



# Selective amplification of x-rays in the energy range 50-65 keV

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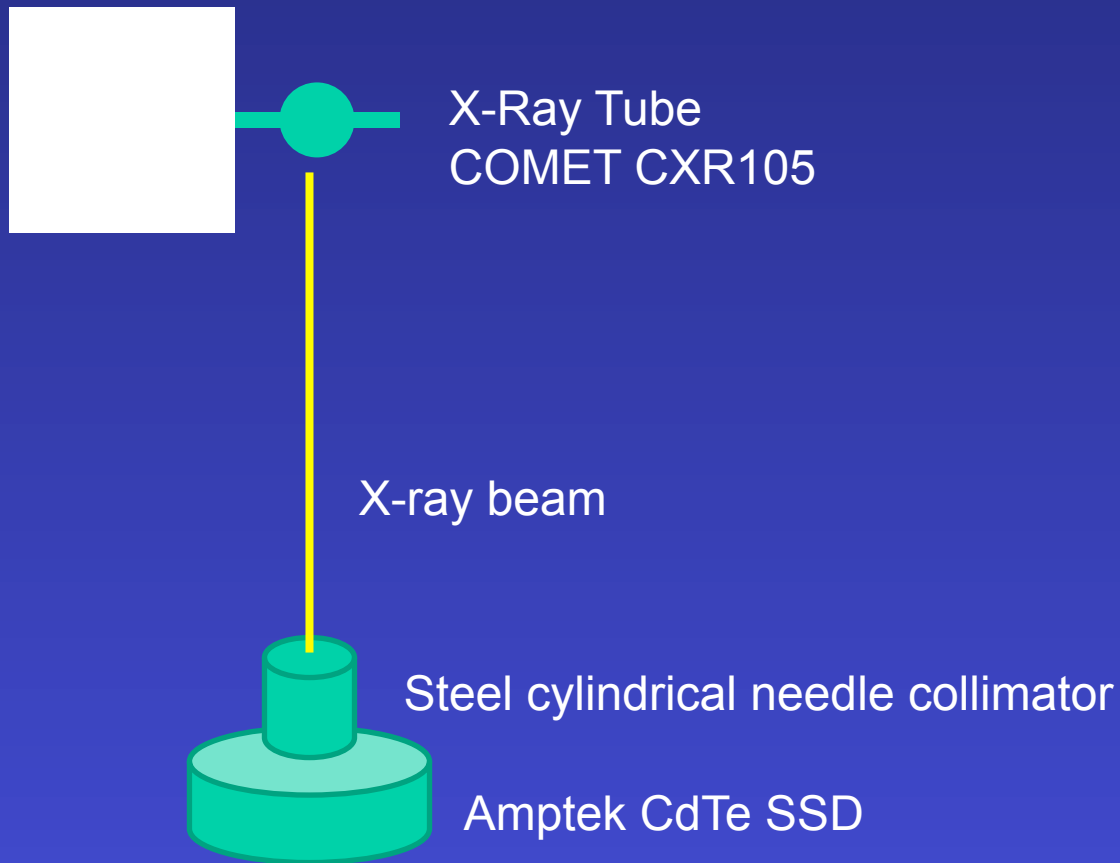
# OUTLOOK

- Experimental results
- Theoretical Model
  - Description of Polarization
  - Scalar and Vector Models
  - The Codes
- Interpretation of Experimental Data

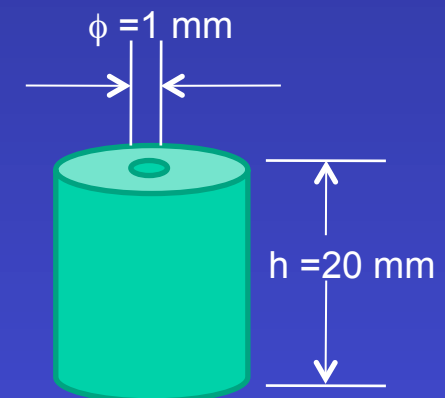
# EXPERIMENTAL RESULTS

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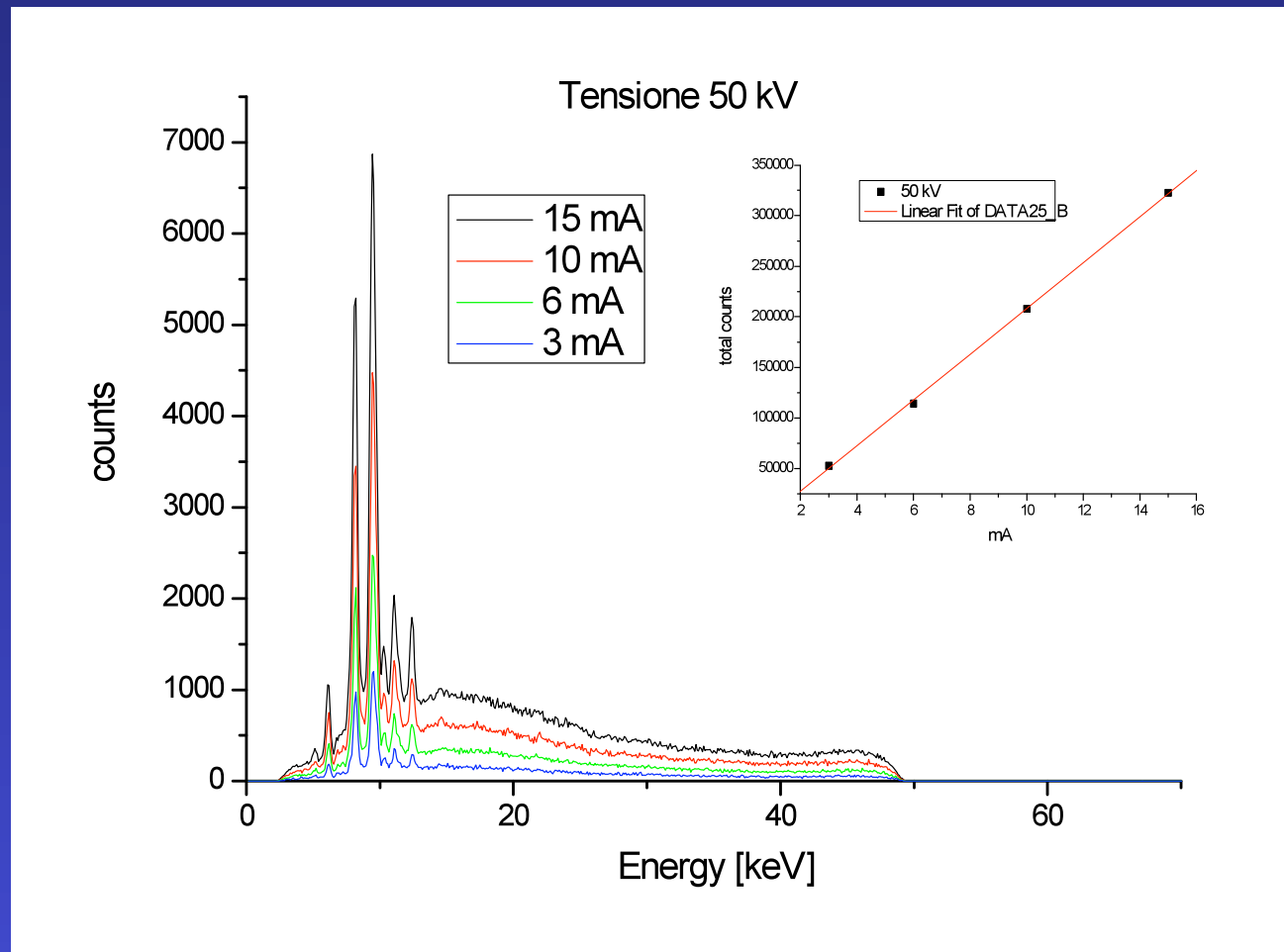
# Direct Measurement of X-Ray Spectra



