

X-ray photon spectroscopy calculations

**Prof. Jorge E. Fernandez,
Laboratorio of Montecuccolino, DIN**

keywords

- X-rays -> Photon transport
- Multiple scattering
- Unpolarised & polarised radiation
- X-ray interactions
- X-ray spectrometry
- Monte Carlo & Deterministic codes

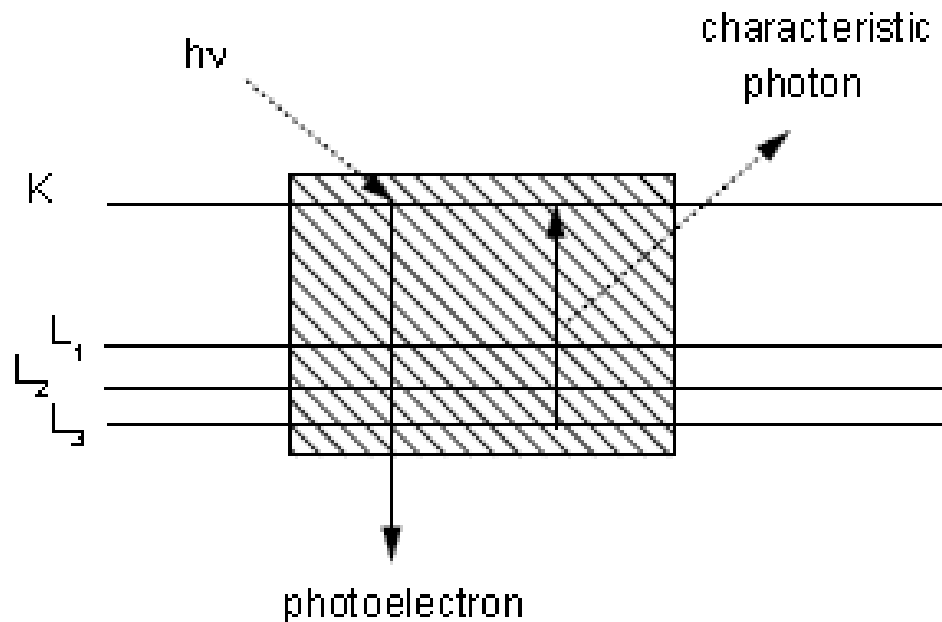
X-RAYS

- electromagnetic radiation
- X-rays penetrate deeply into the matter, and interact with the atoms without changing their chemical state
- in a thick medium, give place to a phenomenon known as **multiple scattering**.

MULTIPLE SCATTERING

- Multiple scattering models describe the influence of the prevailing interactions in the x-ray regime (**photoelectric effect, Compton scattering and Rayleigh scattering**)
- The photoelectric effect itself is a 'scattering process'

Photoelectric effect as 'scattering'



