# X-ray photon spectroscopy calculations

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# keywords

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

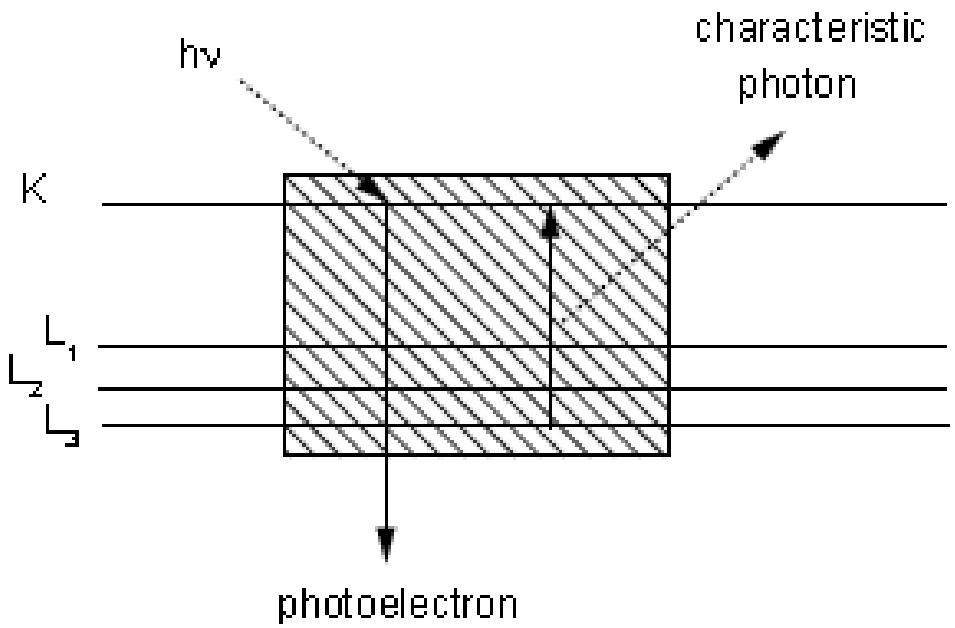
# X-RAYS

- **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

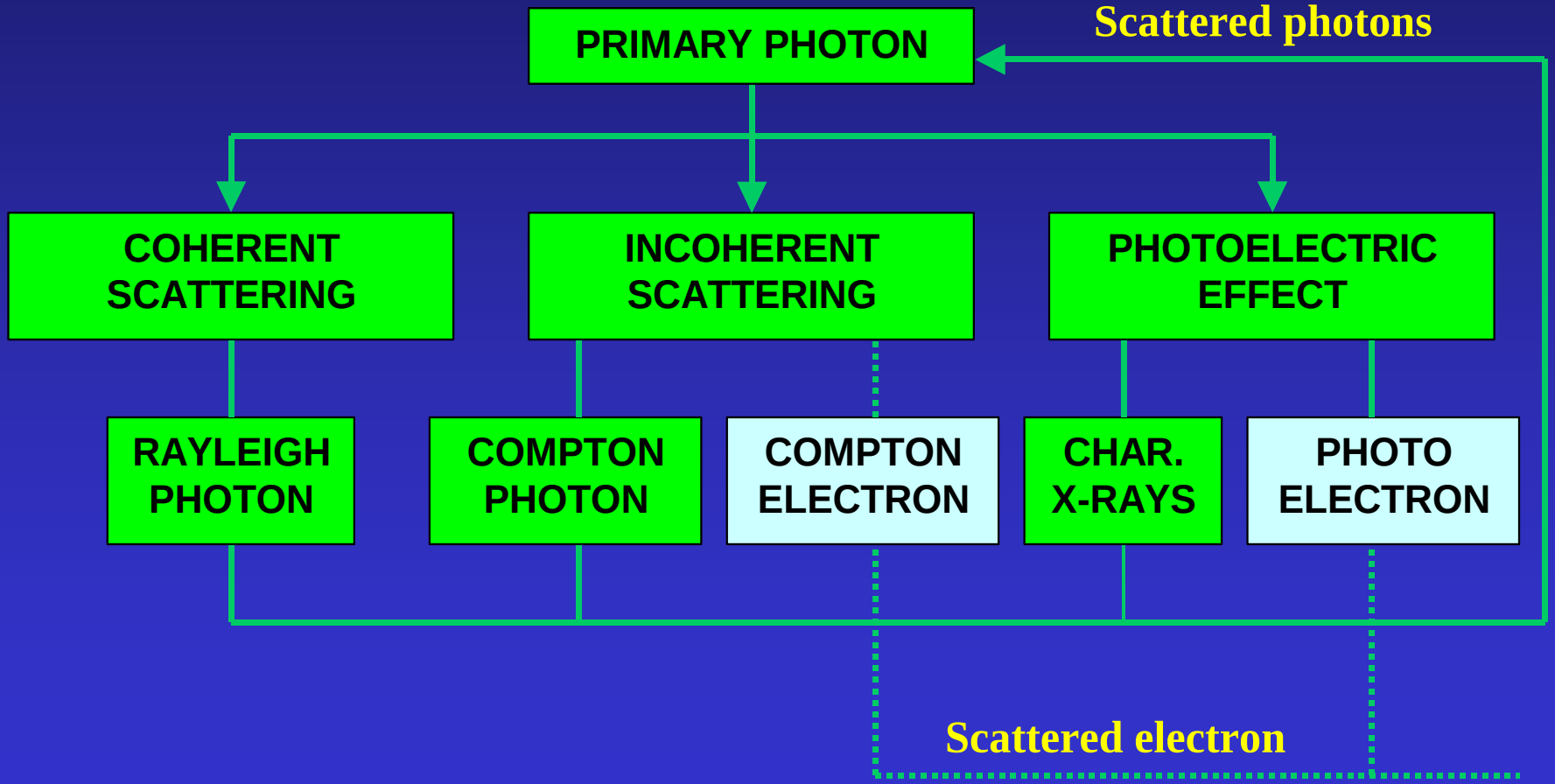
- Multiple scattering models describe the influence of the prevailing interactions in the x-ray regime (photoelectric effect, Compton scattering and Rayleigh scattering)
- The photoelectric effect itself is a ‘scattering process’