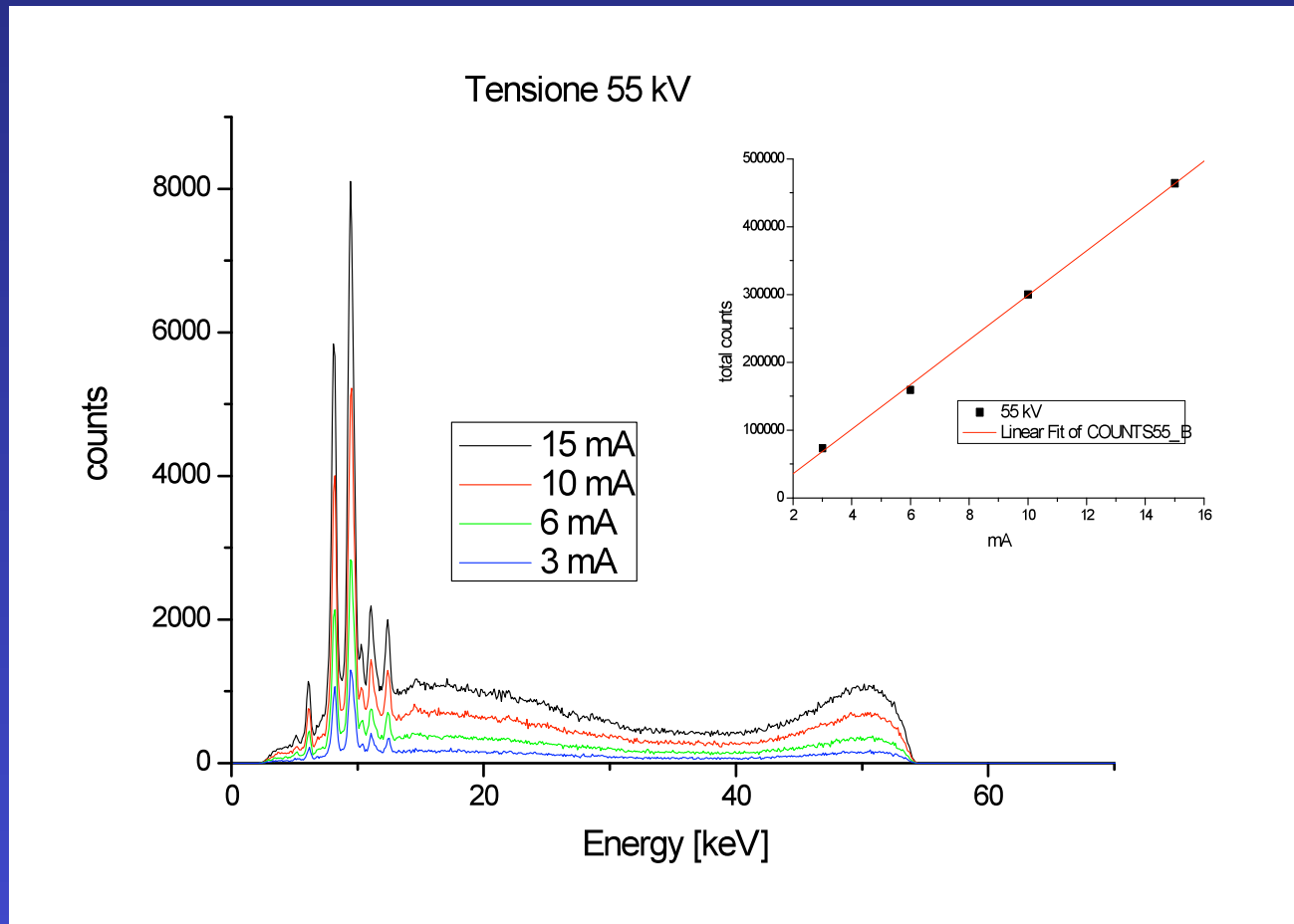
## Set-up #1 Cylindrical Collimator



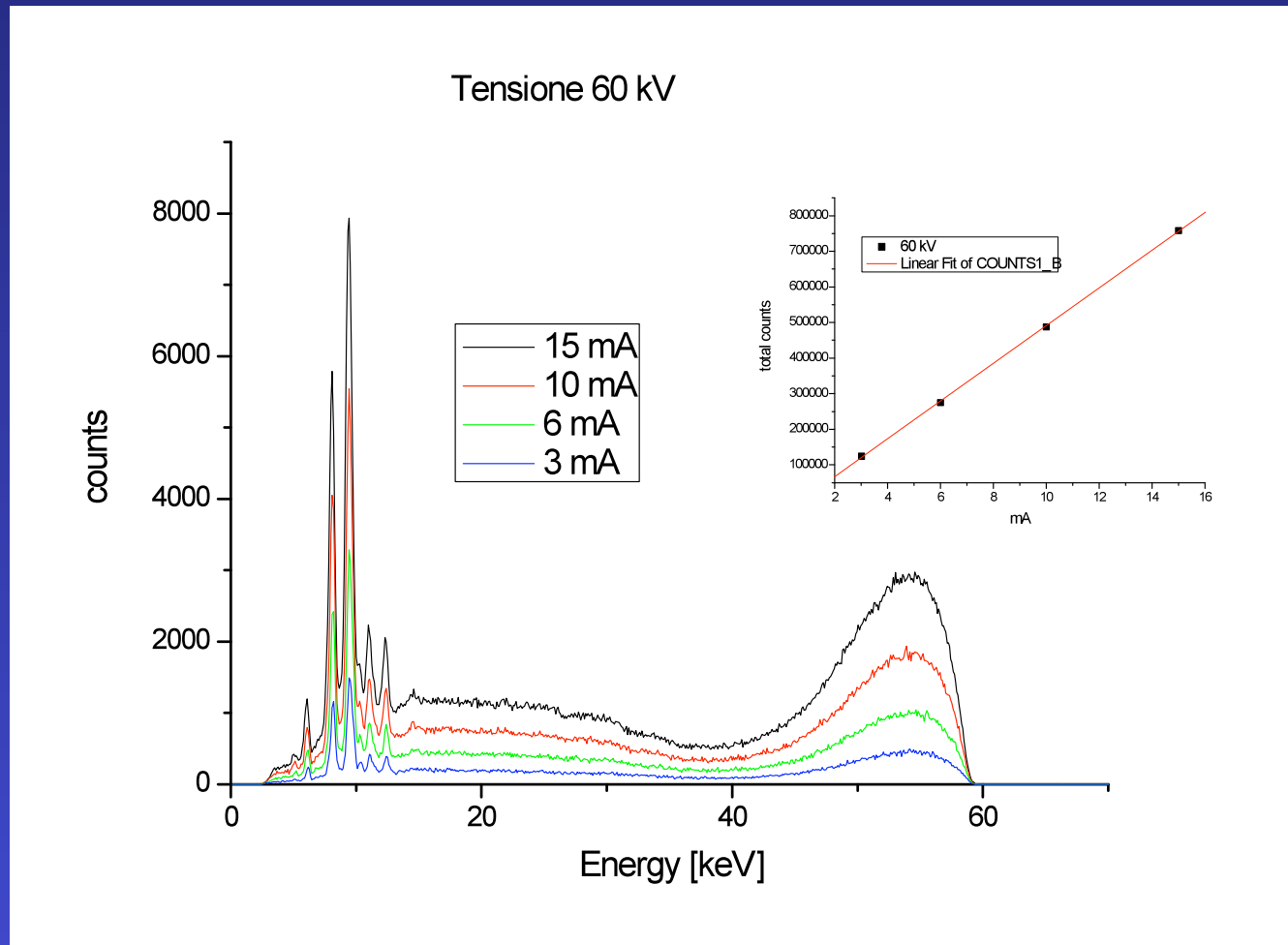
# 50 kV



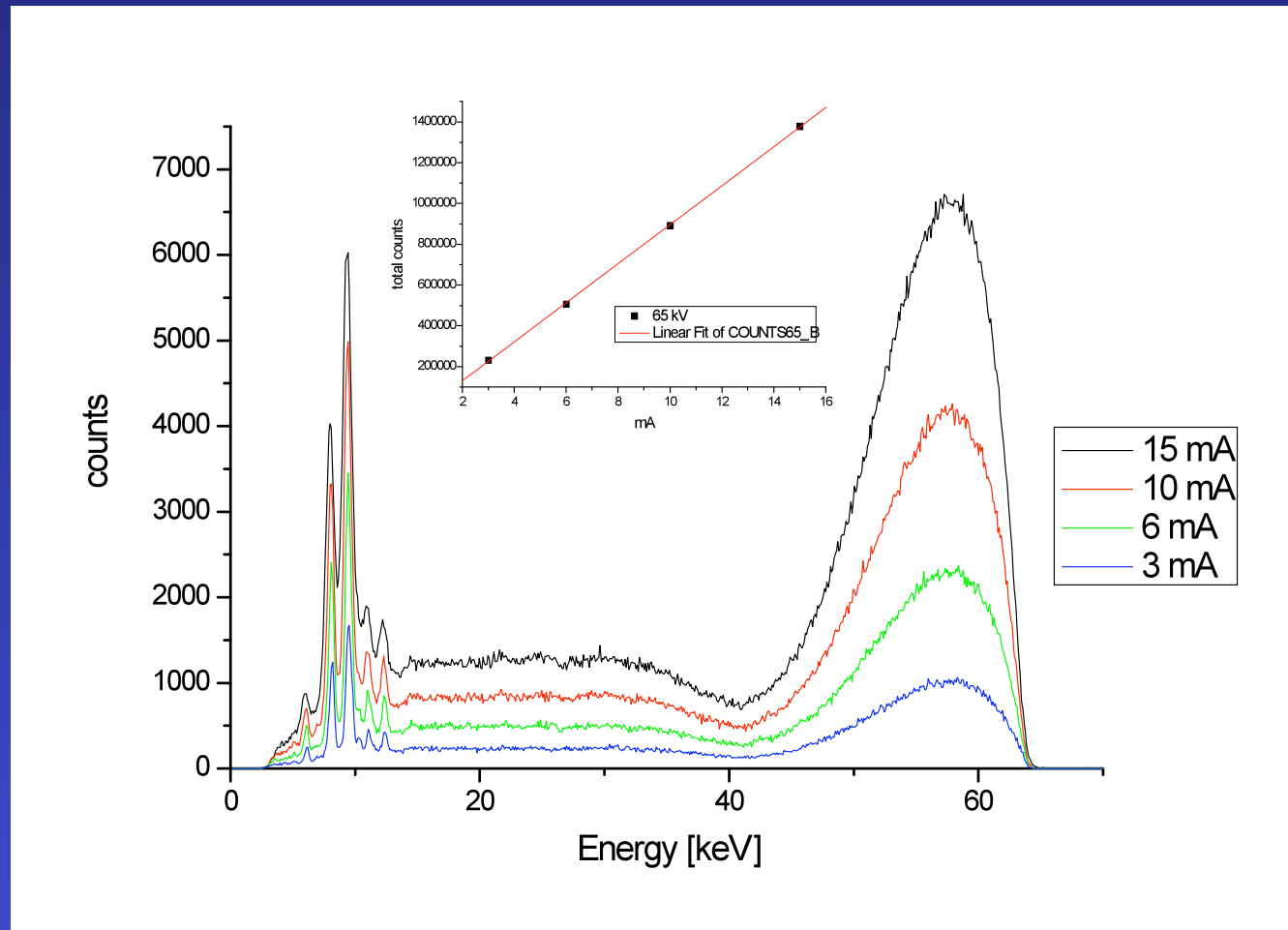
# 55 kV



# 60 kV

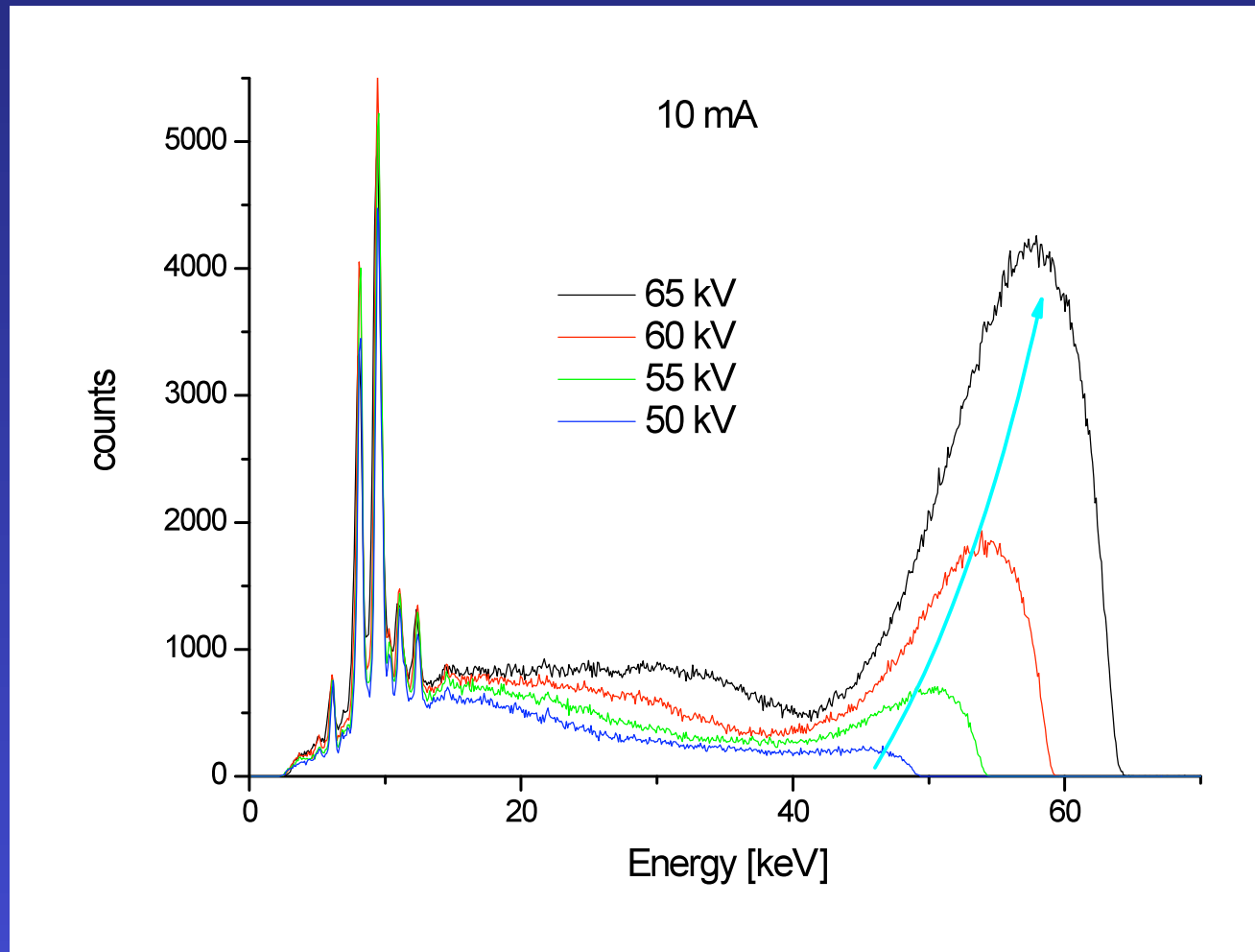


