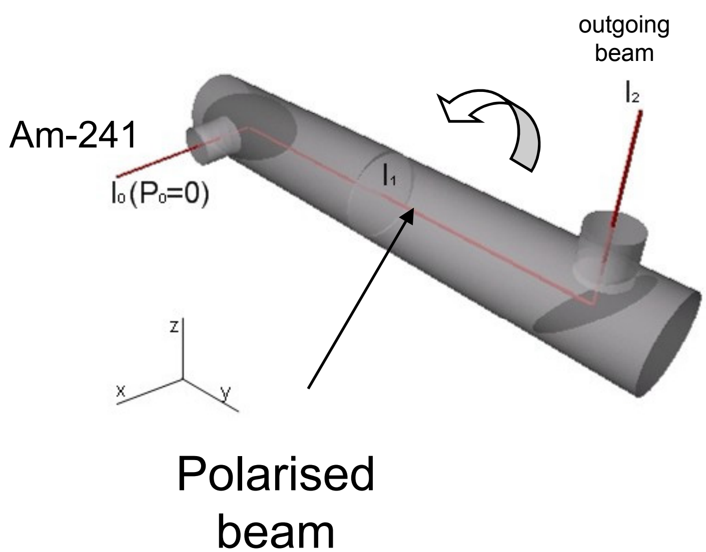
Source: Am-241 γ-source (59.54 keV)
unpolarised