# Photoelectric effect as ‘scattering’

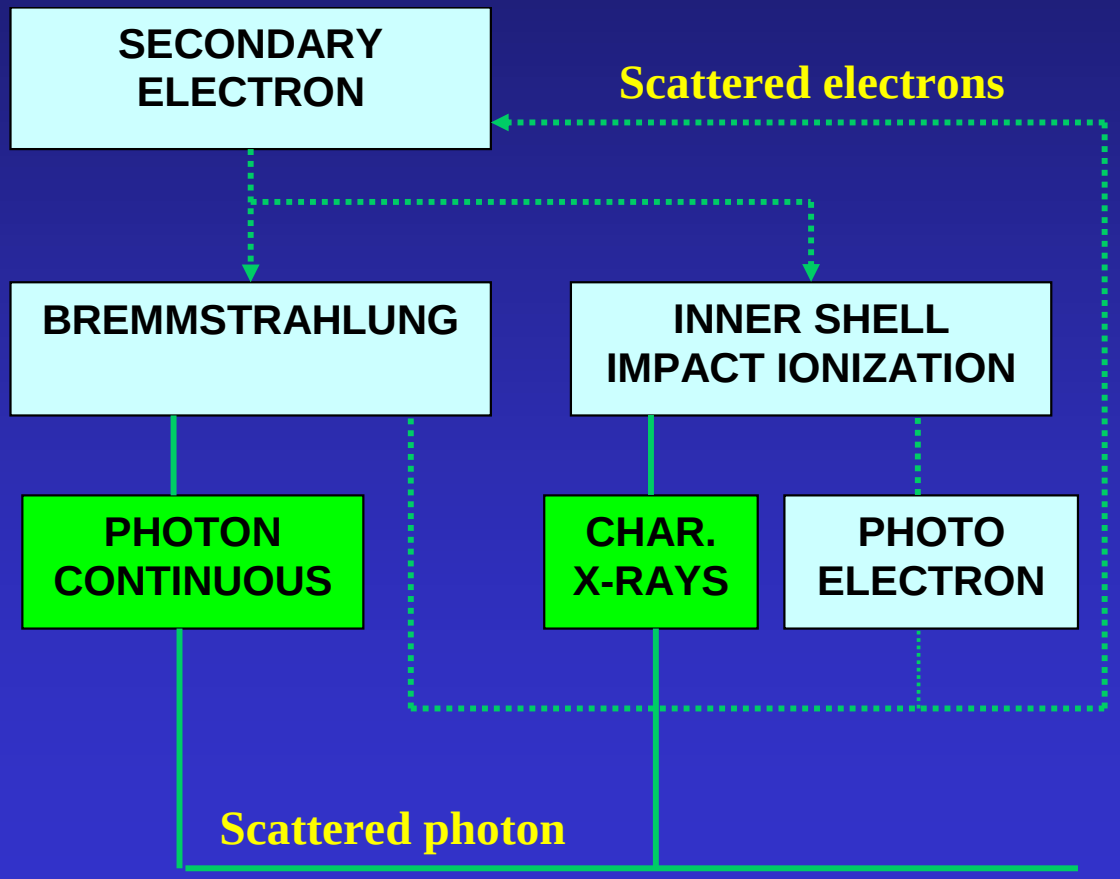



photoelectric absorption + radiative transition = photoelectric 'scattering'