photoelectric
absorption

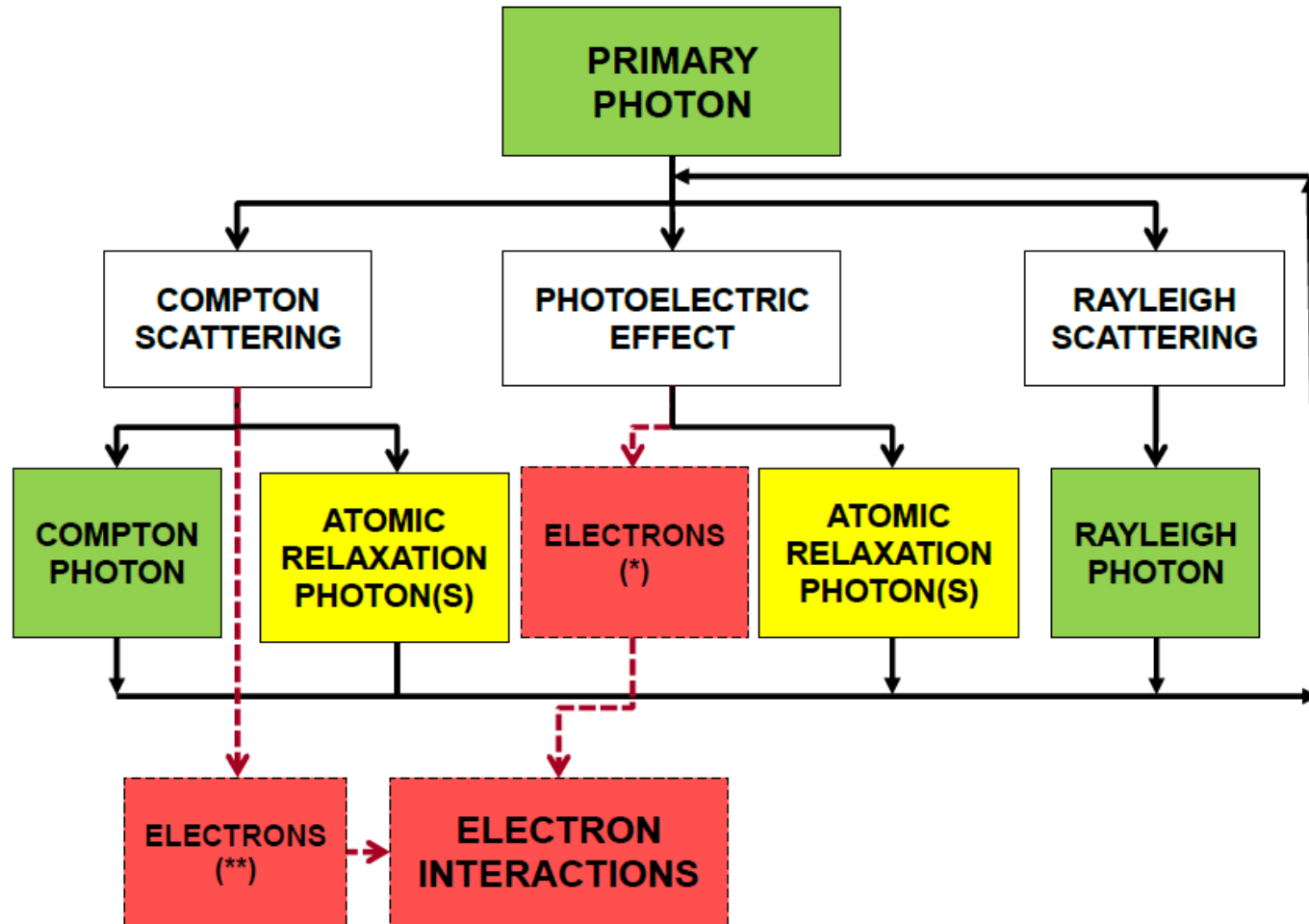
+

radiative
transition

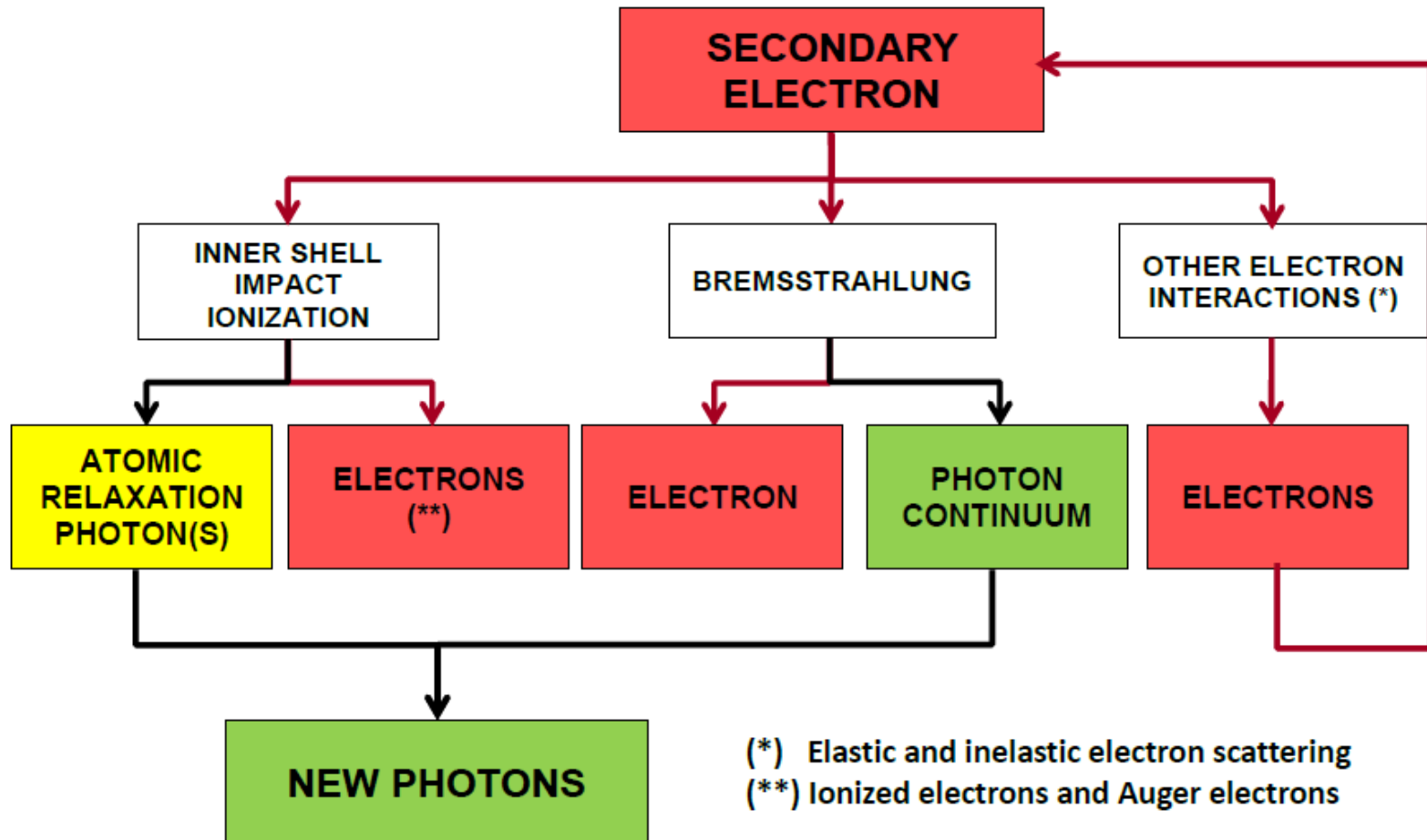
=

photoelectric
'scattering'

DETAILED INTERACTIONS IN THE X-RAY REGIME



Electron-photon coupling



X-RAY SPECTROMETRY TECHNIQUES

X-RAY TECHNIQUES (USING A X-RAY SOURCE)

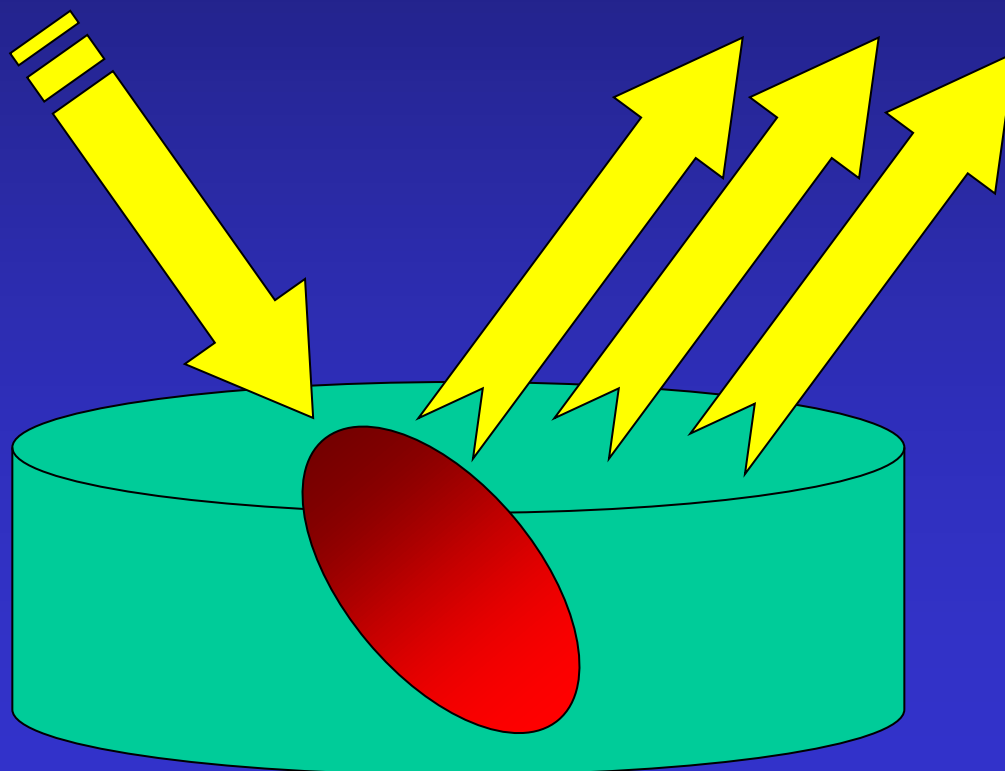
(ATOMIC INFORMATION)