Geometry: incidence 45°
(at each taret) take-off 45°



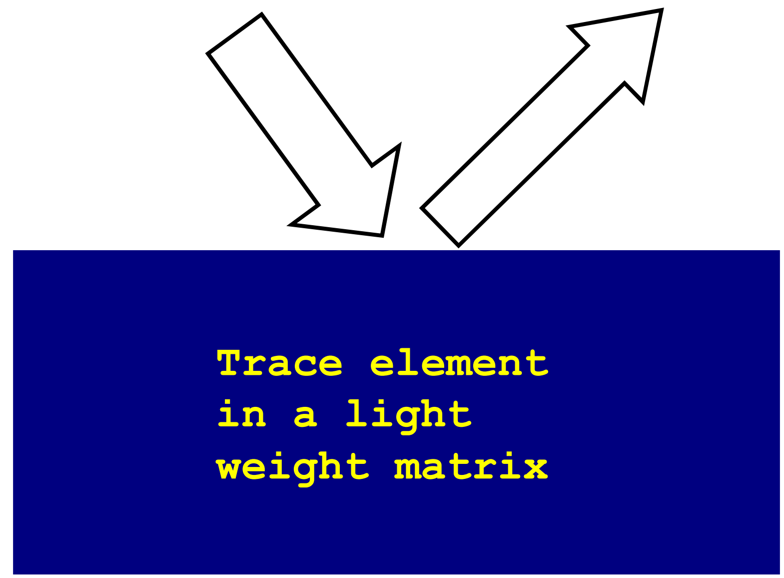
polarised source vs unpolarised source

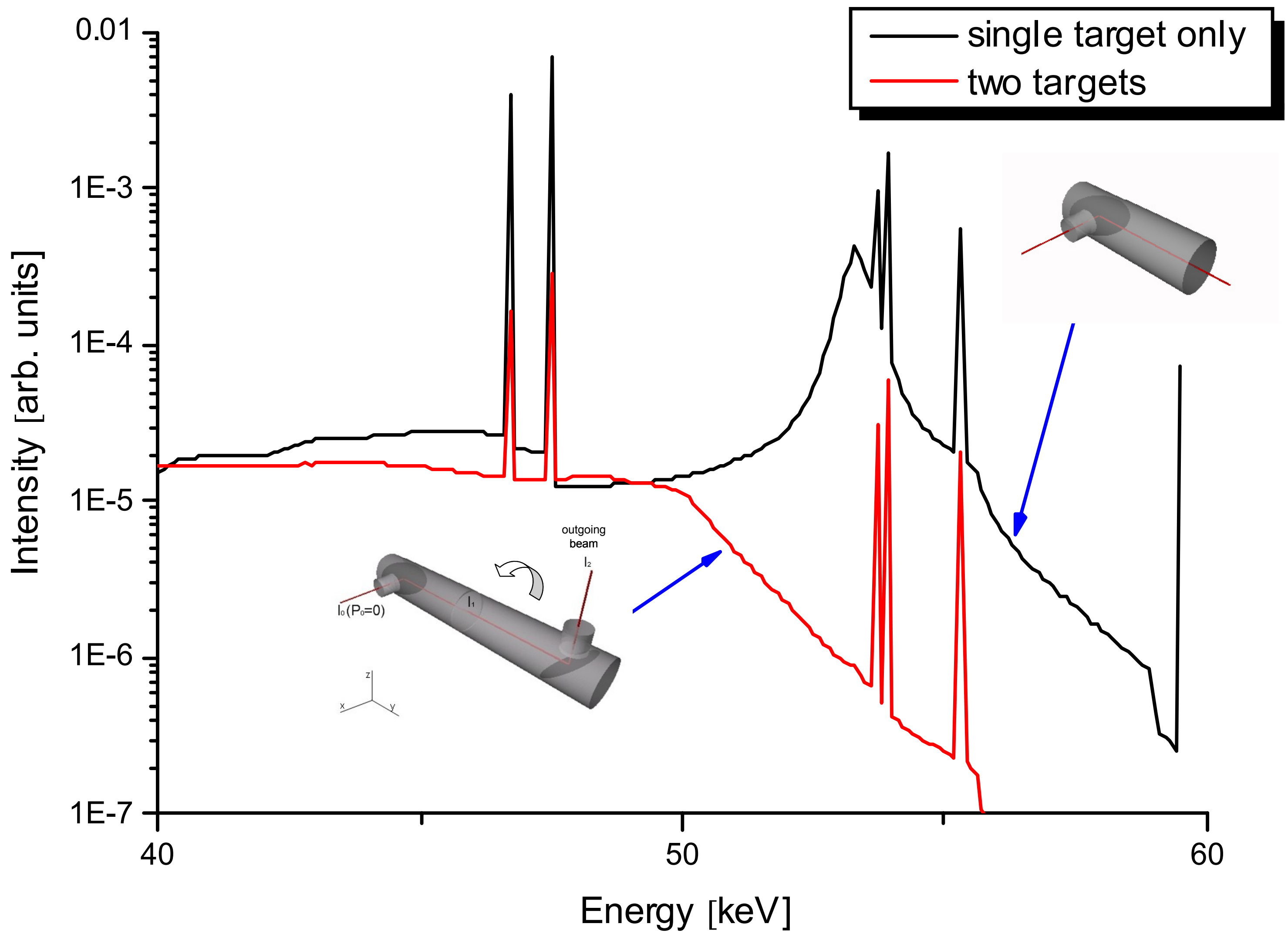
using scattering to polarise the beam



vs

Am-241
unpolarised beam




single target only