# THE PREVAILING INTERACTIONS IN THE *X-RAY* REGIME



# Electron-photon coupling



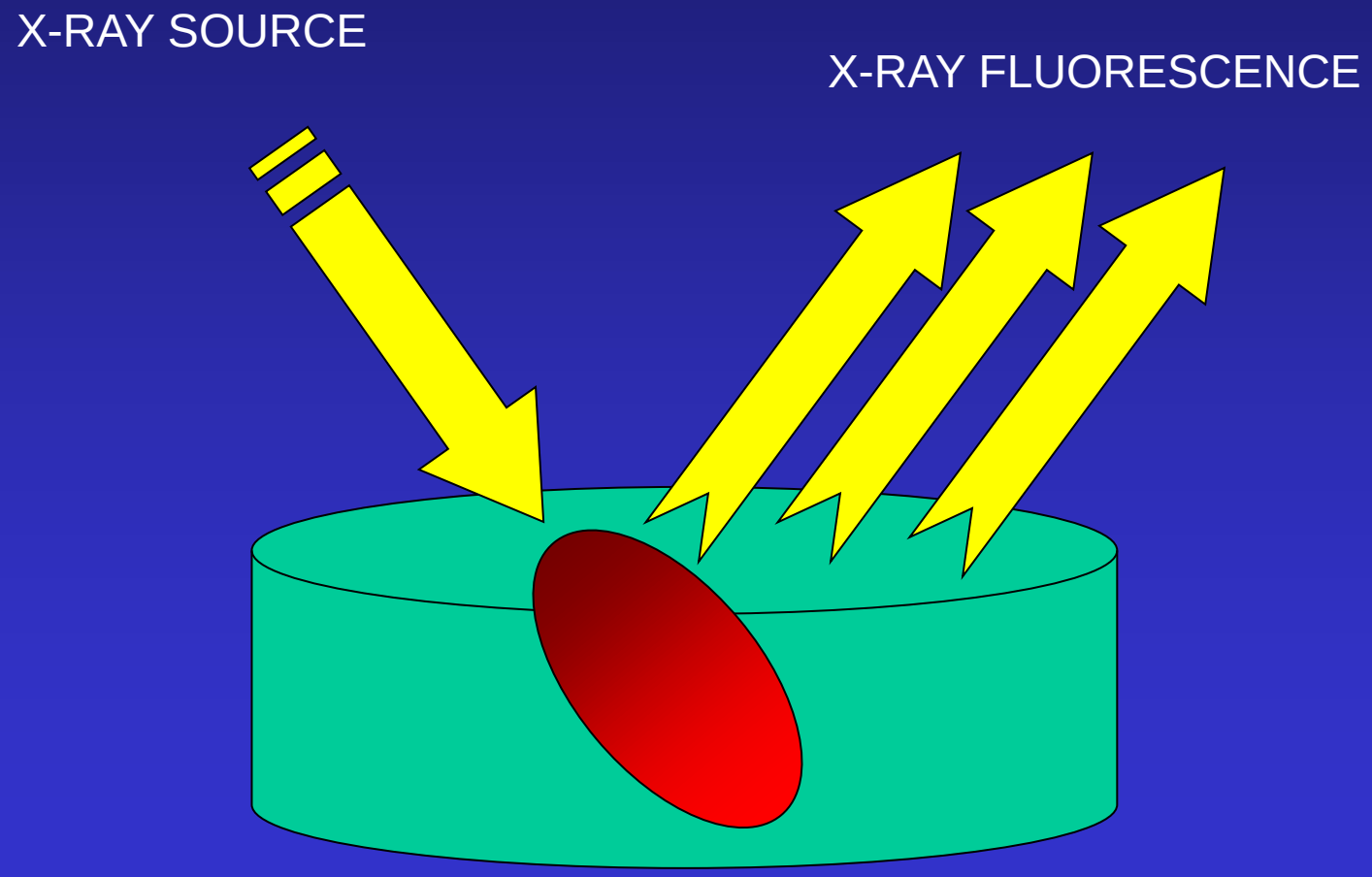
# X-RAY SPECTROMETRY TECHNIQUES

# 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 FLUORESCENCE

SOURCE: INCOHERENT
UNPOLARIZED OR POLARIZED

GEOMETRY: REFLECTION

INTEREST COLLISION: PHOTOELECTRIC EFFECT (GIVING CHARACTERISTIC LINES)

PENETRATION: LOW-MEDIUM

MEASURE: ELEMENTAL COMPOSITION IN A VOLUME

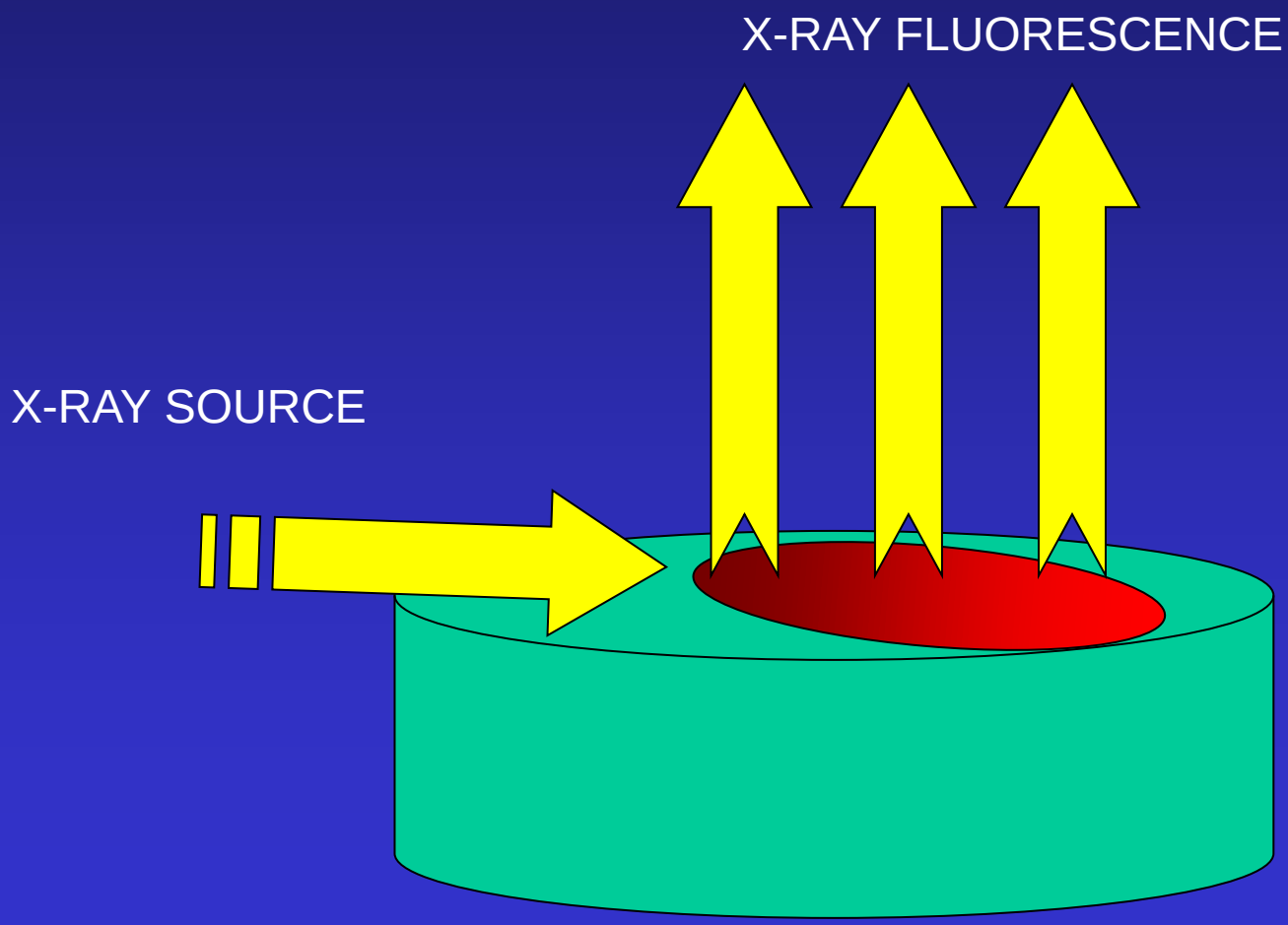
MAPPING: YES (2-D), 3D WITH CONFOCAL XRF