- **X-RAY FLUORESCENCE (XRF)**
- **TOTAL REFLECTION FLUORESCENCE (TXRF)**
- **X-RAY SCATTERING**
- **X-RAY RADIOGRAPHY**
- **PHASE CONTRAST RADIOGRAPHY**
- **X-RAY TOMOGRAPHY**
 - **ATTENUATION TOMOGRAPHY**
 - **XRF TOMOGRAPHY**

X-RAY FLUORESCENCE (XRF)

X-RAY SOURCE

X-RAY FLUORESCENCE



X-RAY FLUORESCENCE

SOURCE: INCOHERENT

UNPOLARIZED OR POLARIZED

GEOMETRY: REFLECTION

INTEREST COLLISION: PHOTOELECTRIC EFFECT
(GIVING CHARACTERISTIC LINES)

PENETRATION: LOW-MEDIUM

MEASURE: ELEMENTAL COMPOSITION IN A
VOLUME

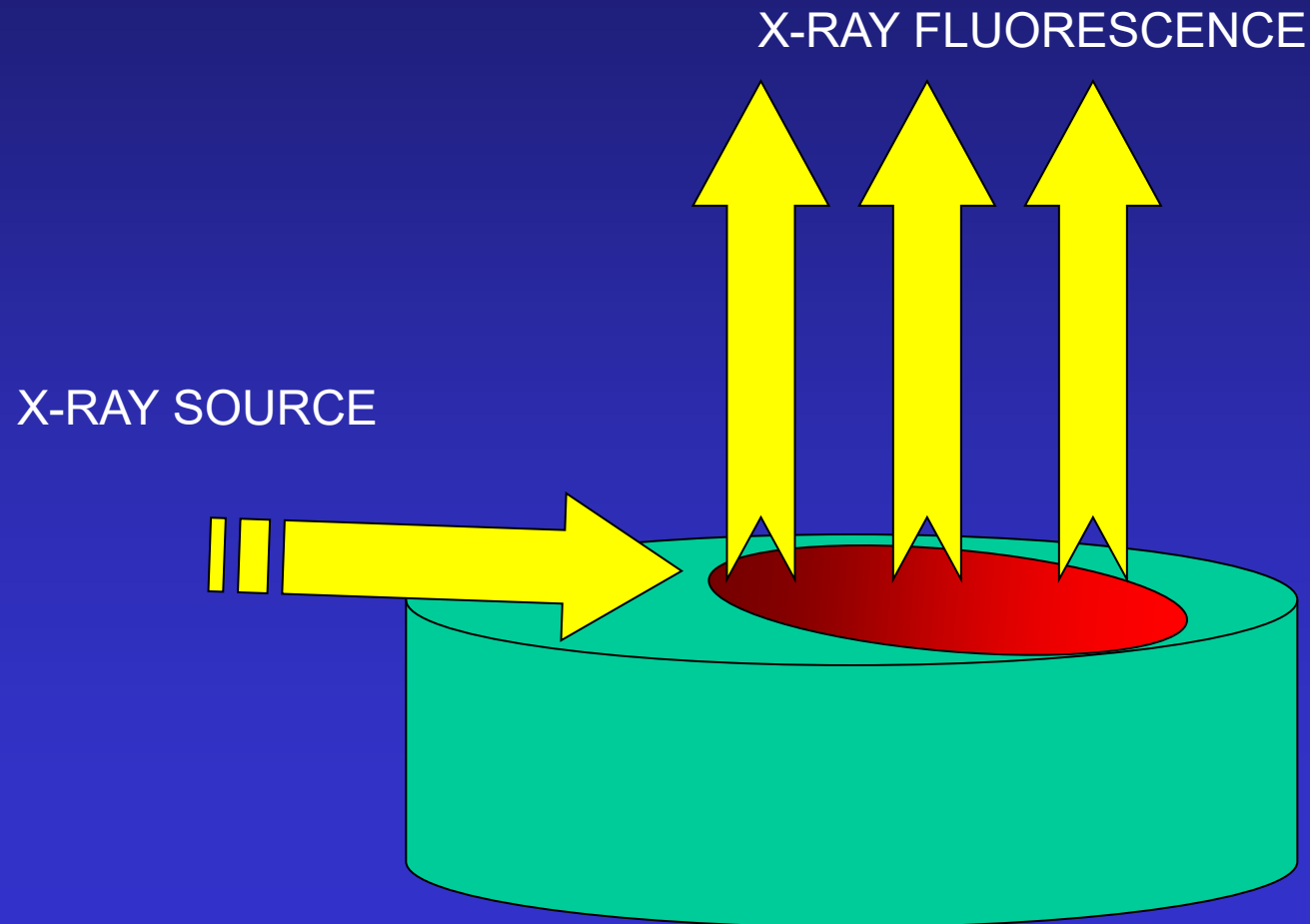
MAPPING: YES (2-D), 3D WITH CONFOCAL XRF

MATERIALS: PAINTINGS, GLASSWORKS, METALS,
FRESCOES, ETC.

EQUIPMENT: PORTABLE

DATA HANDLING: LIGHT (SEMI-QUANTITATIVE)
HEAVY (QUANTITATIVE OR 2D)

TOTAL REFLECTION X-RAY FLUORESCENCE (TXRF)



TOTAL REFLECTION X-RAY FLUORESCENCE

SOURCE: INCOHERENT

UNPOLARIZED OR POLARIZED

GEOMETRY: GRAZING INCIDENCE, REFLECTION

INTEREST COLLISION: PHOTOELECTRIC EFFECT
(GIVING CHARACTERISTIC LINES)