two targets
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
Intensity [arb. units]
40
50
60
Energy [keV]
outgoing
beam
I_2
I_1
$I_0(P_0=0)$
z
x
y

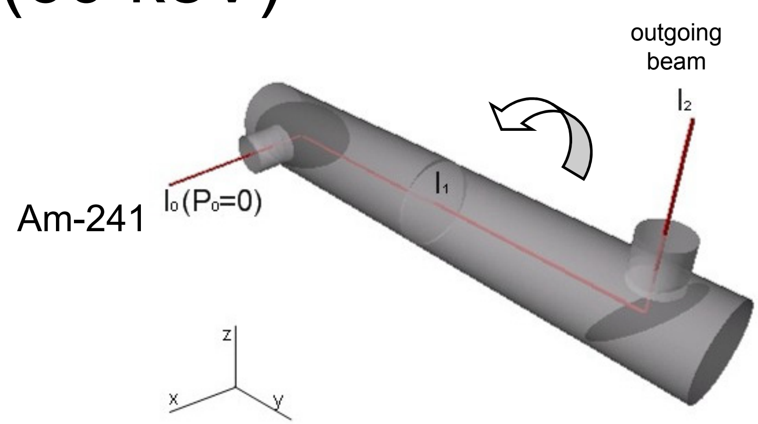
Example 2: rotational study of multiple scattering in the 2nd target