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

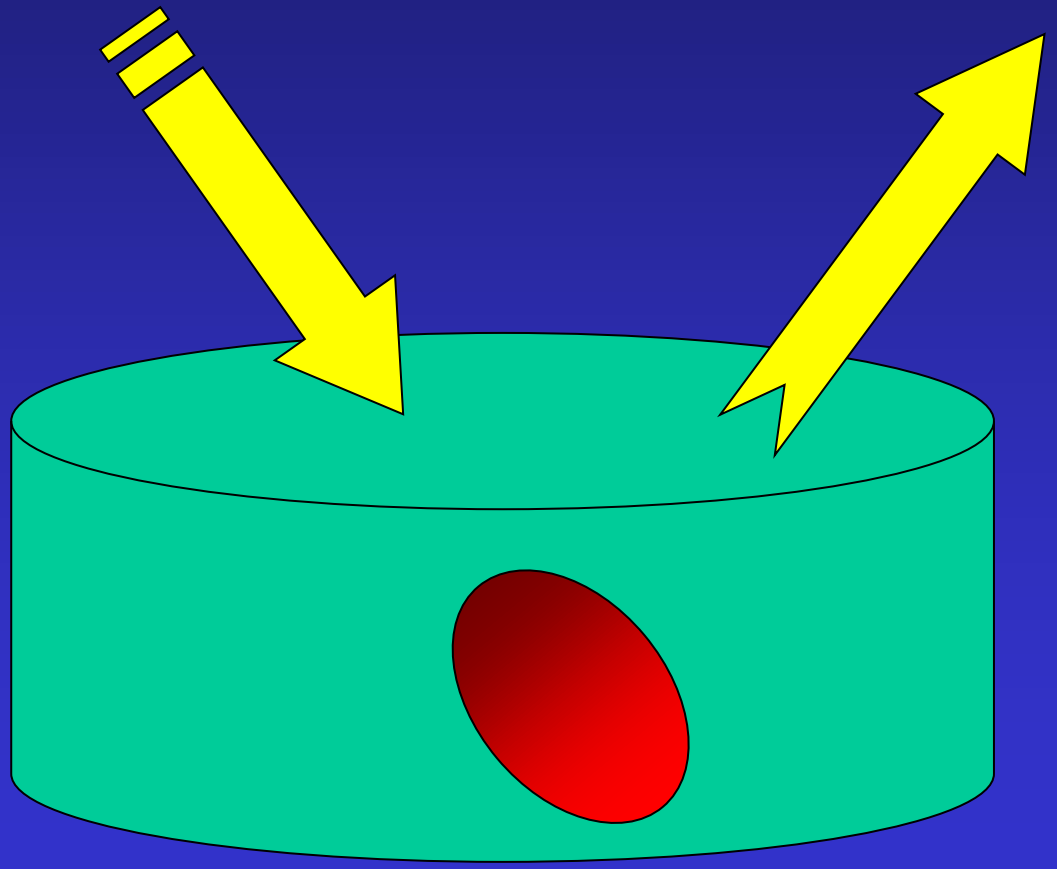
EQUIPMENT: LABORATORY (ALIGNEMENT IS DELICATE)

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

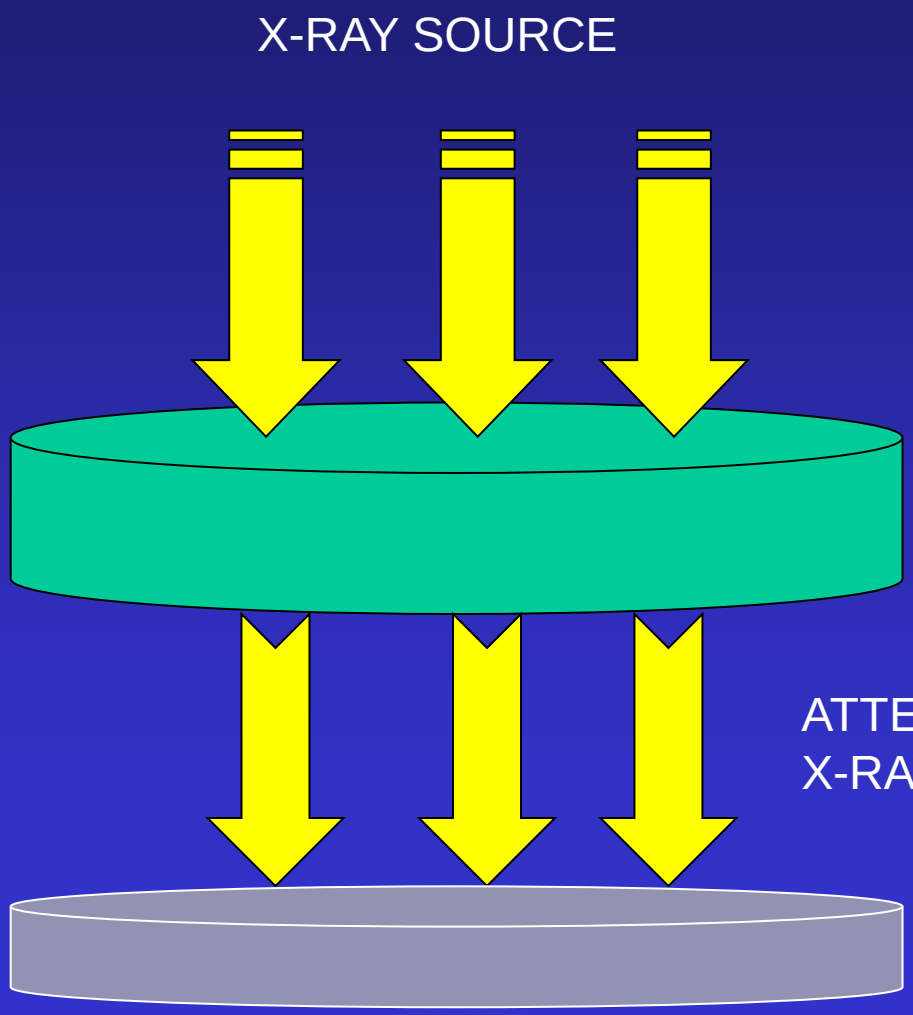
MAPPING: YES (2-D)

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

EQUIPMENT: PORTABLE

DATA HANDLING: HEAVY (STATISTICAL METHODS)

