

Advanced Characterization Methods II : Radiation interactions with matter

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1- Introduction

2- Electronic structure

3- Interactions: general overview

4- Photon-matter interactions

- 4.1- Atomic scale
- 4.2- Structural effects

5- Electrons-matter interactions

6- Neutron-matter interactions

1- Introduction

Particles that are used for characterization

- Photons
- Electrons
- Neutrons
- Ions

2 types of interactions

- Elastic interaction: no energy transfer
- Inelastic interaction: energy transfer

Energy transfer depends on

- The nature of the interaction
- The interaction mechanism
- Frequency and probability of the interaction

Diffraction

- Atoms organized in space
 - incoming radiation will be scattered in some specific direction
 - study of organization of the scattered radiation will provide input on atom layout in space

Spectroscopy

- Atoms or structures absorb part of the incoming radiation and emit other radiations
 - study of the absorption / scattering energies
 - information on chemistry, vibrations, etc

Microscopy

- The interaction depends on location in the sample
 - formation of 2D or 3D images

2- Electronic structures

Atom with atomic number Z

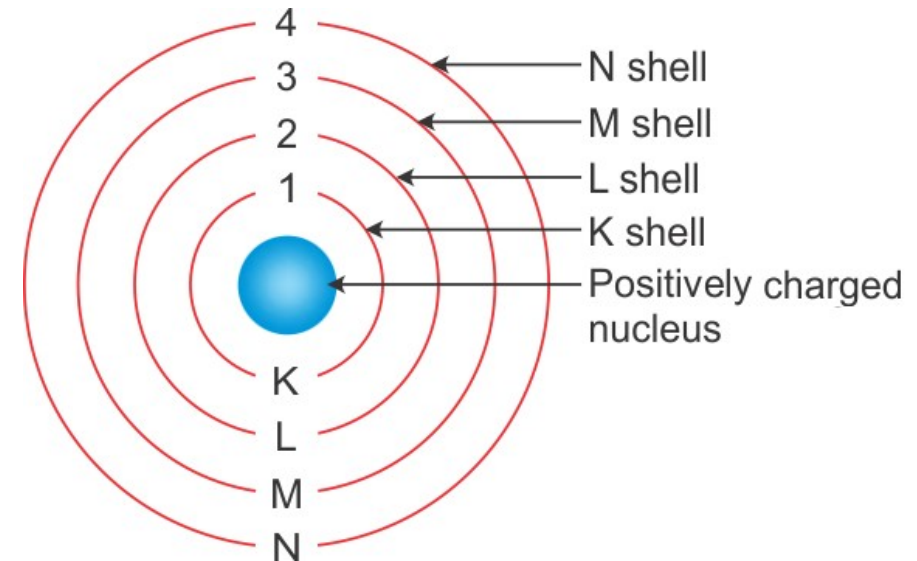
- Positive charge in the nucleus Ze (Z protons and some neutrons)
- Electron cloud with charge $-Ze$

Schrödinger equation, quantum mechanics

- Electrons are placed at quantified energy levels, shells and subshells
- Quantum numbers n, l, m, s