First target (polariser): water target

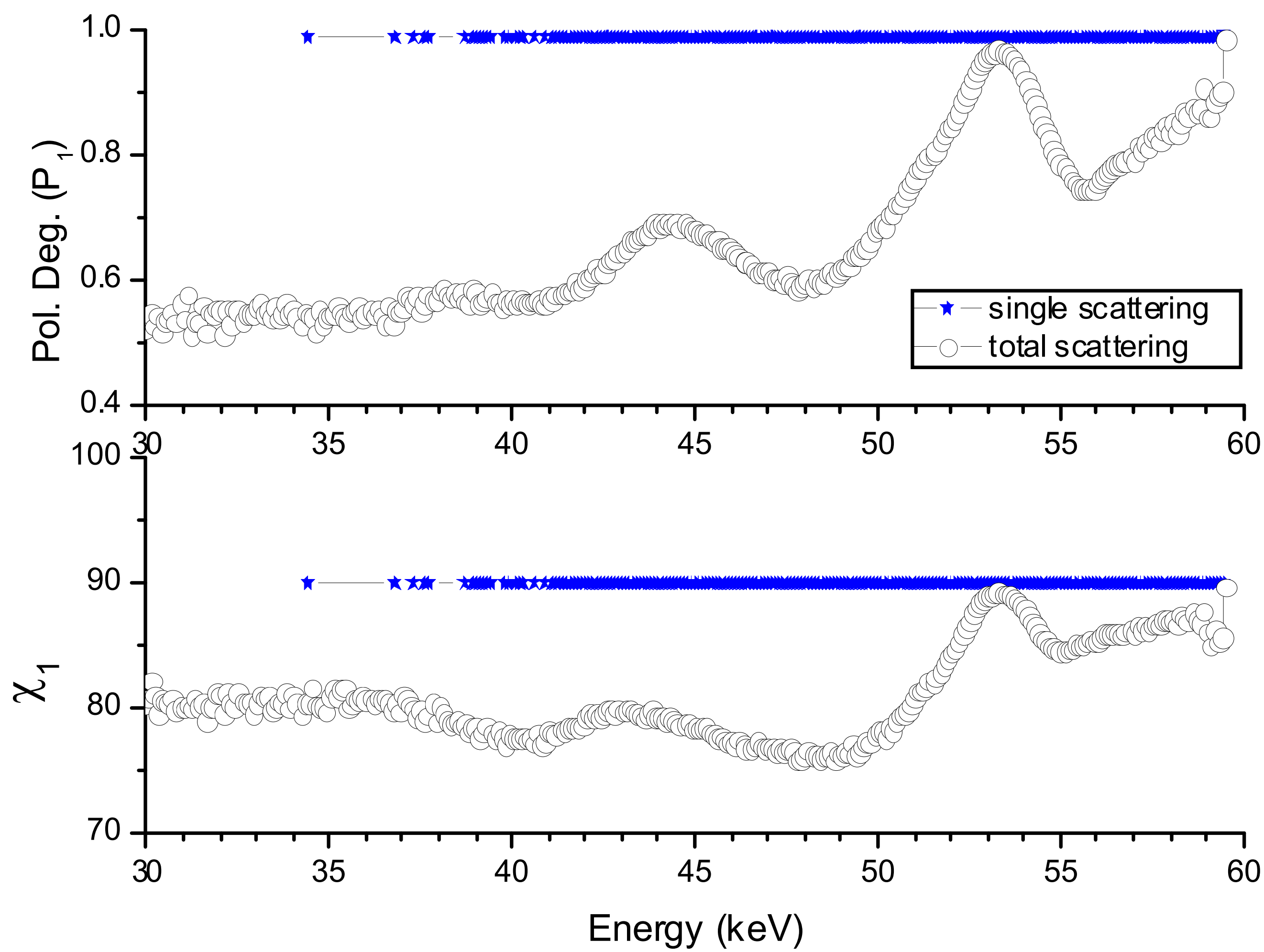
Second target (specimen): water target

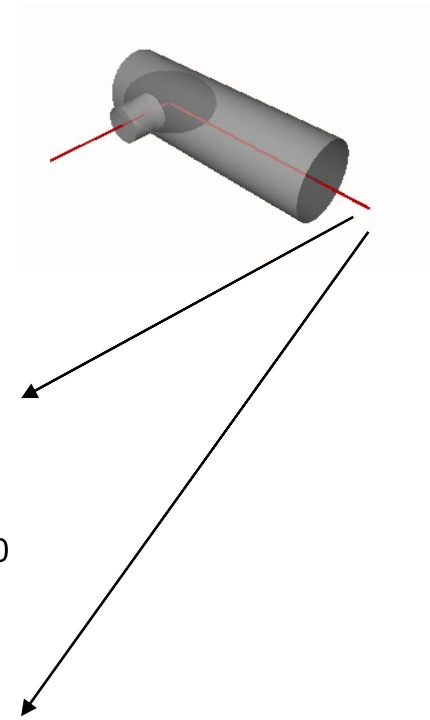
Source: Am-241 γ-source (60 keV)
unpolarised