# 65 kV

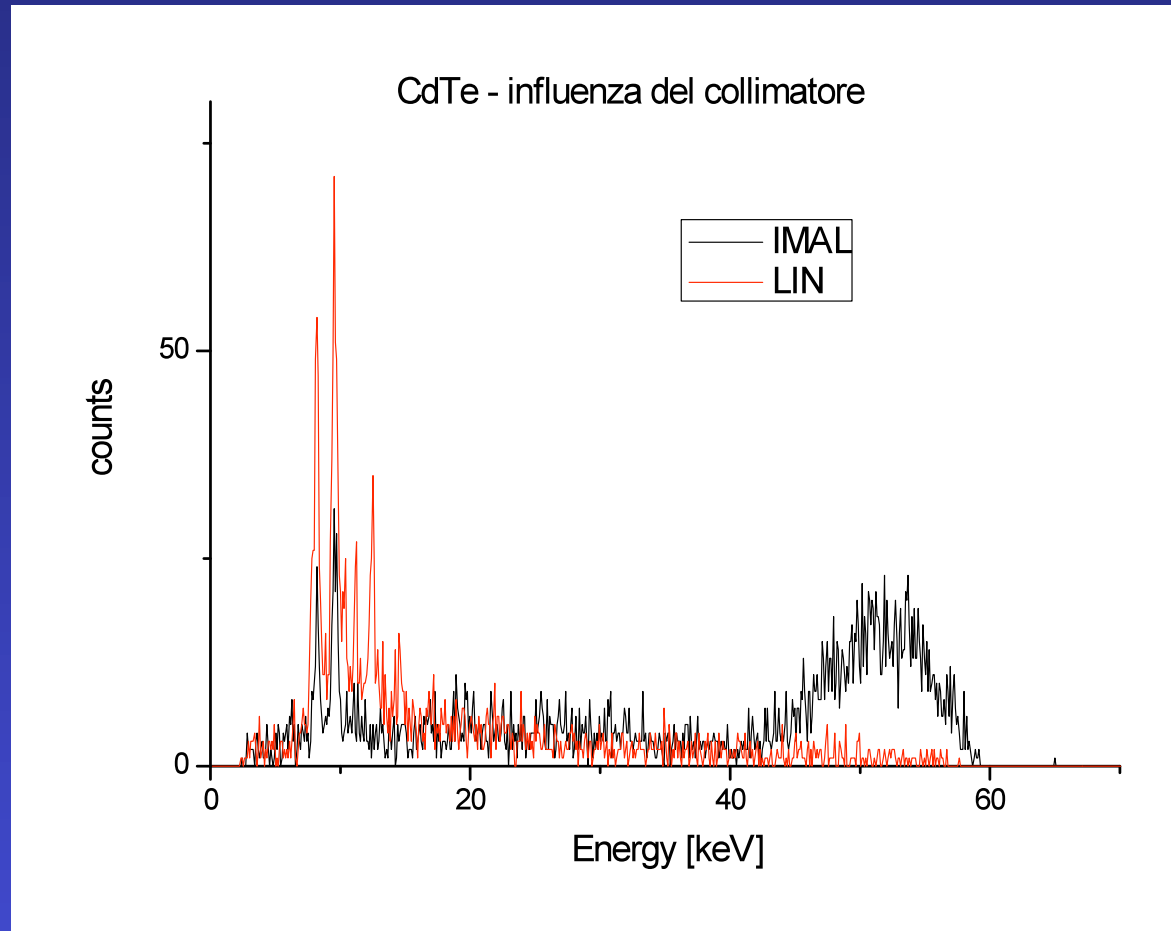




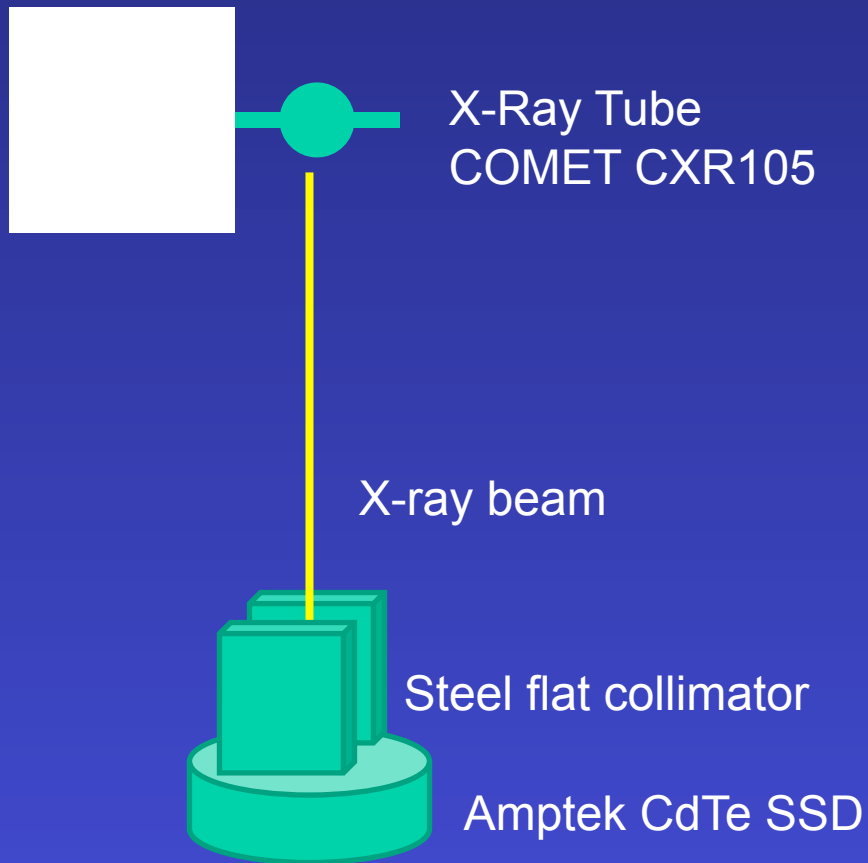
# Variation with KV



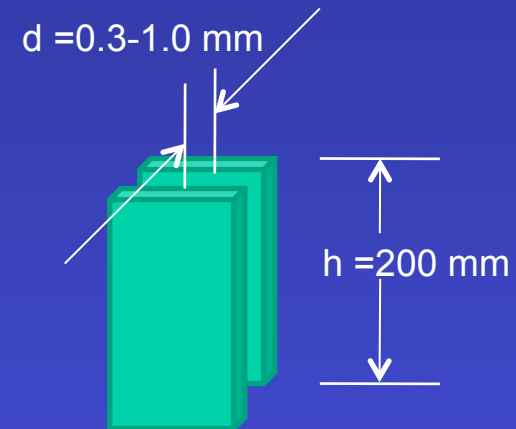
# Comparison between needle and trap collimators



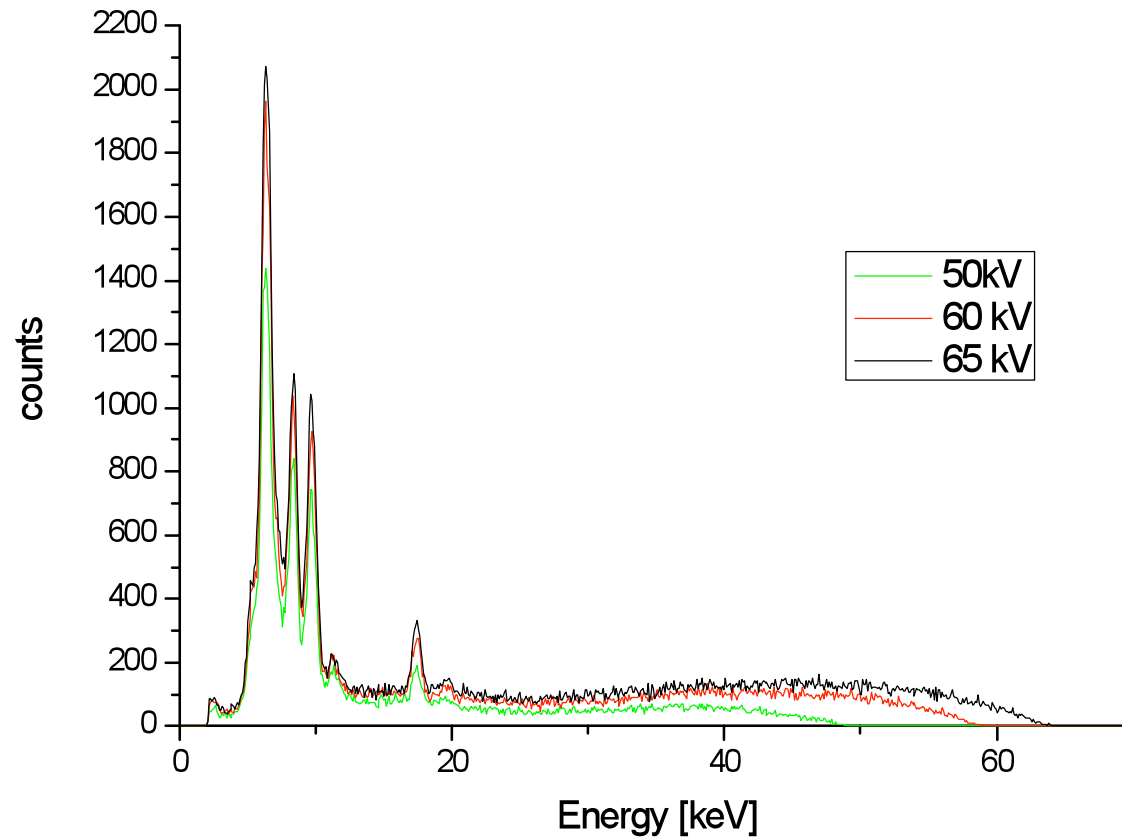