PENETRATION: LOW

MEASURE: SURFACE, TRACE ELEMENTS

MAPPING: MORE DIFFICULT

MATERIALS: COATINGS

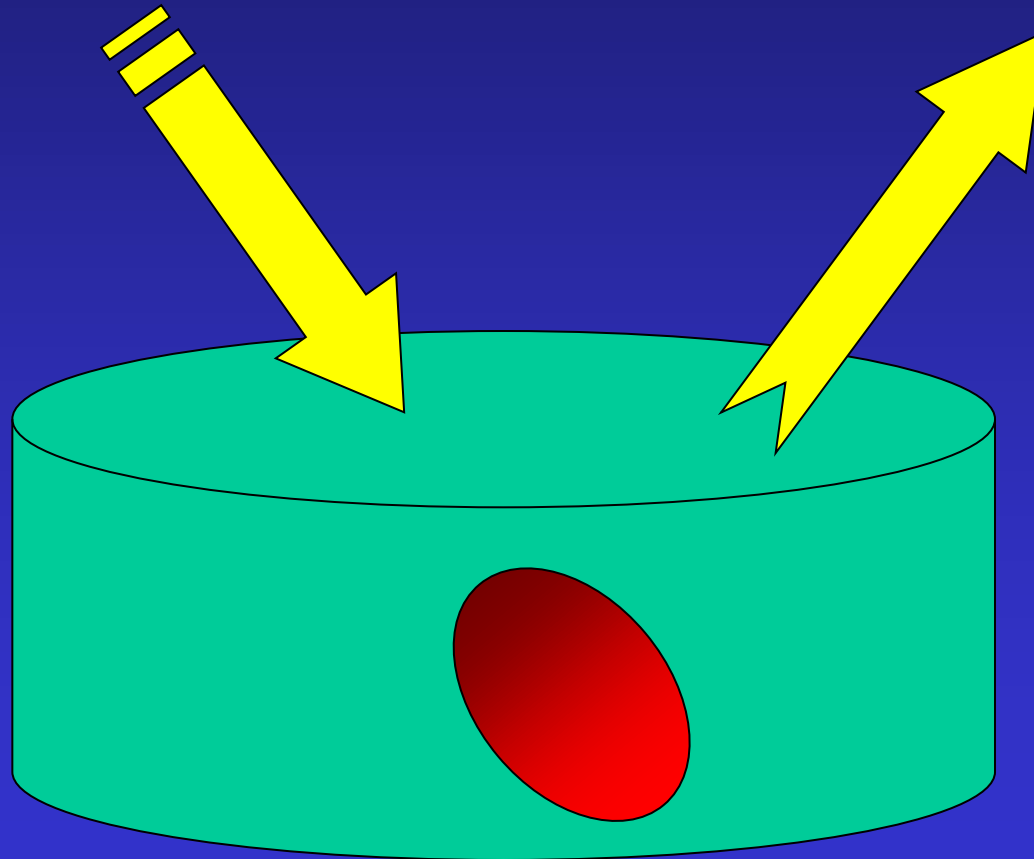
EQUIPMENT: LABORATORY (ALIGNEMENT IS
DELICATE)

DATA HANDLING: LIGHT

X-RAY SCATTERING

HIGH ENERGY
X-RAY SOURCE

X-RAY FLUORESCENCE



X-RAY SCATTERING

SOURCE: INCOHERENT

UNPOLARIZED OR POLARIZED

GEOMETRY: REFLECTION AND TRANSMISSION

INTEREST COLLISION: COMPTON SCATTERING

(SOMETIMES USED TOGETHER WITH RAYLEIGH SCATTERING AND COMPTON TAIL)

PENETRATION: MEDIUM-HIGH

MEASURE: DENSITY

MAPPING: YES (2-D)

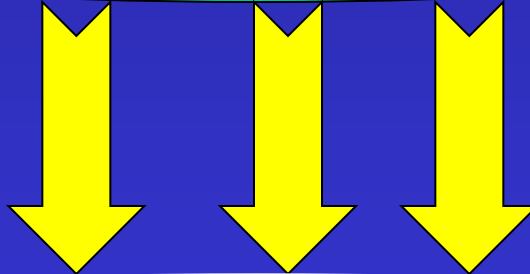
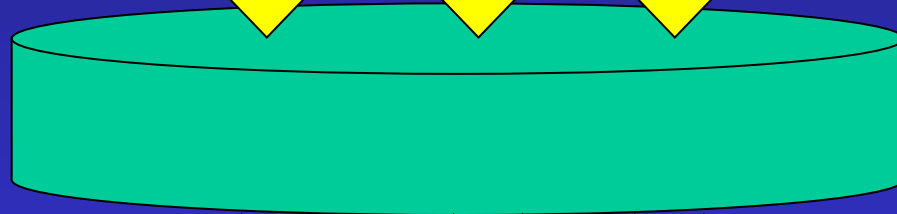
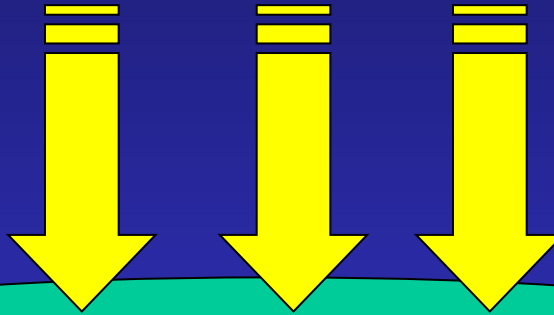
MATERIALS: MARBLES, STONES, MURAL SUPPORT OF FRESCOES, ETC.

EQUIPMENT: PORTABLE

DATA HANDLING: HEAVY (STATISTICAL METHODS)

X-RAY RADIOGRAPHY

X-RAY SOURCE



ATTENUATED
X-RAY BEAM

SENSITIVE PLATE
OR CCD (DIGITAL)



X-RAY RADIOGRAPHY

SOURCE: INCOHERENT

UNPOLARIZED

GEOMETRY: TRANSMISSION

INTEREST COLLISION: FULL EFFECT OF
ATTENUATION (NOT A SINGLE
COLLISION)

PENETRATION: MEDIUM-HIGH

MEASURE: CONTRAST IS ATTENUATION

MAPPING: YES (2-D)