Pauli exclusion principle

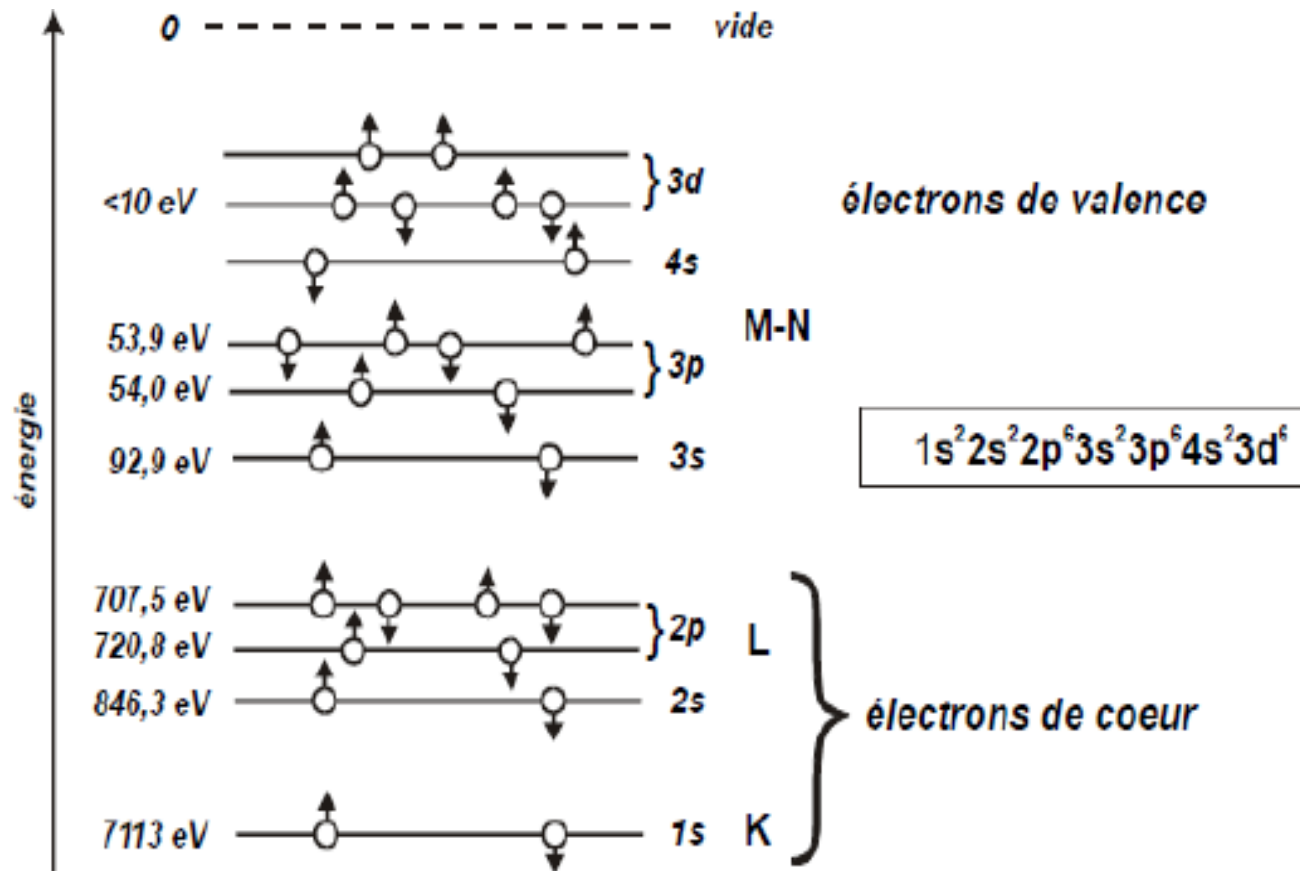
- 2 electrons can not be in the same state



Electron shells

- $n=1$ (K), max 2 e^-
- $n=2$ (L), max 8 e^-
- $n=3$ (M), max 18 e^-
- $n=4$ (N), max 32 e^-
- $n=5$ (O), max 50 e^-
- etc

Illustration: iron electronic structure



**Structure électronique
d'un atome de fer**

Energy scale:
energy required to eject the electron from the atom

3- General concepts

I : intensity = number of particles per time unit

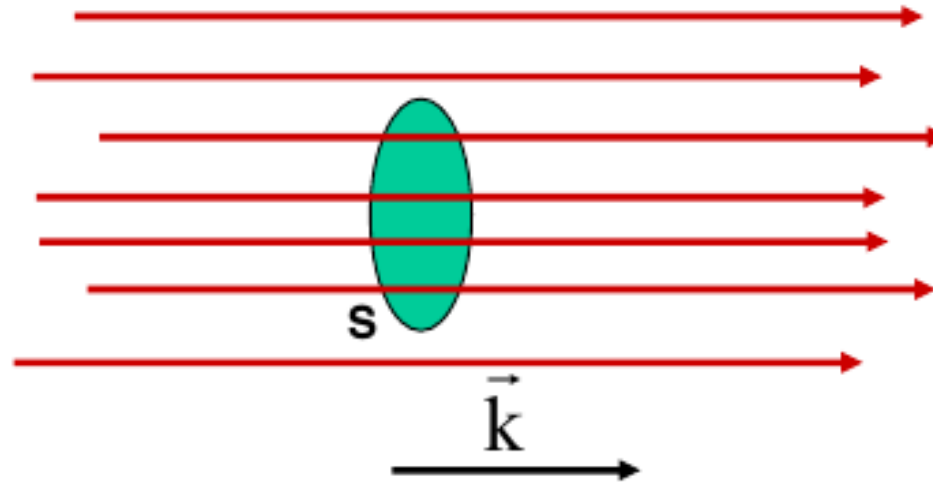
F : flux = number of particles per time and surface unit