# Direct Measurement of X-Ray Spectra



## Set-up #2 Plate Collimator



# Variation with KV



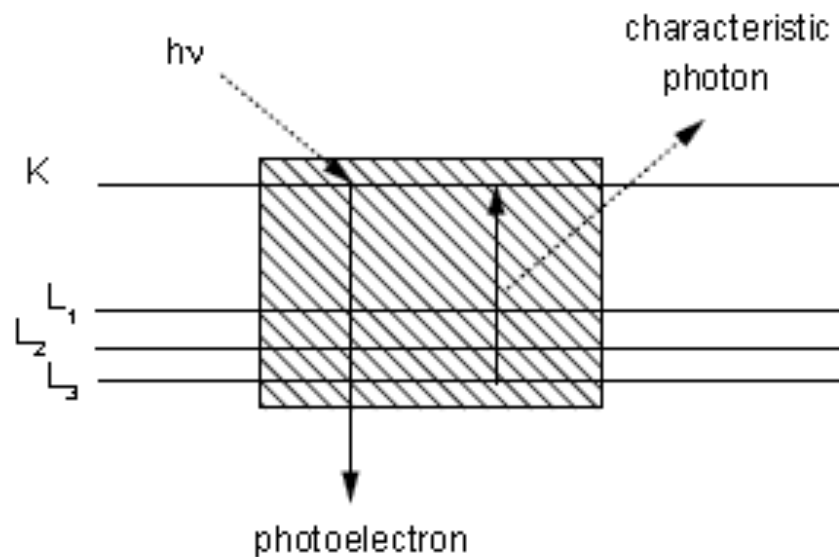
# THEORETICAL MODEL

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# 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'