# X-RAY RADIOGRAPHY



# X-RAY RADIOGRAPHY

SOURCE: INCOHERENT
UNPOLARIZED

GEOMETRY: TRANSMISSION

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

PENETRATION: MEDIUM-HIGH

MEASURE: CONTRAST IS ATTENUATION

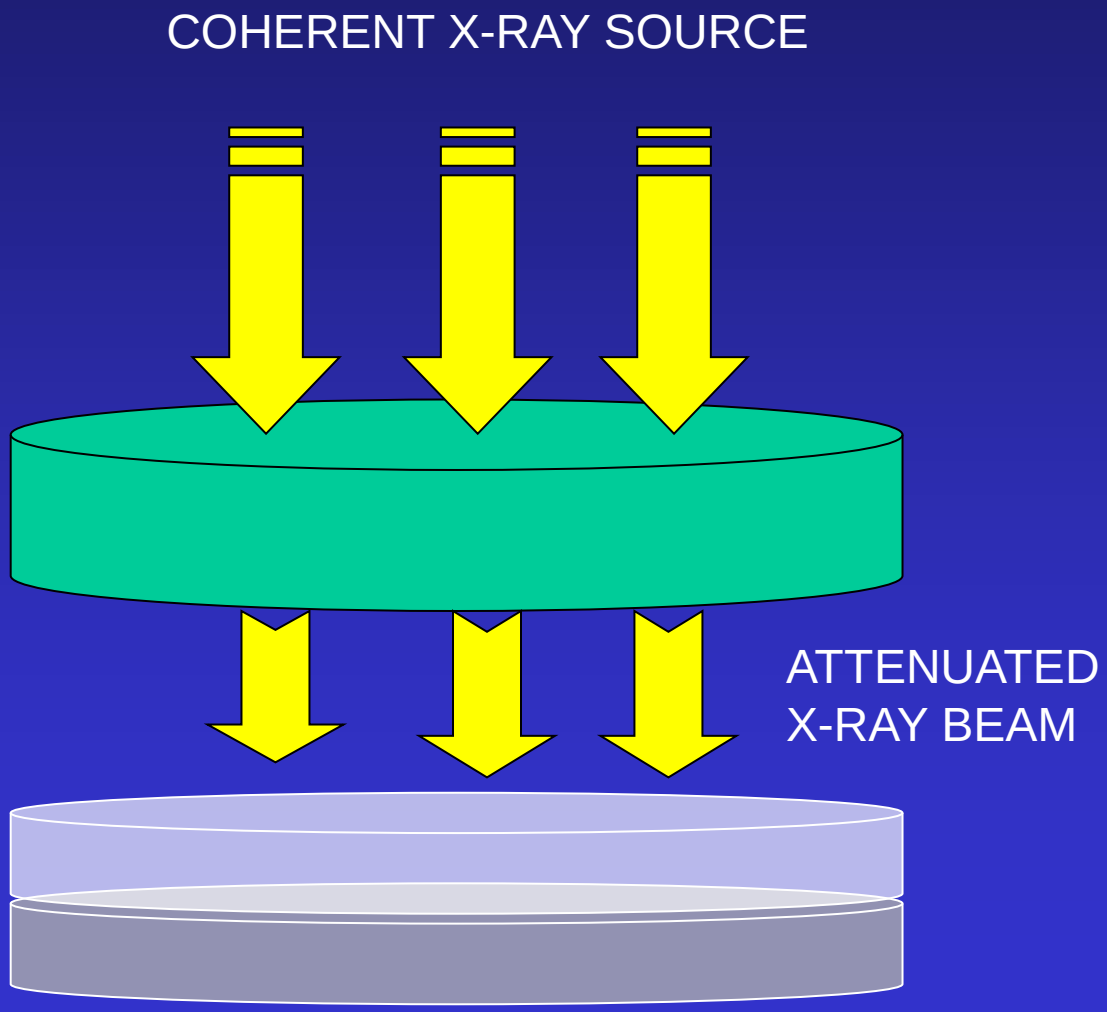
MAPPING: YES (2-D)