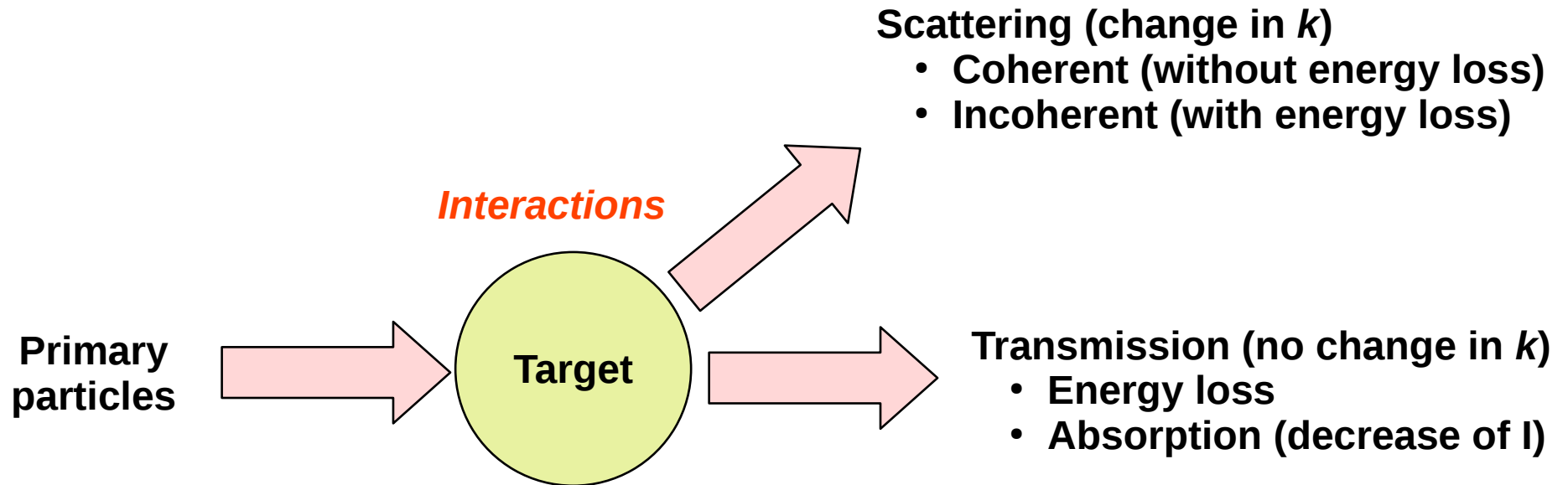
E : incoming particles energy

$\mathbf{k}$: wave vector

- Direction of the incoming flux
- Norm proportional to energy

temps t :
 n particules
 $I = n/t$
 $F = I/S = n/(tS)$





Effects on target

- Local heating (meV)
- Excitation of vibrations and rotations (vibrons, rotons) (1-100 meV)
- Elastic waves (phonons, plasmons) (1-10 eV)
- Excitation of external electronic levels (1-100 eV)
- Excitation of core electronic levels (100 eV – 100 keV)
- Atomic displacement
- Etc