photoelectric  
absorption

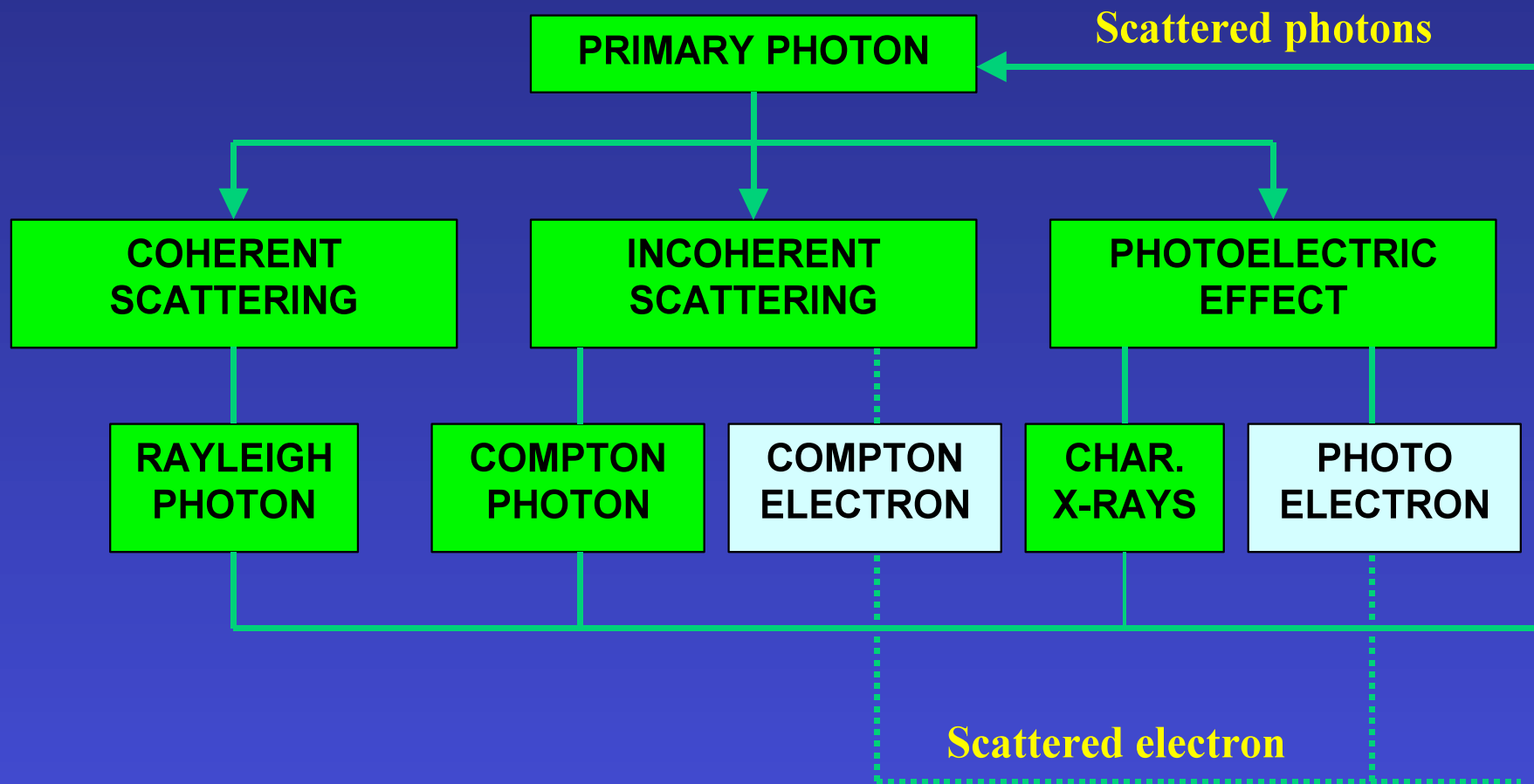
+

radiative  
transition

=

photoelectric  
'scattering'

# PREVAILING INTERACTIONS IN THE X-RAY REGIME





# DESCRIPTION OF POLARIZATION

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# WHY POLARIZATION?

Polarization state  wave nature of photons

By considering polarization we  
improve the model of photon  
diffusion

**Without polarization photons are considered only as particles**



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

# Polarization state definition

Four parameters:

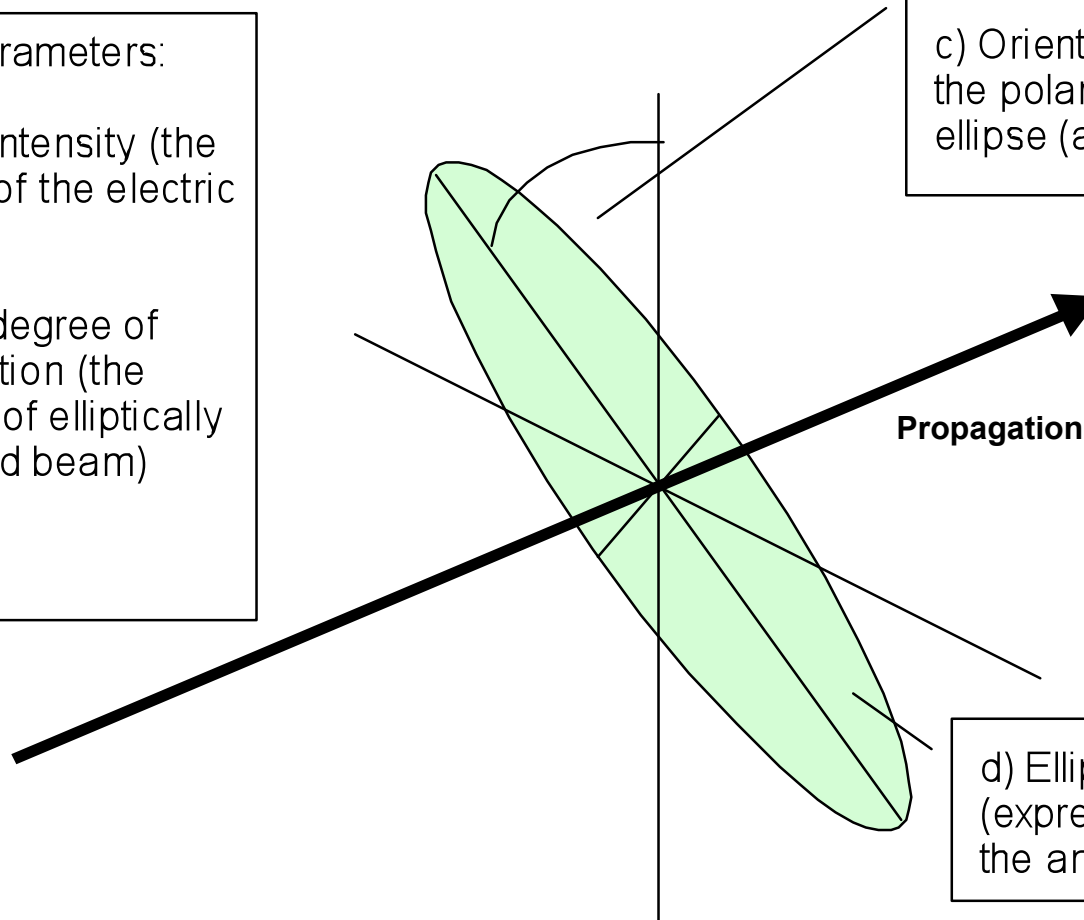
a) The intensity (the square of the electric field)

b) The degree of polarization (the fraction of elliptically polarized beam)

c) Orientation of the polarization ellipse (angle  $\chi$ )

Propagation vector

d) Ellipticity (expressed by the angle  $\beta$ )

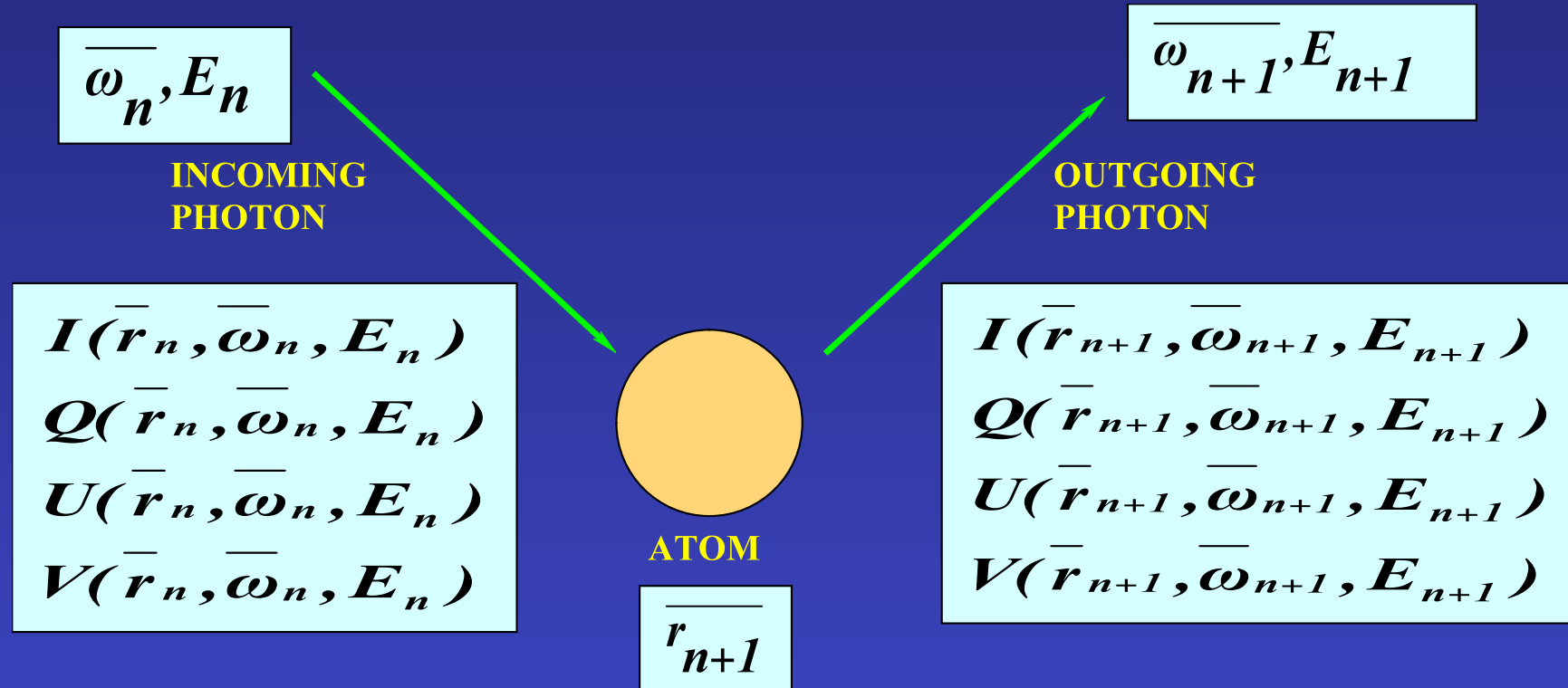


# REPRESENTATION OF POLARIZED RADIATION

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 3-D EQUATION IS SHOWN HERE)

$$\begin{aligned}\vec{\omega} \cdot \nabla \vec{f}^{(S)}(\vec{r}, \vec{\omega}, \lambda) = & -\mu(\vec{r}, \lambda) \vec{f}^{(S)}(\vec{r}, \vec{\omega}, \lambda) \\ & + \int_0^{\infty} d\lambda' \int_{4\pi} d\omega' H^{(S)}(\vec{r}, \vec{\omega}, \lambda, \vec{\omega}', \lambda') \vec{f}^{(S)}(\vec{r}, \vec{\omega}', \lambda') \\ & + \vec{S}^{(S)}(\vec{r}, \vec{\omega}, \lambda)\end{aligned}$$

where

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



# VECTOR TRANSPORT EQUATION (CONT.)

where

$$H^{(S)}(\vec{r}, \vec{\omega}, \lambda, \vec{\omega}', \lambda') = L^{(S)}(\pi - \psi) K^{(S)}(\vec{r}, \vec{\omega}, \lambda, \vec{\omega}', \lambda') L^{(S)}(-\psi')$$