MATERIALS: LIGHT ELEMENTS

EQUIPMENT: LABORATORY

DATA HANDLING: LIGHT

# PHASE CONTRAST RADIOGRAPHY



# PHASE CONTRAST RADIOGRAPHY

SOURCE: COHERENT
UNPOLARIZED OR POLARISED

GEOMETRY: TRANSMISSION

INTEREST COLLISION: RAYLEIGH SCATTERING

PENETRATION: MEDIUM-HIGH

MEASURE: CONTRAST IS ATTENUATION

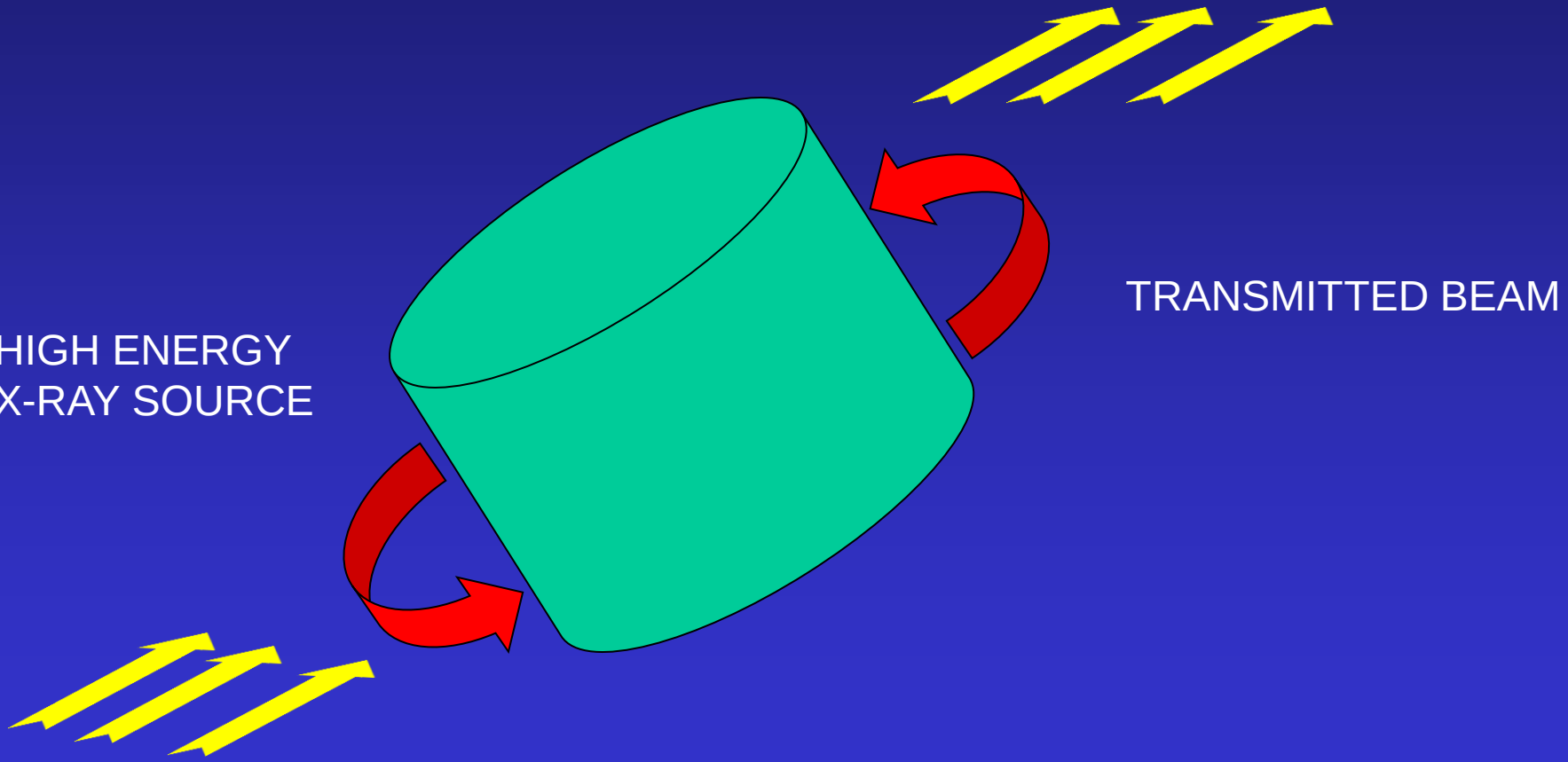
MAPPING: YES (3-D EFFECTS)

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

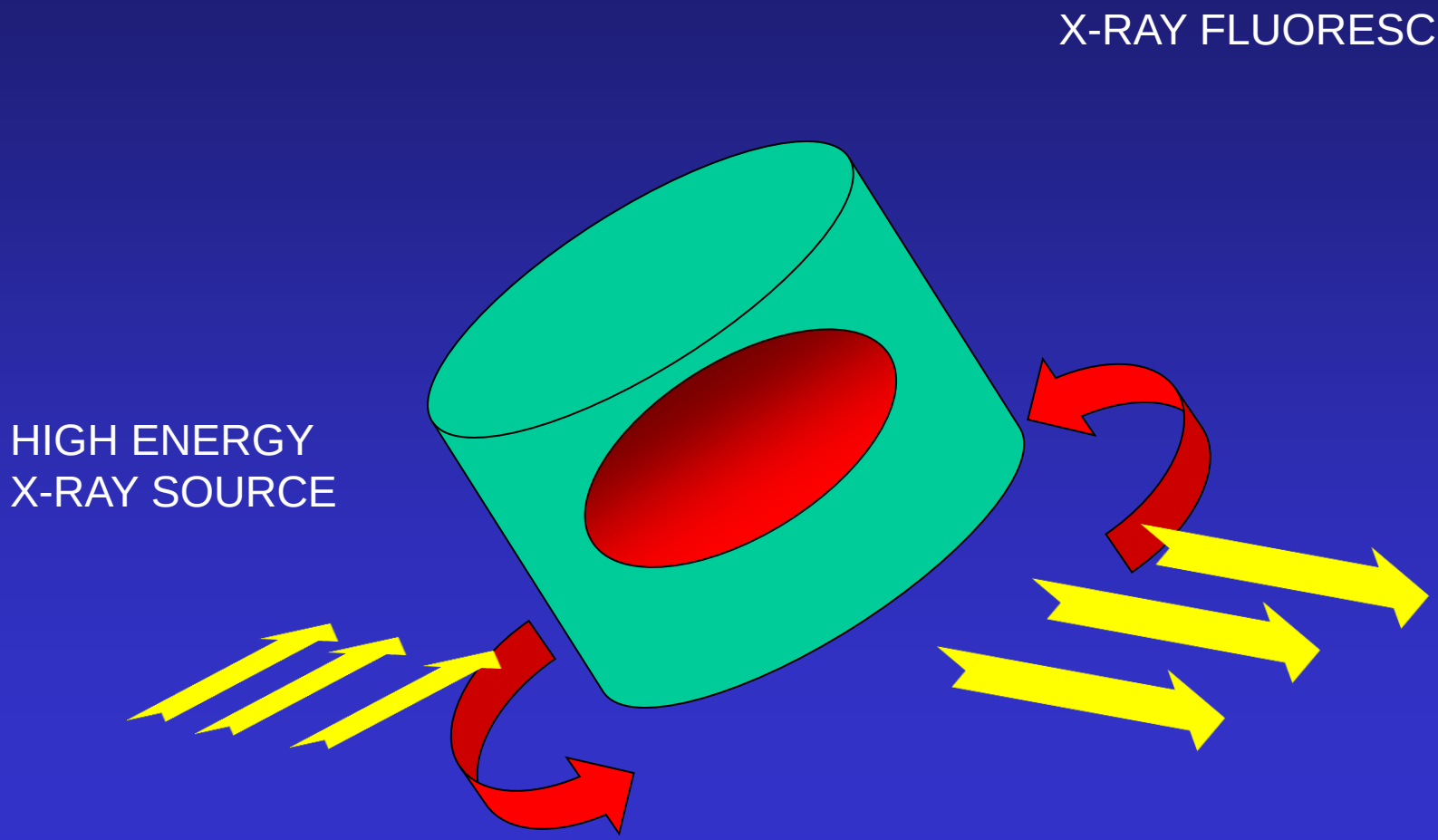
MAPPING: YES (3-D ATTENUATION COEFFICIENT)