Geometry: incidence 45°
take-off 45°

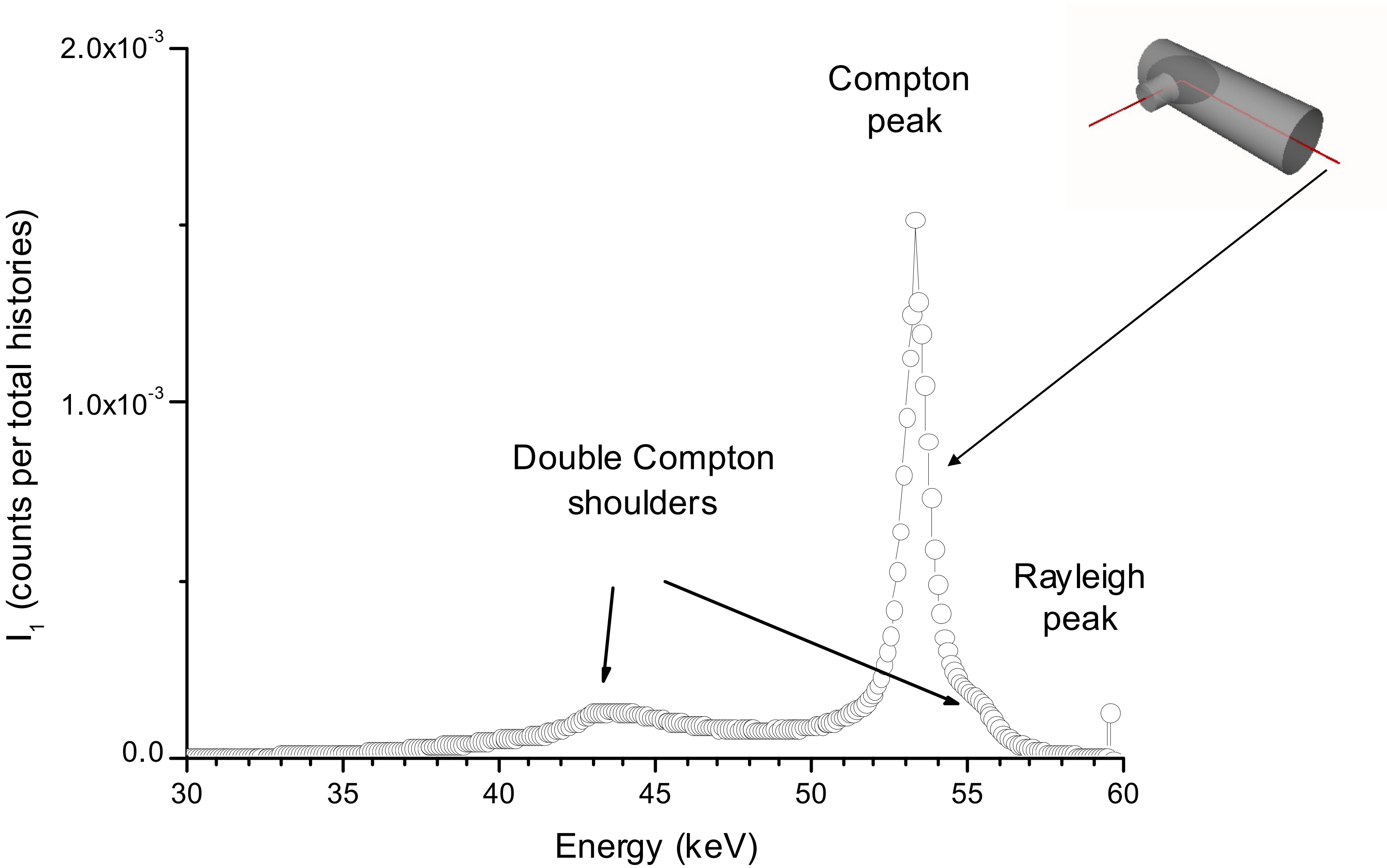


Polarisation degree and electrical field vector after scattering in the 1st target