$H^{(S)}$  = 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)

# SCALAR and VECTOR MODELS

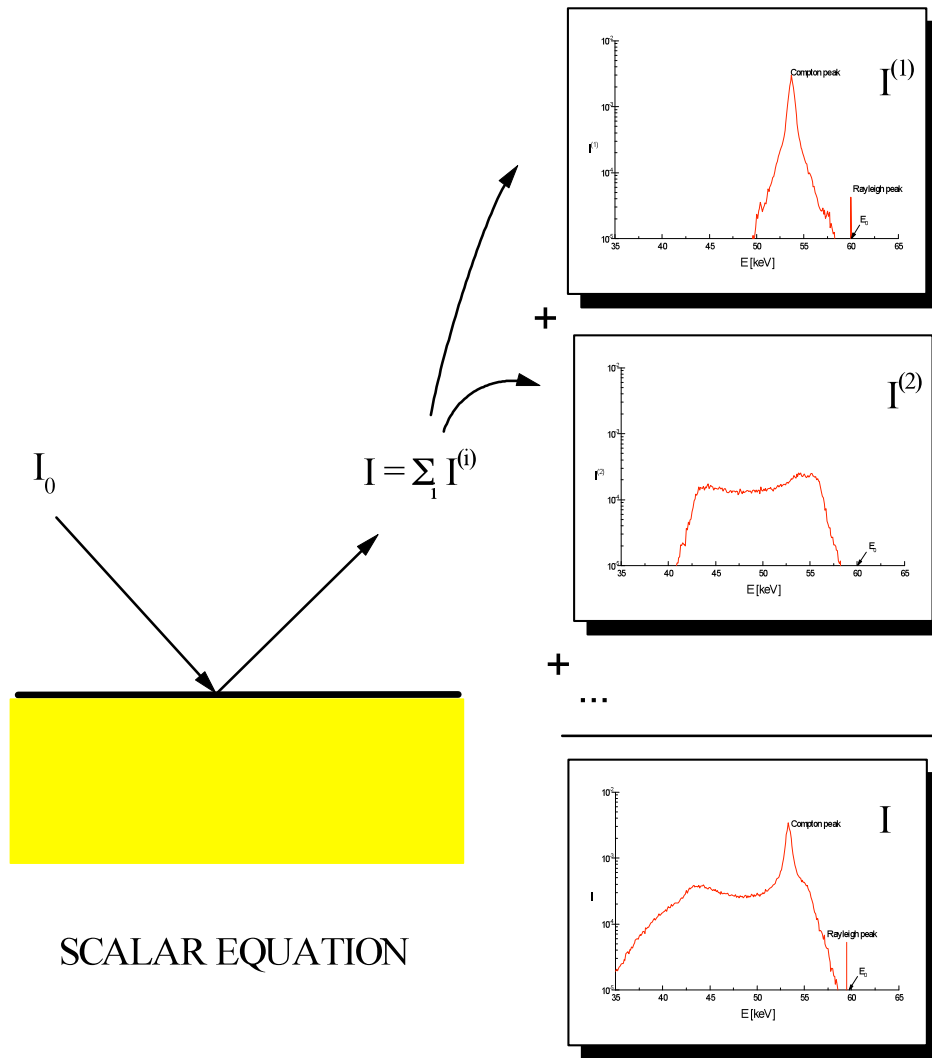
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# MODELS

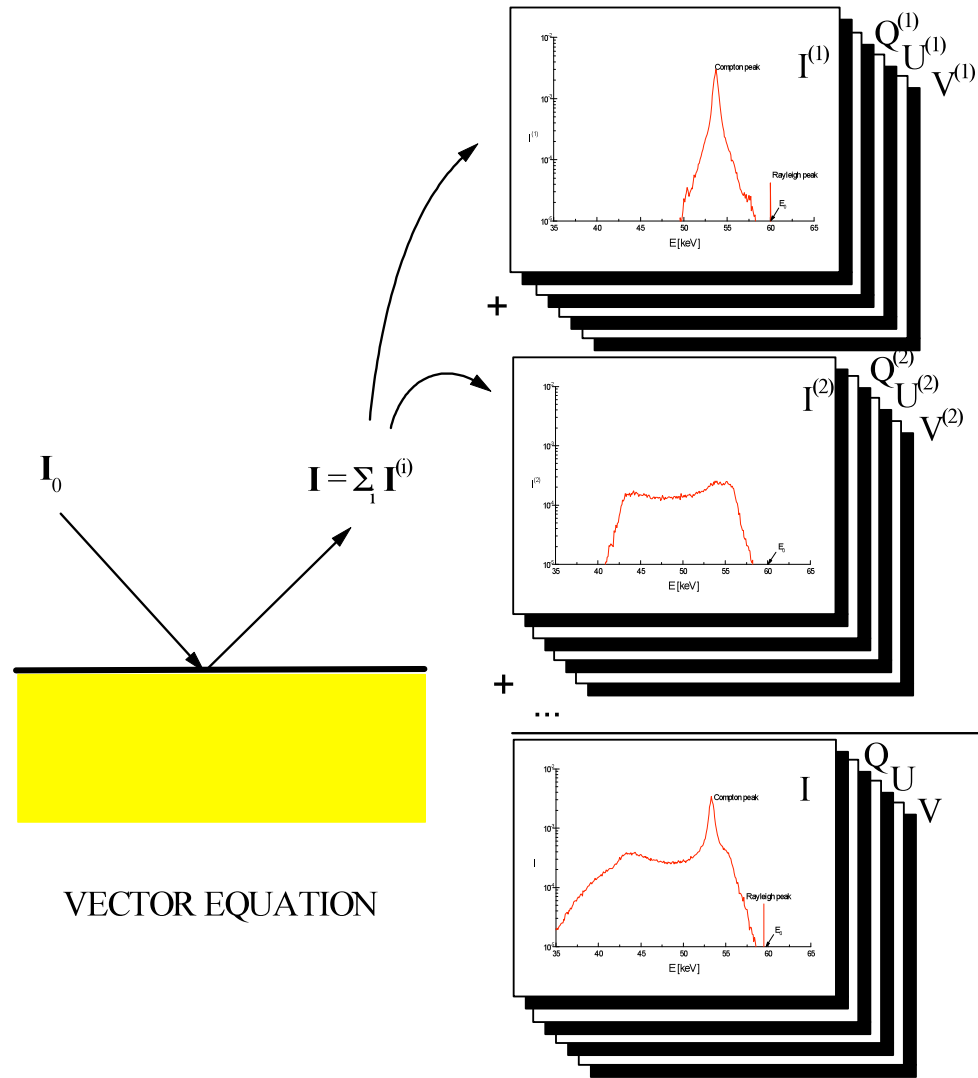
Different degrees of approximation to describe the diffusion photons:

- ***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

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# SOLUTION TECHNIQUES

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



**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>

The screenshot shows a Netscape browser window titled "SHAPe codes home page - Netscape". The address bar contains "http://shape.ing.unibo.it/index.htm". The page features the University of Bologna logo (Alma Mater Studiorum, A.D. 1088) and the main heading "SHAPe codes for radiation transport" in a stylized font. Below this is a dark grey button labeled "home page".

On the left side, there is a vertical navigation menu with the following items: home, overview, SHAPe, MCSHAPe, 3D deterministic codes, atomic database, data tables, downloads, links, our group, and publications.

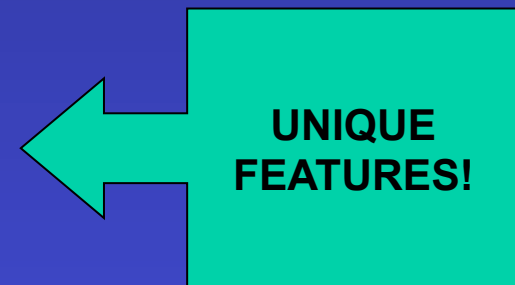
The main content area is divided into three columns:

- Left Column:** A section titled "Deterministic and Monte Carlo photon transport codes" in red. It contains two paragraphs of text describing the multiple scattering description of polarised photon diffusion and the development of several codes for photon transport. A blue link "more..." is at the bottom.
- Middle Column:** A large, faded watermark of the University of Bologna seal is visible. At the bottom of this column, the text "SHAPE.ING.UNIBO.IT" is displayed.
- Right Column:** A section titled "LATEST VERSIONS" in yellow. It lists four versions: MCSHAPe v2.50, MCINPUT V2.10, SHAPe v2.20, and MUPLOT V1.03. Below this is a "NEWS" section in yellow, containing three news items with dates and version numbers: September 9th, 2005 - MCSHAPe v2.50; March 9th 2005 - MCINPUT v2.10; and October 28th 2004 - MUPLOT v1.03.