MATERIALS: SMALL SIZE OBJECTS

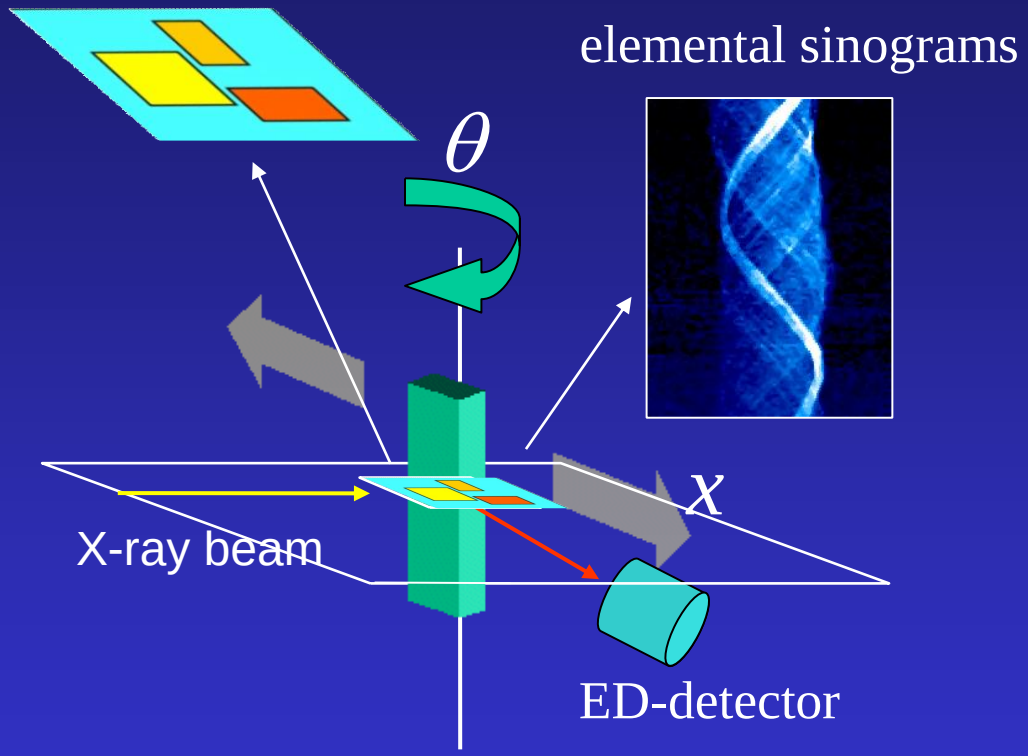
EQUIPMENT: LABORATORY

DATA HANDLING: HEAVY (RECONSTRUCTION METHODS)

# X-RAY FLUORESCENCE TOMOGRAPHY



# 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

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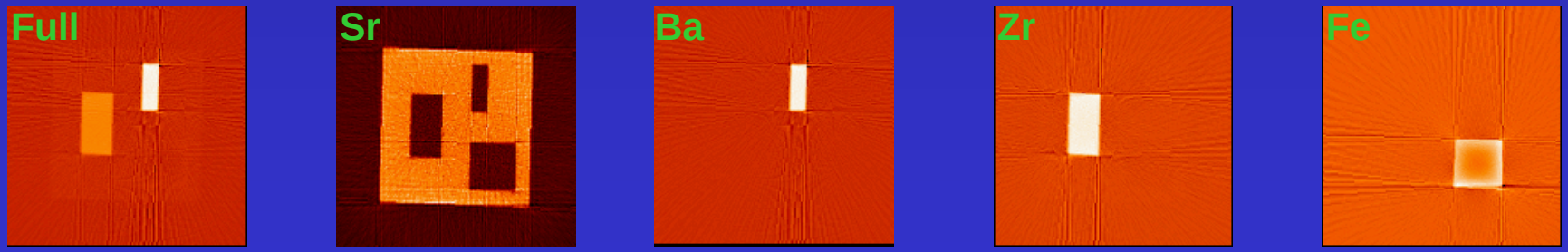
# 3D – MCSHAPE: XRF Tomography

Full spectrum | Sr | Ba | Zr | Fe

120 × 3°

reconstruction

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# 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