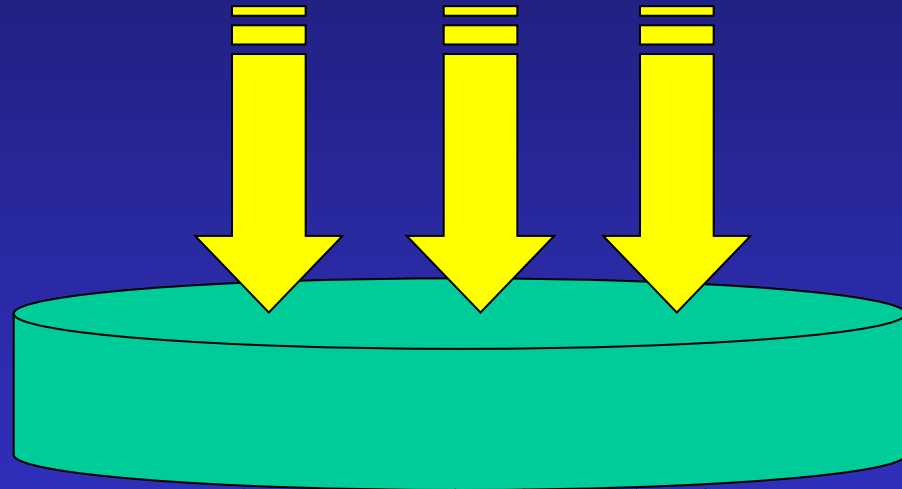
MATERIALS: LIGHT ELEMENTS

EQUIPMENT: LABORATORY

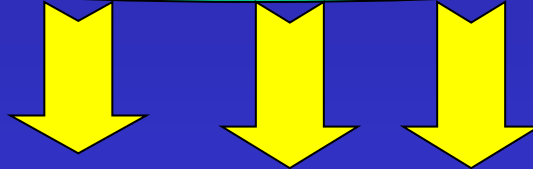
DATA HANDLING: LIGHT

PHASE CONTRAST RADIOGRAPHY

COHERENT X-RAY SOURCE

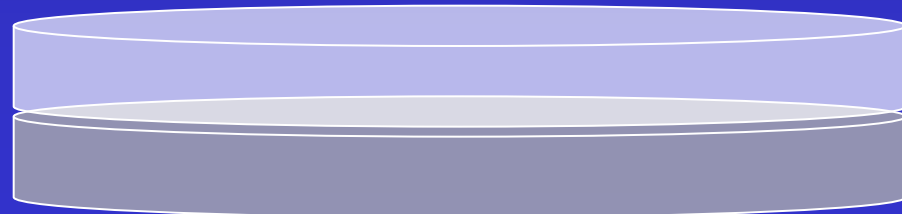


ATTENUATED
X-RAY BEAM



PHASE ANALYSER

CCD



PHASE CONTRAST RADIOGRAPHY

SOURCE: COHERENT

UNPOLARIZED OR POLARISED

GEOMETRY: TRANSMISSION

INTEREST COLLISION: RAYLEIGH
SCATTERING

PENETRATION: MEDIUM-HIGH

MEASURE: CONTRAST IS ATTENUATION

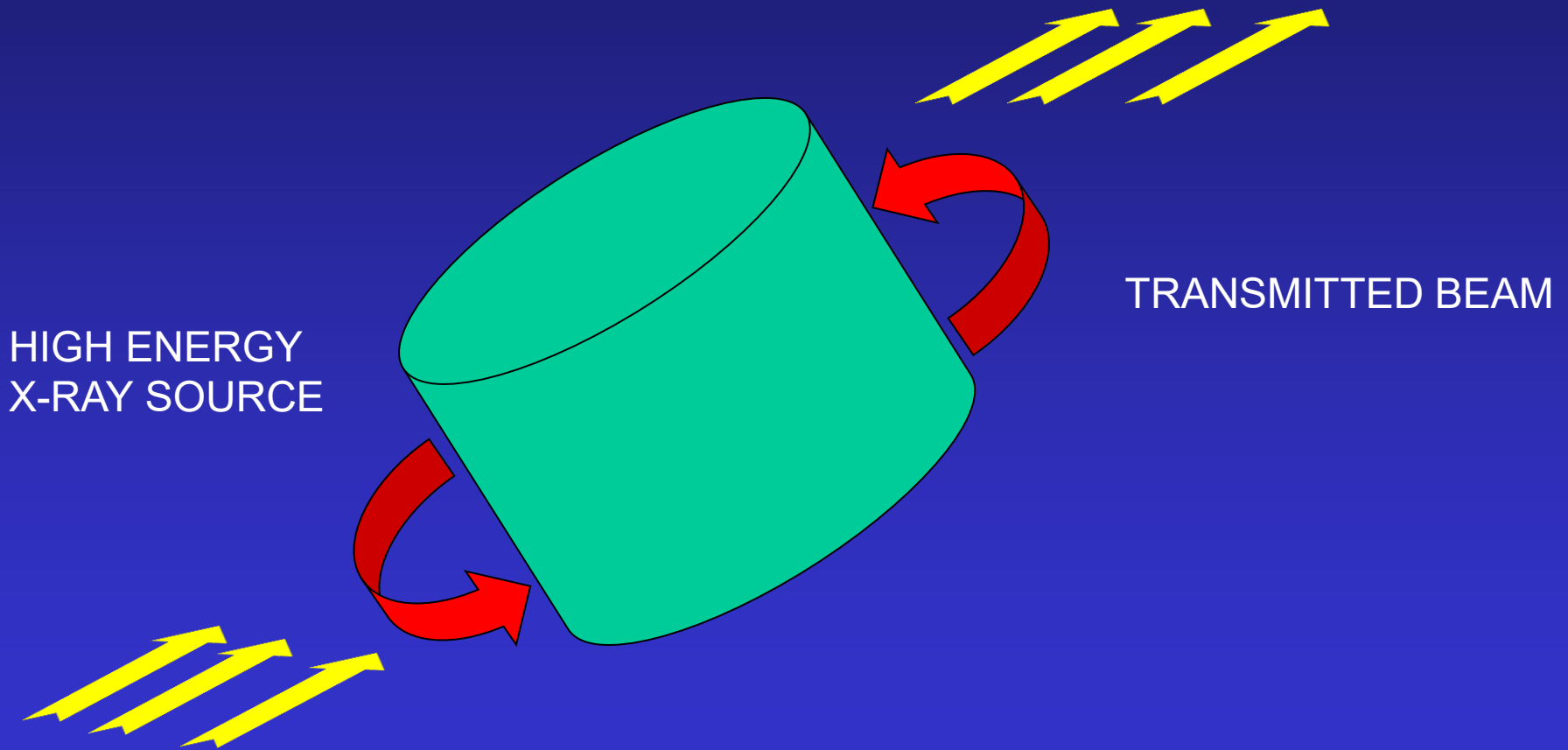
MAPPING: YES (3-D EFFECTS)

MATERIALS: LIGHT ELEMENTS

EQUIPMENT: LABORATORY

DATA HANDLING: HEAVY

X-RAY ATTENUATION TOMOGRAPHY



X-RAY ATTENUATION TOMOGRAPHY

SOURCE: INCOHERENT

UNPOLARIZED OR POLARIZED

GEOMETRY: TRANSMISSION

INTEREST COLLISION: FULL ATTENUATION
EFFECT (NOT A SINGLE COLLISION)