At the bottom of the browser window, a status bar shows "Transferring data from shape.ing.unibo.it..." and a small message "This site was visited".

## CODES COMPARISON (part 1: Physics)

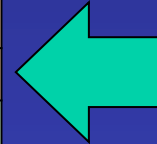
Features	Details	SHAPE v2.20	MCSHAPE v2.62
Physics	photoelectric effect	☒	☒
	~1000 characteristic lines	☒	☒
	line width	☒	☒
	atomic Rayleigh scattering	☒	☒
	atomic Compton scattering	☒	☒
	Compton profile	first collision only	☒
	electron bremsstrahlung	foreseen in v3	foreseen in v3
	open data bases	☒	☒
	user defined elements		foreseen in v3
	infinite thickness targets	☒	☒
	finite thickness targets		☒
	multilayer targets		☒
	polarization representation	Stokes	Stokes
	<b>source polarization state</b>	<b>linear/ unpolarised</b>	<b>arbitrary</b>
	<b>calculated spectrum</b>	intensity component only	<b>full polarization state</b>
	monochromatic source	☒	☒
	polychromatic source	postprocessor	☒
	external detector	solid state Si/Ge	☒
	reflection geometry	☒	☒
	transmission geometry		☒



## CODES COMPARISON (part 2: model and programming)

Features	Details	SHAPE v2.20	MCSHAPE v2.62
Miscellaneous	selective computation of single interaction chains	☒	partial
Transport model	particle	photons	photons
	scalar equation	☒	☒
	vector equation	☒	☒
	solution	deterministic	Monte Carlo
	collisions	3	100
	1-D spatial geometry	☒	☒
	3-D spatial geometry		<b>using MCSHAPE3D</b>
Code	language	DELPHI	FORTRAN 90
	additional libraries	graphics	WINTERACTER
	platform	WINDOWS	WINDOWS / LINUX
	distribution	web site	web site
	parallelization		MPICH v1.0 (only Linux)
Applications	spectroscopy	☒	☒
	analytical chemistry	☒	☒
	radiation metrology	☒	☒
	x-ray optics		with MCSHAPE3D
	dosimetry		with MCSHAPE3D
	radiation transport teaching	☒	☒

**NEW!!**  
3D version  
of MCSHAPE



# INTERPRETATION OF EXPERIMENTAL DATA

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# SIMULATIONS WITH MCSHAPE 1-D

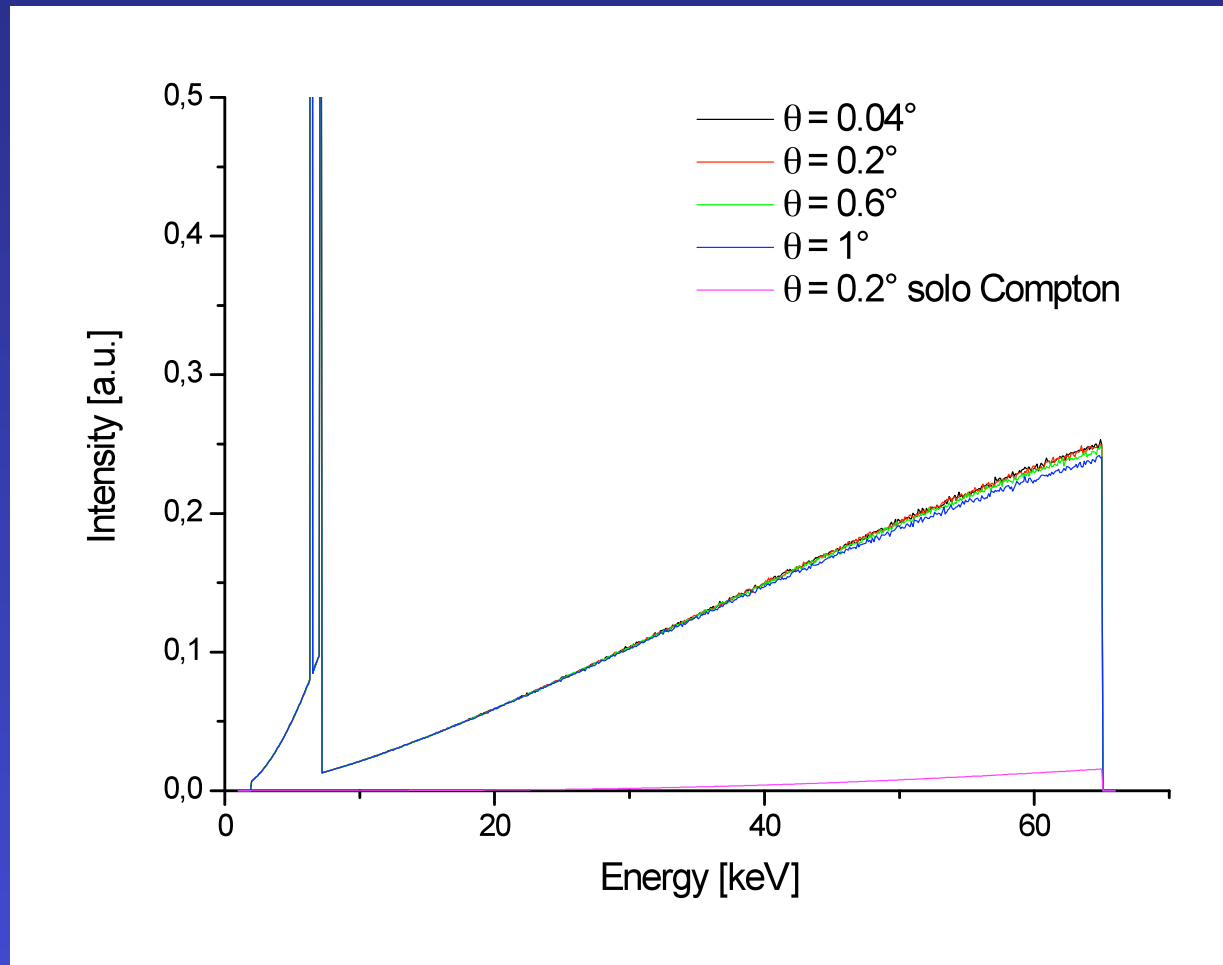
The simulation was performed using the following parameters:

- (1) Pure iron flat collimator
- (2) Incidence and take-off angles in agreement with a scattering angle of:

$$\theta \approx \text{tg}\theta = \frac{\frac{1}{2} \text{collimator diameter}}{\text{distance collimator - tube}} = \frac{\frac{1}{2}(1\text{mm})}{(2000\text{mm})} \approx 2.5 \cdot 10^{-4} \text{ rad}$$

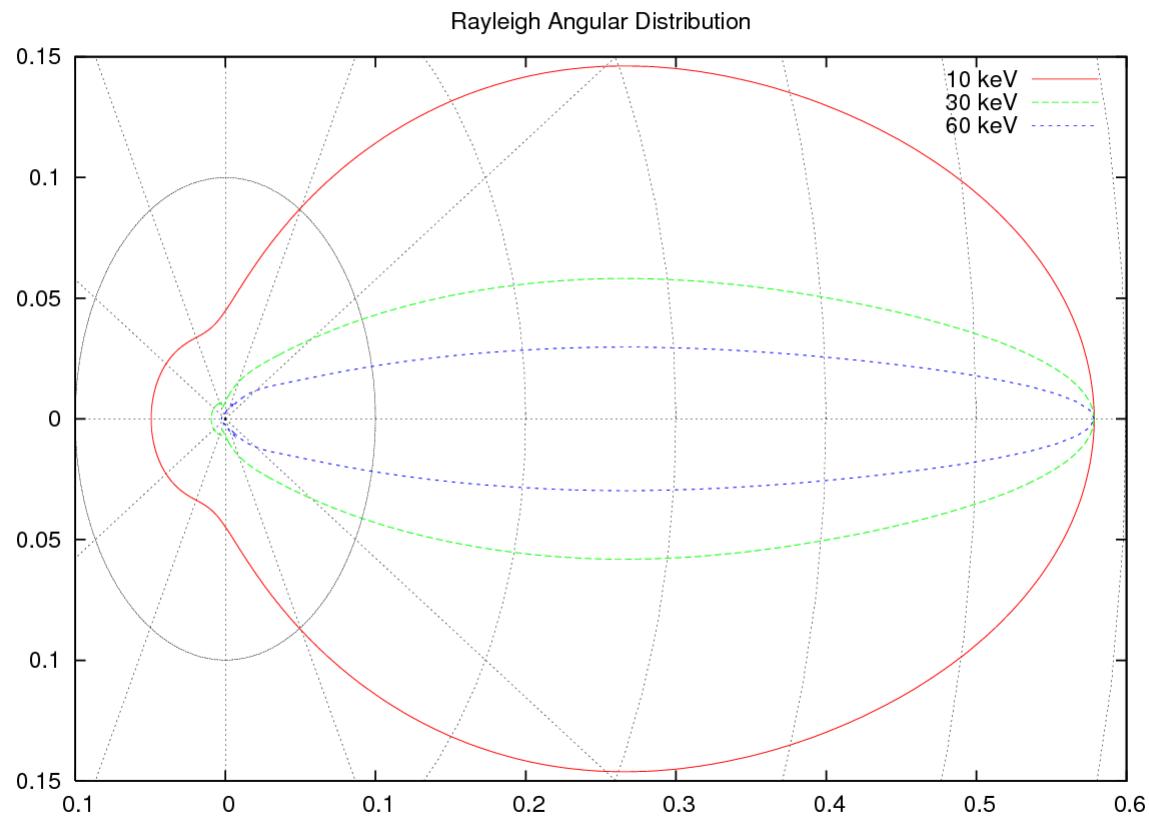
- (3) Polychromatic excitation from 2 to 65 keV