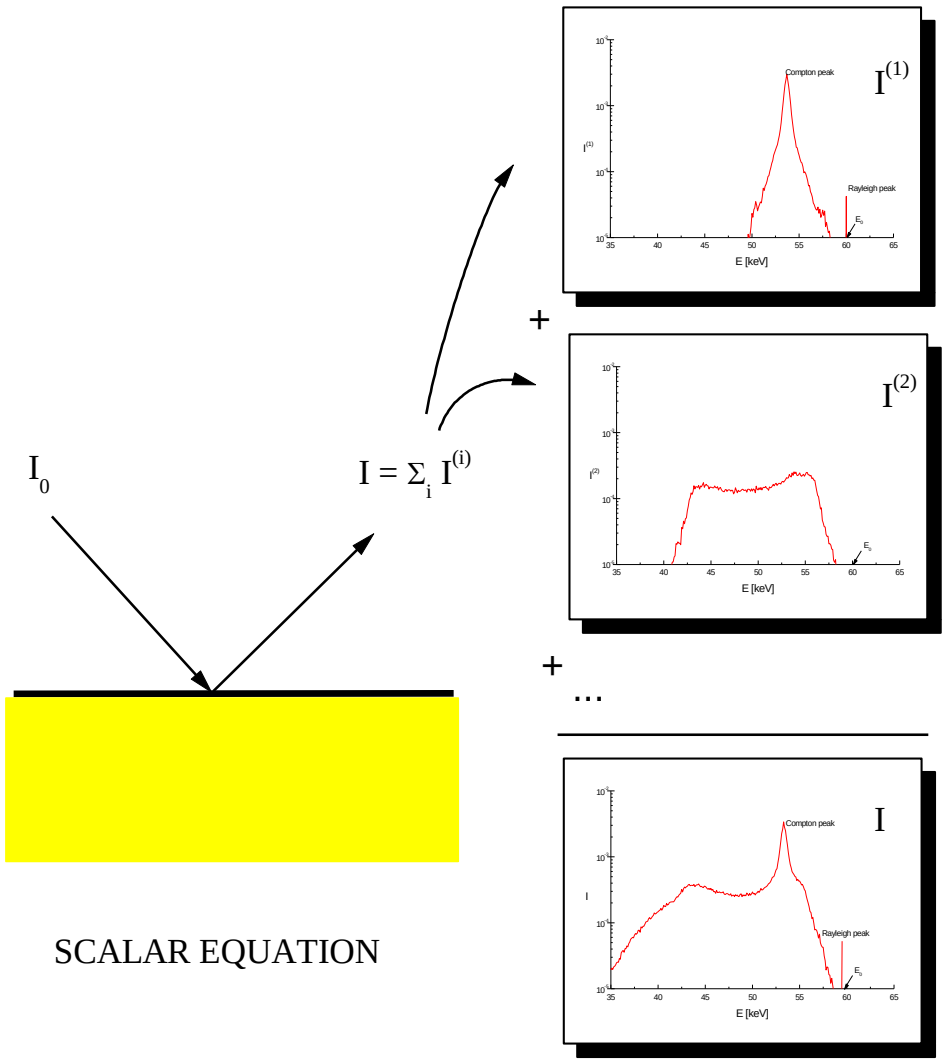
one collision

| a | Photoelectric effect | Rayleigh scattering | Compton scattering |
|---|---|---|---|
| | (P)<br>characteristic lines<br>(discrete) | (R)<br>Rayleigh peak<br>(discrete) | (C)<br>Compton peak<br>(continuous) |

two collisions

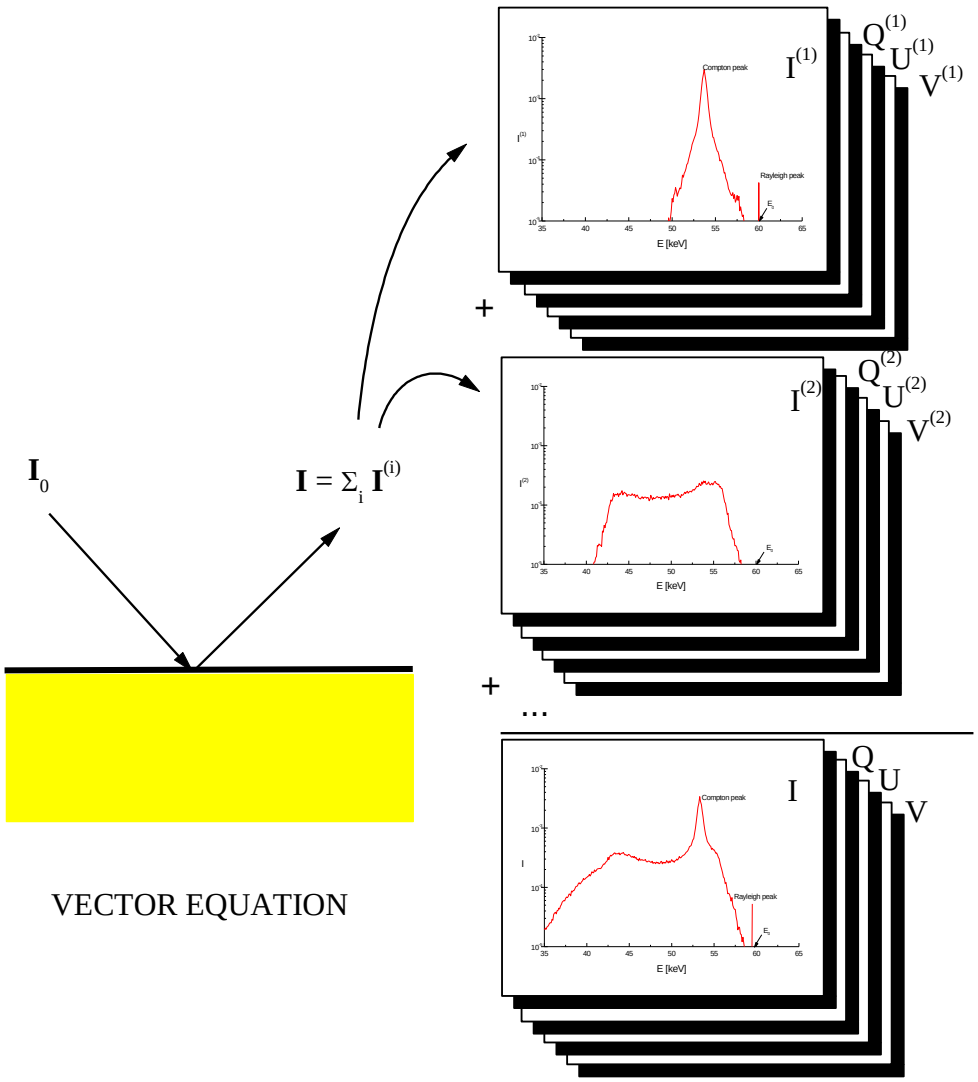
| a \ b | Photoelectric effect | Rayleigh scattering | Compton scattering |
|---|---|---|---|
| Photoelectric effect | (P,P)<br>XRF secondary enhancement<br>(discrete on XRF line) | (P,R)<br>XRF enhancement due to scattering<br>(discrete on XRF line) | (P,C)<br>XRF enhancement due to scattering<br>(continuous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

# Scalar transport equation




SCALAR EQUATION

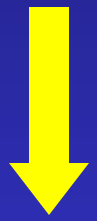
# Vector transport equation




VECTOR EQUATION

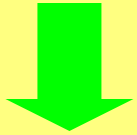
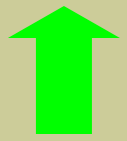
# SOLUTION TECHNIQUES

**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.