PENETRATION: MEDIUM-HIGH

MEASURE: VOLUME

MAPPING: YES (3-D ATTENUATION COEFFICIENT)

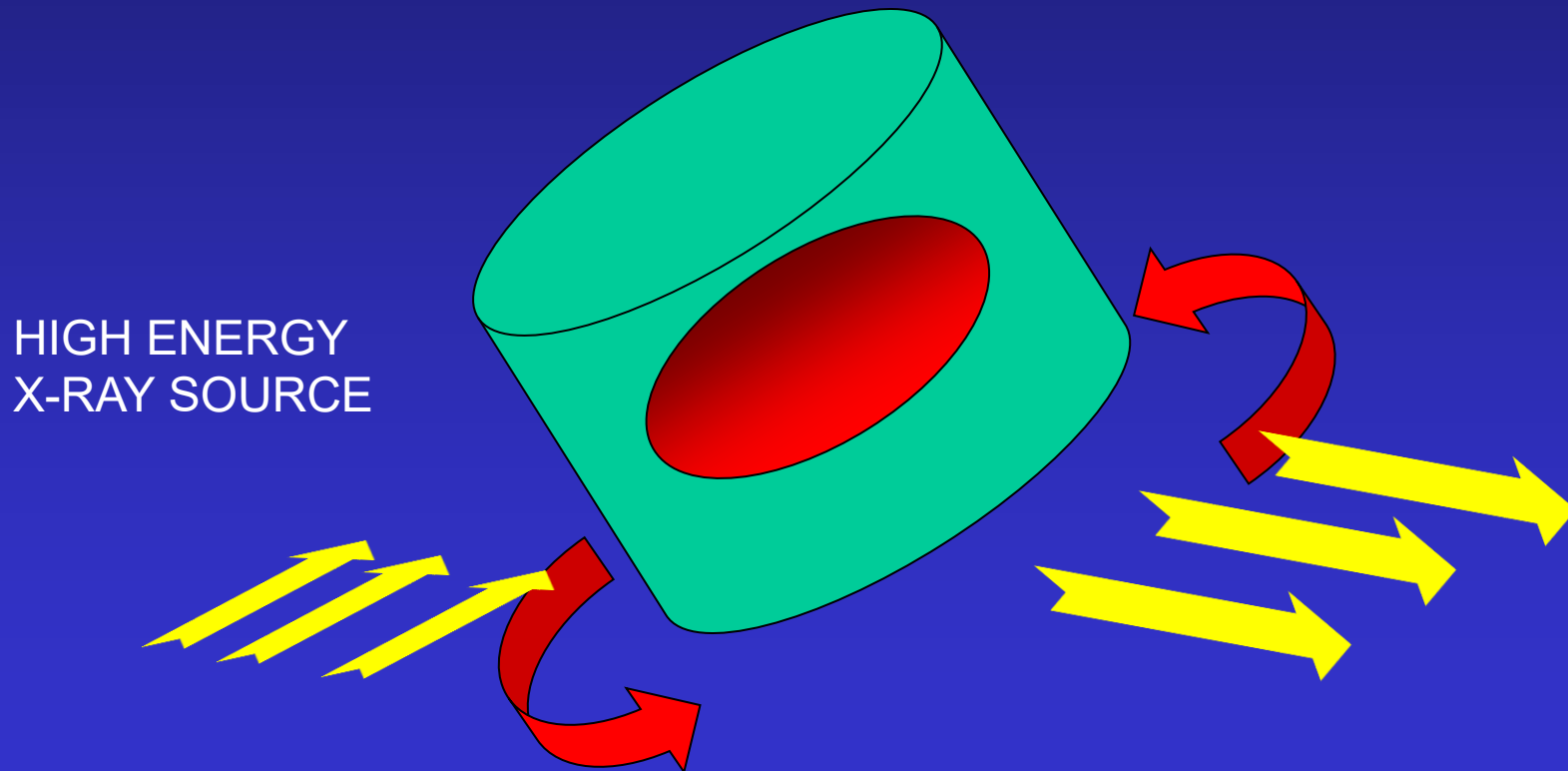
MATERIALS: SMALL SIZE OBJECTS

EQUIPMENT: LABORATORY

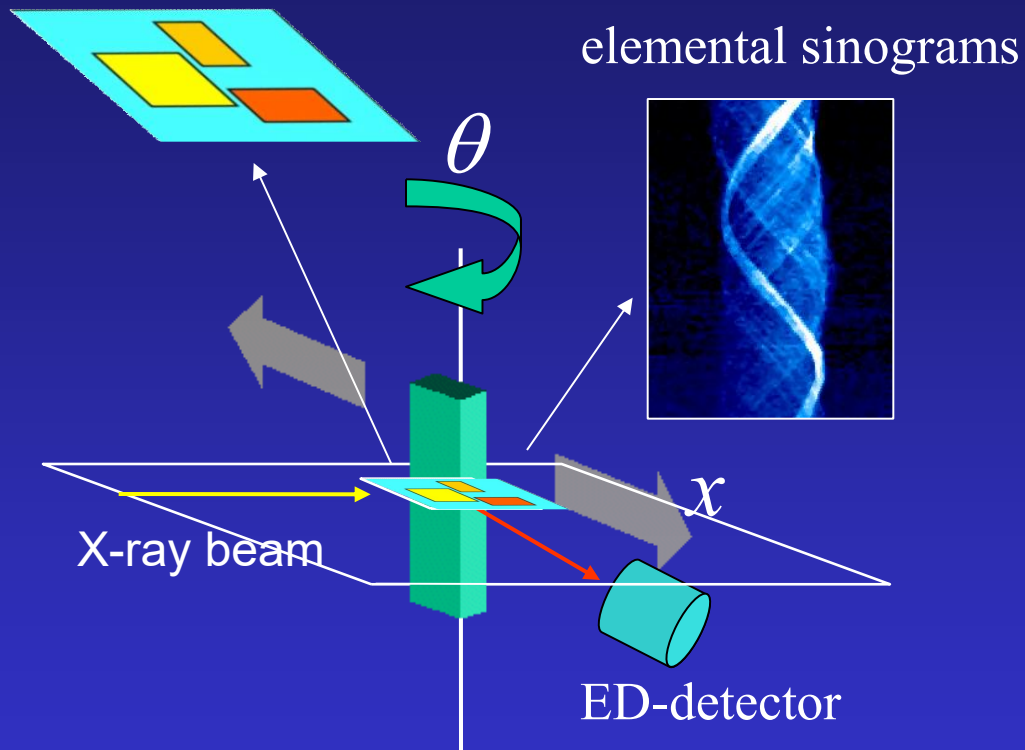
DATA HANDLING: HEAVY (RECONSTRUCTION
METHODS)