# SIMULATION WITH MCSHAPE 1-D

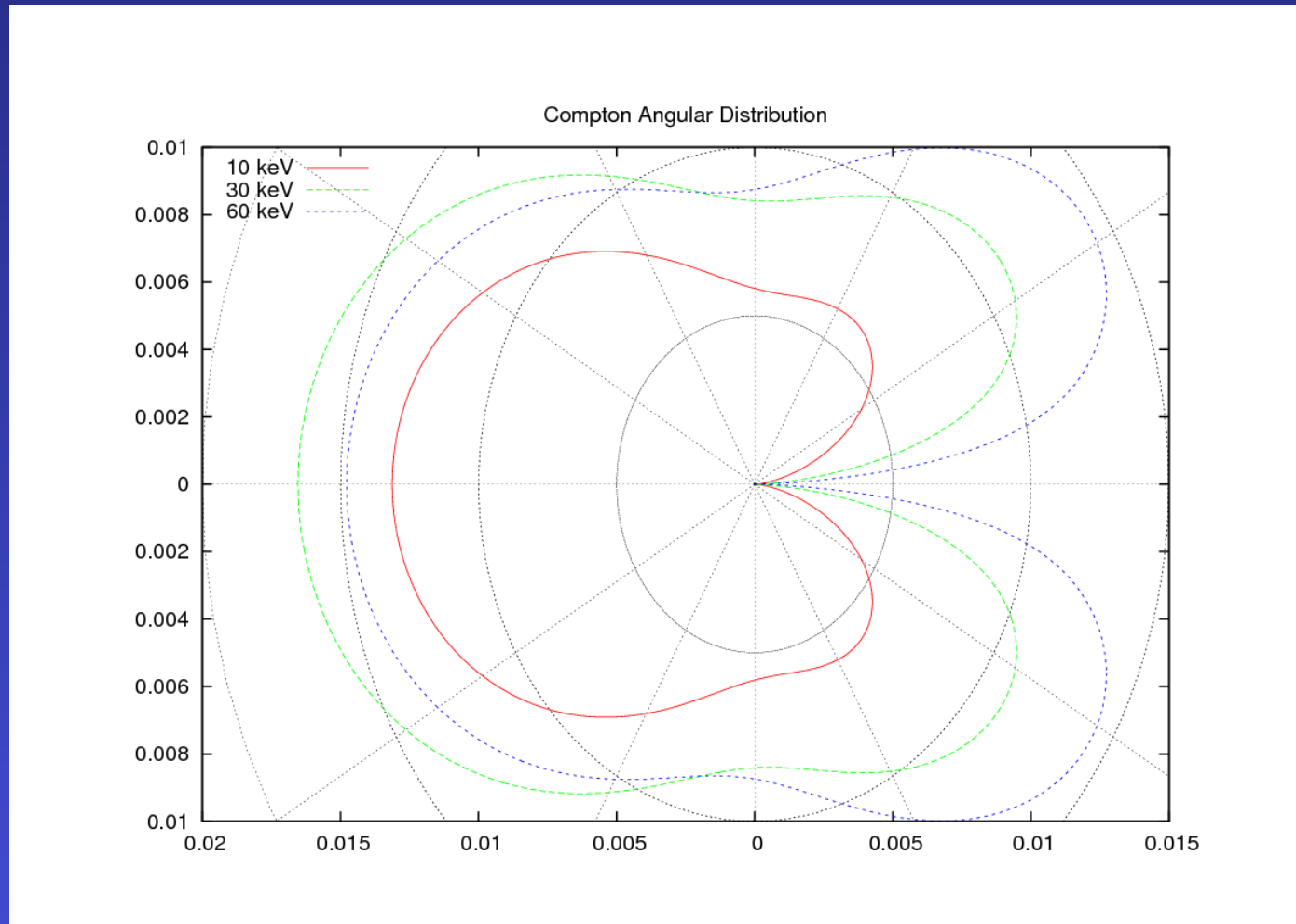




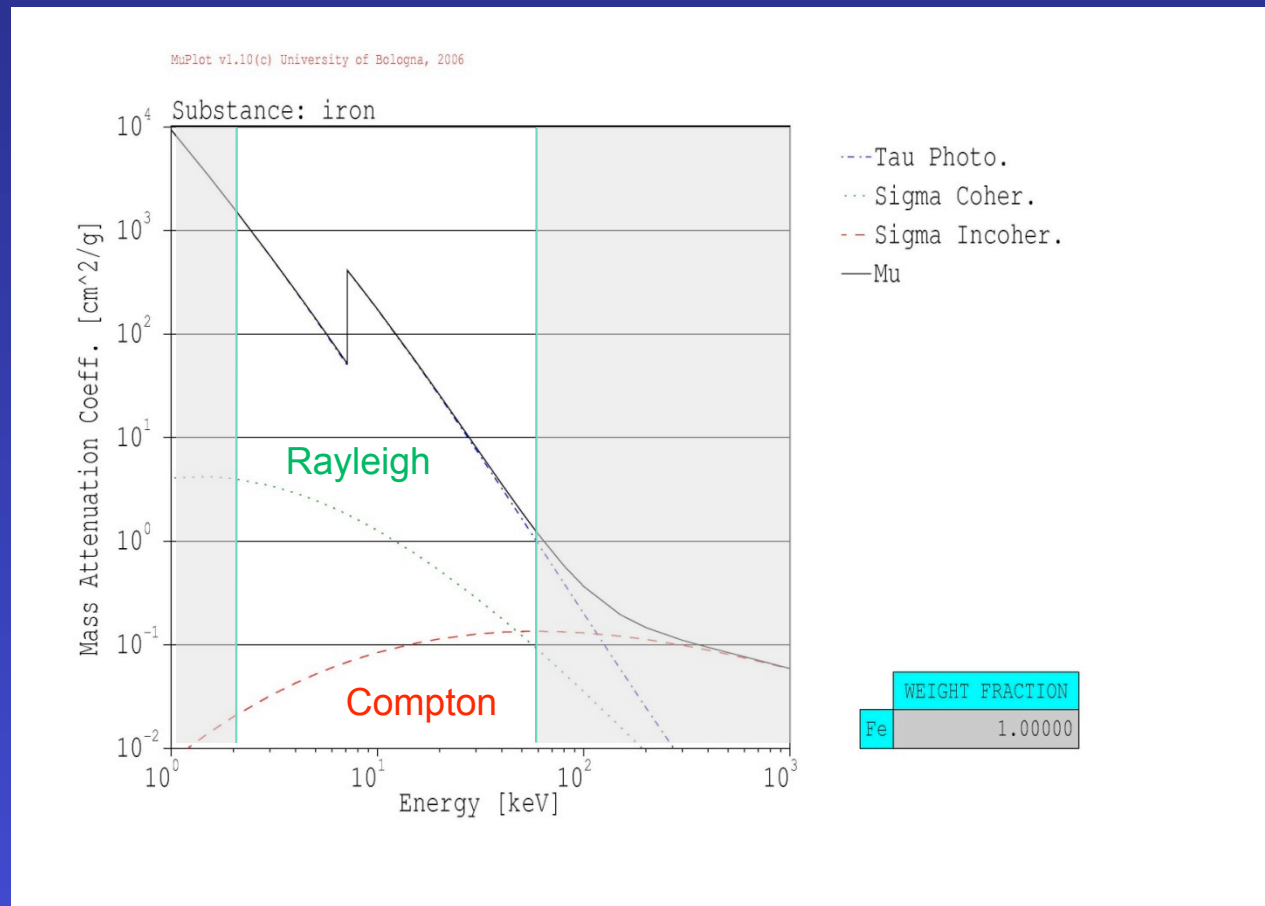
# Atomic Rayleigh scattering always prevails in forward scattering



# Atomic Compton scattering is negligible in forward scattering



In addition, Rayleigh scattering prevails (or is equivalent) to Compton in the energy range considered



# CONCLUSIONS

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## CONCLUSIONS (1/2)

- **Needle collimators can be used to remarkably enhance the intensity of the x-ray beam in the high energy side of x-ray spectra**
- **At 65 kV operation, the enhancement of the spectrum is equivalent to the whole incident spectrum and is concentrated on the high energy side.**
- **Plate collimators produce a similar but weaker effect.**
- **The effect has been tested in the range 50-65 keV**

## CONCLUSIONS (2/2)

- The MCSHAPE 1-D code was used to interpret the physical reasons of this effect.
- The enhancement can be explained as due to multiple scattering, in particular, atomic Rayleigh scattering in the forward direction (small angle scattering).
- The measured enhancement exceeds the theoretical prediction of the 1-D code but is consistent with a 3-D estimation.

*Thank you for your attention!*