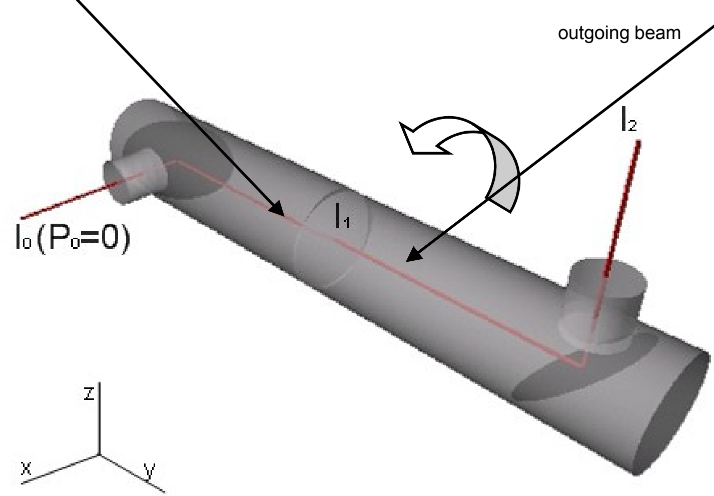


Scatter spectrum after the 1st target

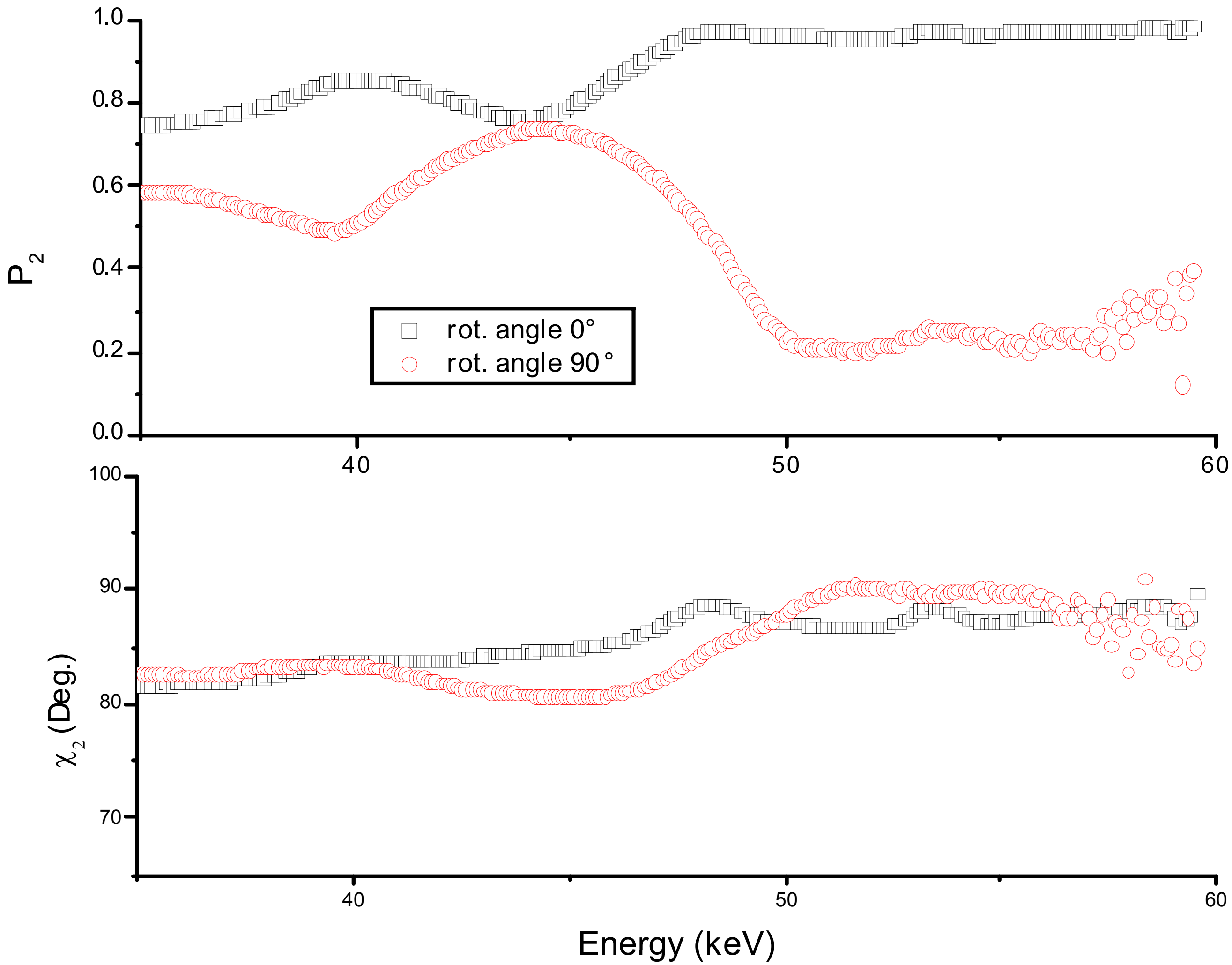


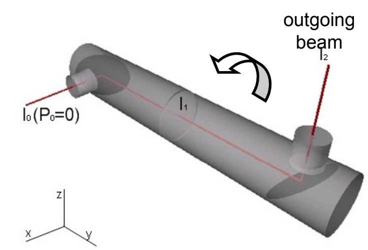
Two-target device

Scatter in the 1st target → Source for the second target

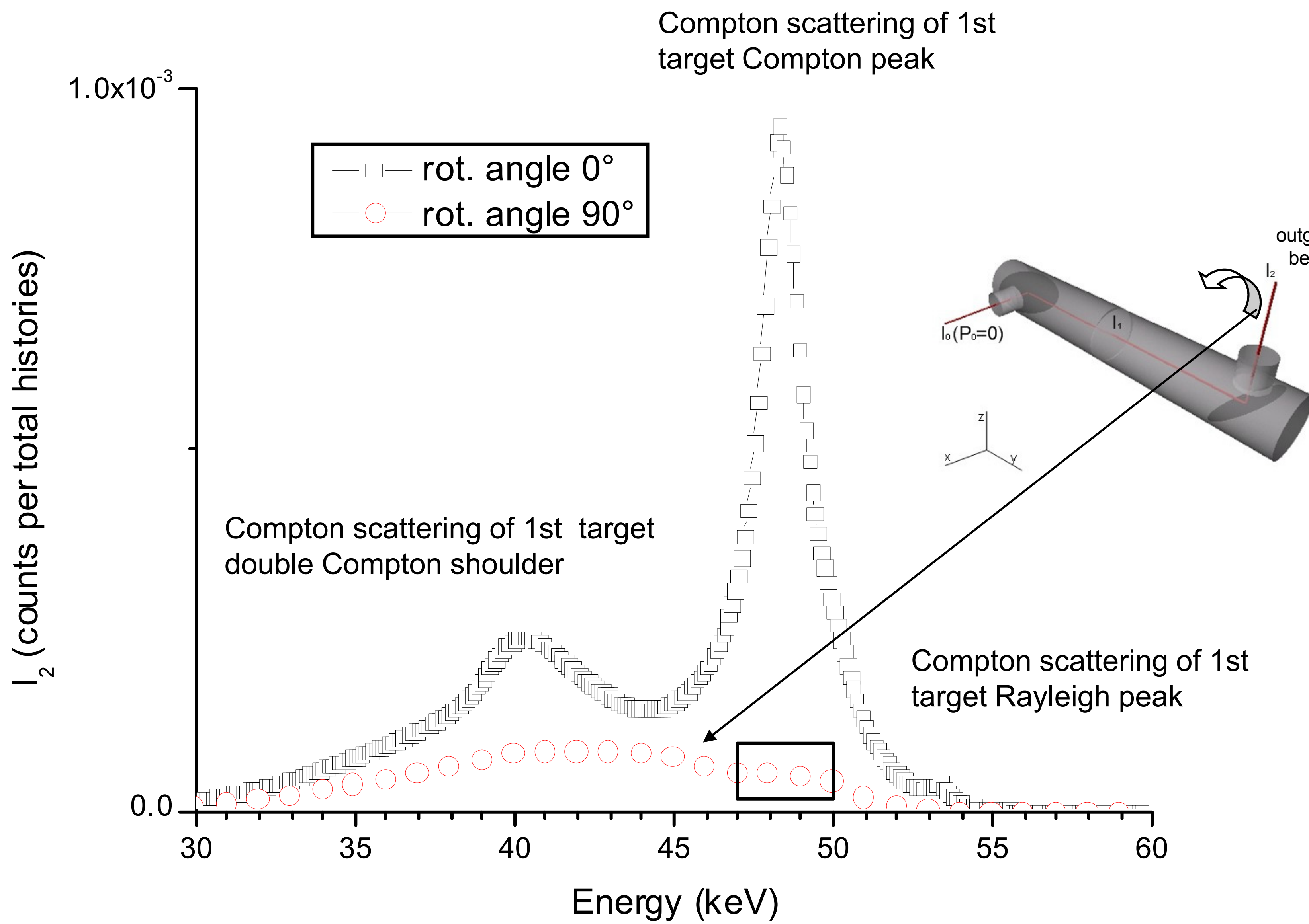