X-RAY FLUORESCENCE TOMOGRAPHY

X-RAY FLUORESCENCE



3D – MCSHAPE: XRF Tomography



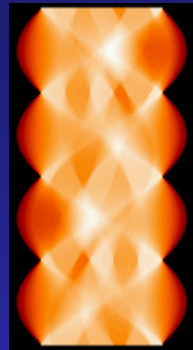
- **Total dimension:** 0.1 x 0.1 x 0.01 cm
- **Composition:**
 - Region **A**: C + 0.1%Sr, $\rho = 1.0 \text{ g/cm}^3$
 - Other elements:
 - Region **B**: SiO_2 + 1%Fe, $\rho = 2.23 \text{ g/cm}^3$
 - Region **C**: SiO_2 + 1%Ba, $\rho = 2.23 \text{ g/cm}^3$
 - Region **D**: SiO_2 + 1%Zr, $\rho = 2.23 \text{ g/cm}^3$
- **Source:**
 - energy: 59.54 keV
 - type: point source
 - unpolarized
- **Detector:**
 - type: disk with 30 mm² of total area
 - no collimator

3D – MCSHAPE: XRF Tomography

Full spectrum



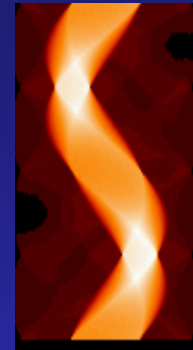
Sr



Ba



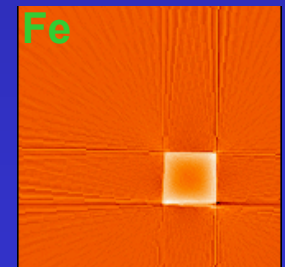
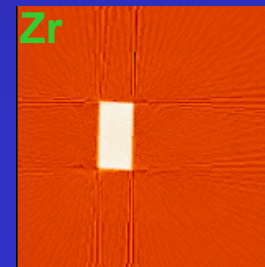
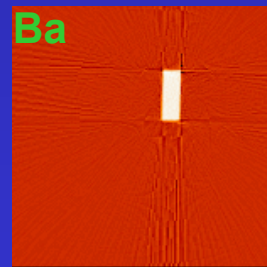
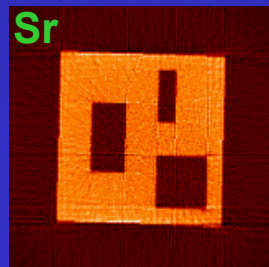
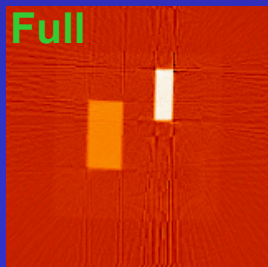
Zr



Fe



reconstruction



X-RAY FLUORESCENCE TOMOGRAPHY

SOURCE: INCOHERENT

UNPOLARIZED OR POLARIZED

GEOMETRY: REFLECTION

INTEREST COLLISION: PHOTOELECTRIC
EFFECT

PENETRATION: MEDIUM-HIGH

MEASURE: VOLUME

MAPPING: YES (3-D SINGLE ELEMENT)

MATERIALS: SMALL SIZE OBJECTS

EQUIPMENT: LABORATORY

DATA HANDLING: HEAVY
(RECONSTRUCTION METHODS)

OTHER X-RAY TECHNIQUES (USING A X-RAY SOURCE)

(STRUCTURE INFORMATION)

- **X-RAY DIFFRACTION (XRD)**

(MOLECULAR INFORMATION)

- **RAMAN SCATTERING**
- **EXAFS**
- **ANOMALOUS SCATTERING ABSORPTION**
- **RAYLEIGH & COMPTON SCATTERING
TOMOGRAPHY**

THEORETICAL MODELS

MODELS TO DESCRIBE PHOTON TRANSPORT

Different degrees of approximation to describe the diffusion of photons:

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

Both models follow a multiple scattering scheme

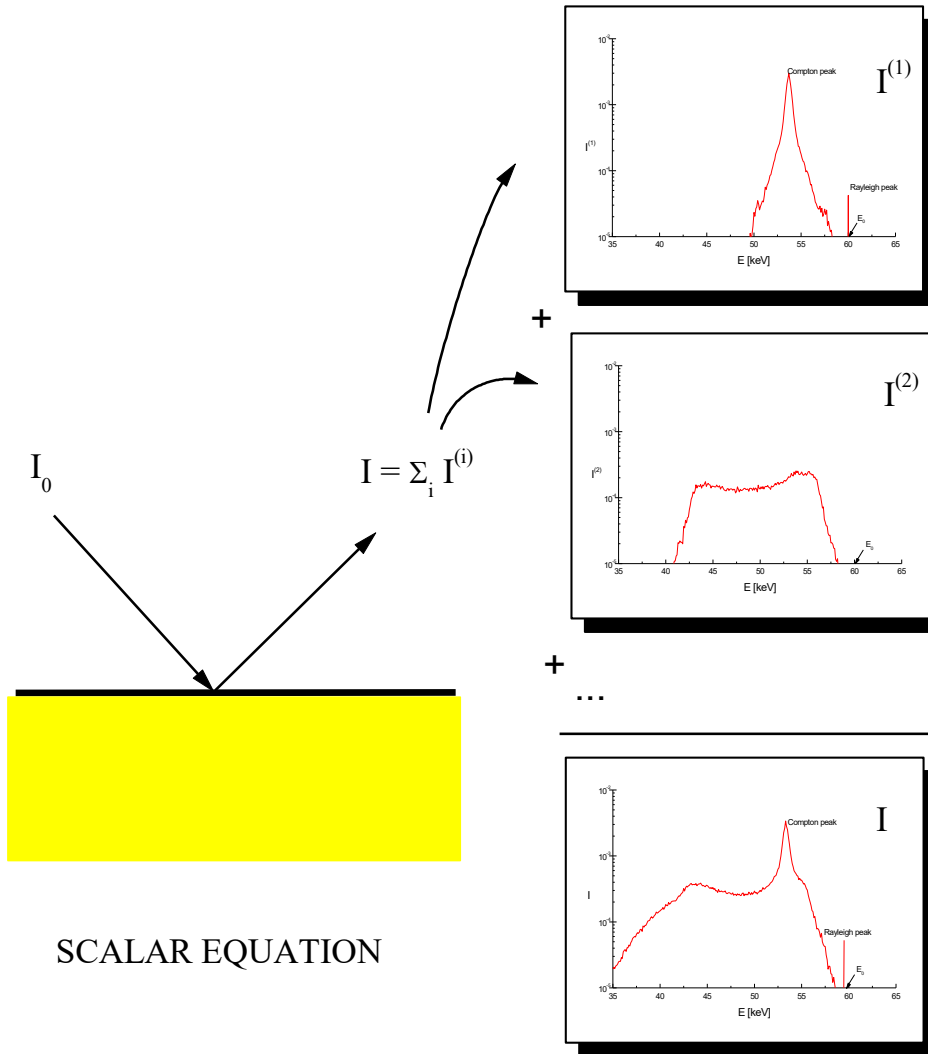
one collision

a	Photoelectric effect	Rayleigh scattering	Compton scattering
	(P) characteristic lines (discrete)	(R) Rayleigh peak (discrete)	(C) Compton peak (continuous)

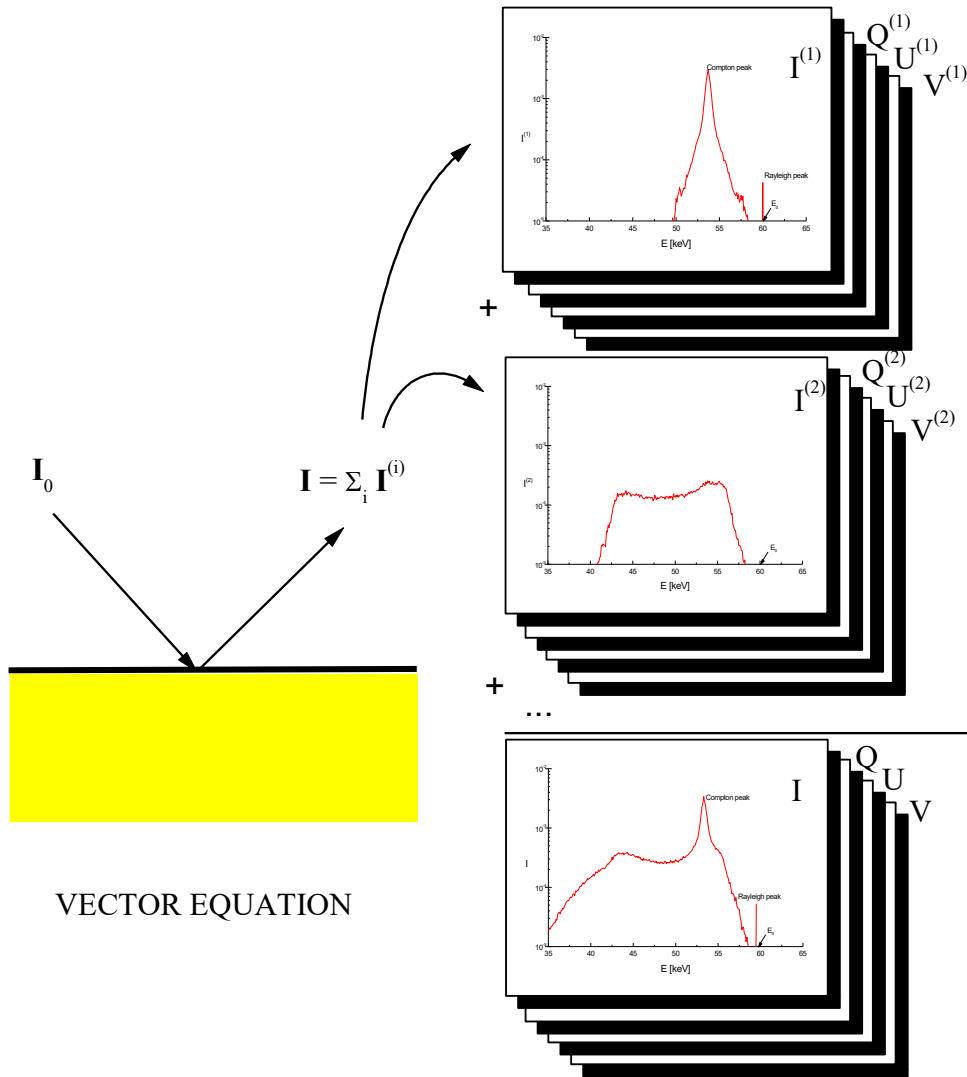
two collisions

	b	Photoelectric effect	Rayleigh scattering	Compton scattering
a				
Photoelectric effect		(P,P) XRF secondary enhancement (discrete on XRF line)	(P,R) XRF enhancement due to scattering (discrete on XRF line)	(P,C) XRF enhancement due to scattering (continuous on XRF line)
Rayleigh scattering		(R,P) XRF enhancement due to scattering (discrete on XRF line)	(R,R) second order scattering (discrete on Rayleigh peak)	(R,C) second order scattering (continuous on Compton peak)
Compton scattering		(C,P) XRF enhancement due to scattering (discrete on XRF line)	(C,R) second order scattering (continuous on Compton peak)	(C,C) second order scattering (continuous on Compton peak)

Scalar transport equation



Vector transport equation





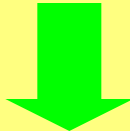
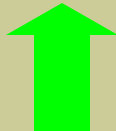
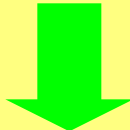

SOLUTION TECHNIQUES

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

Bibliography

- Fano U, Spencer LV and Berger MJ (1959) Penetration and diffusion of X-rays. In *Encyclopedia of Physics*, Vol 38/2, p. 660. Springer Verlag, Berlin.
- Fernández JE and Molinari VG (1991) X-Ray Photon spectroscopy calculations. In: *Advances in Nuclear Science and Technology*, Vol. 22, J Lewins, M Becker eds., Plenum Press, New York, pp. 45-104 (the copy distributed)

Bibliography (polarization effects)

- Pomraning GC (1973) *The equations of radiation hydrodynamics*, Pergamon Press, Oxford.
- Fernández JE, Hubbell JH, Hanson AL and Spencer LV (1993) Polarization effects on multiple scattering gamma transport. *Rad. Phys. Chem.* **41**, 579-630.
- Fernández JE (1999) Polarization effects in multiple scattering photon calculations using the Boltzmann vector equation. *Rad. Phys. Chem.* **56**, 27-59.