Polarisation degree and electrical field vector after scatter in the 2nd target

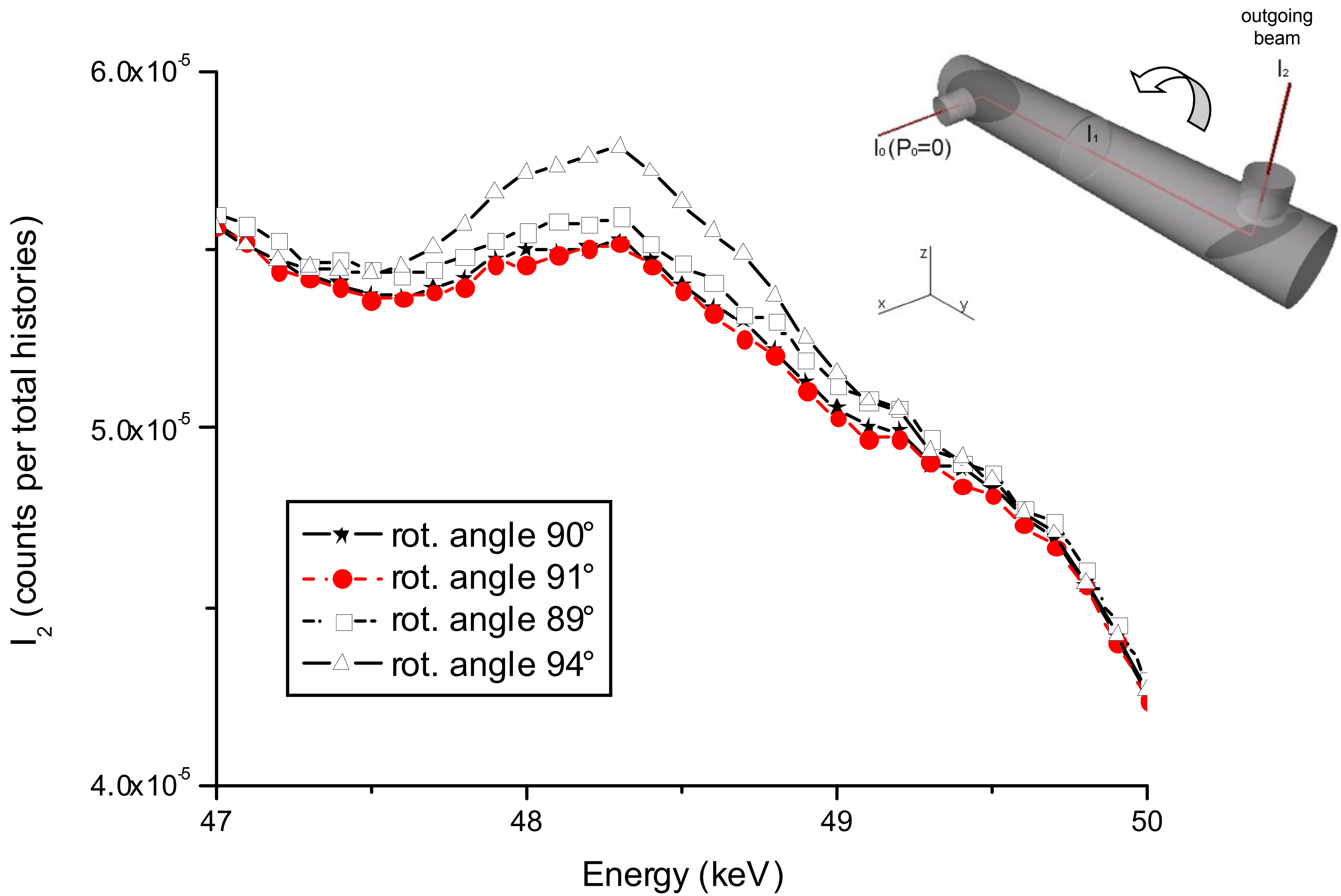




Scatter spectrum after the 2nd target



Zoomed view: multiple scattering background on 2° target for several angles



Conclusions

- A model with polarization is necessary to describe properly scatter (i.e. the angular distribution) at this geometry
- Multiple scattering does not behave as the first scattering

Future developments

- More studies are necessary to characterize the influence of polarization on the radiation field in dosimetry applications