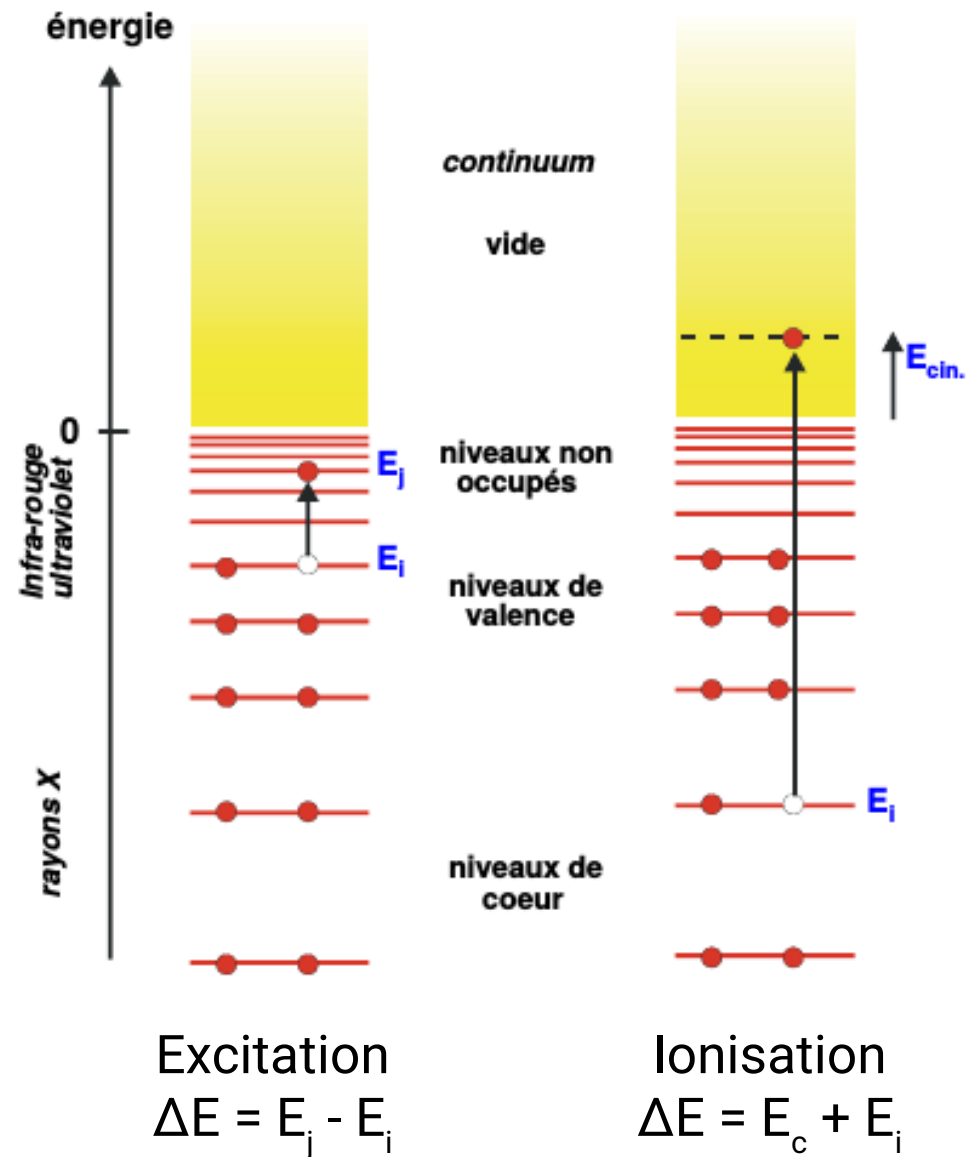
Excitation vs. ionization

Excitation

- Electron transfer to a higher energy level
- No charge change for the atom
- Energy given to the electron = energy difference between both levels

Ionization

- Ejection of the electron
- Charge change for the atom
- Energy given to the electron > ionization energy



4- Interactions of photons with matter

Infrared

- 1 mm to 0.7 μm
- 10^{-3} to 1 eV

Visible light

- 400 to 700 nm
- 1 to 3 eV

Ultraviolet

- 10 nm to 400 nm
- 3 to 100 eV

Soft-X-rays

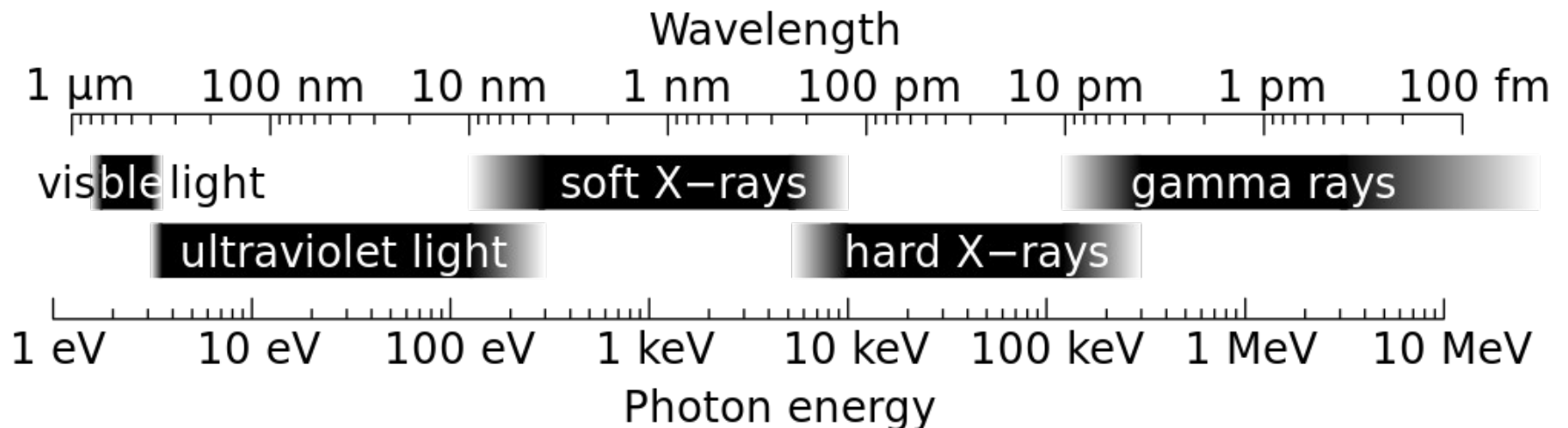
- 0.1 nm to 10 nm
- 100 eV to 10 keV

Hard-X-rays

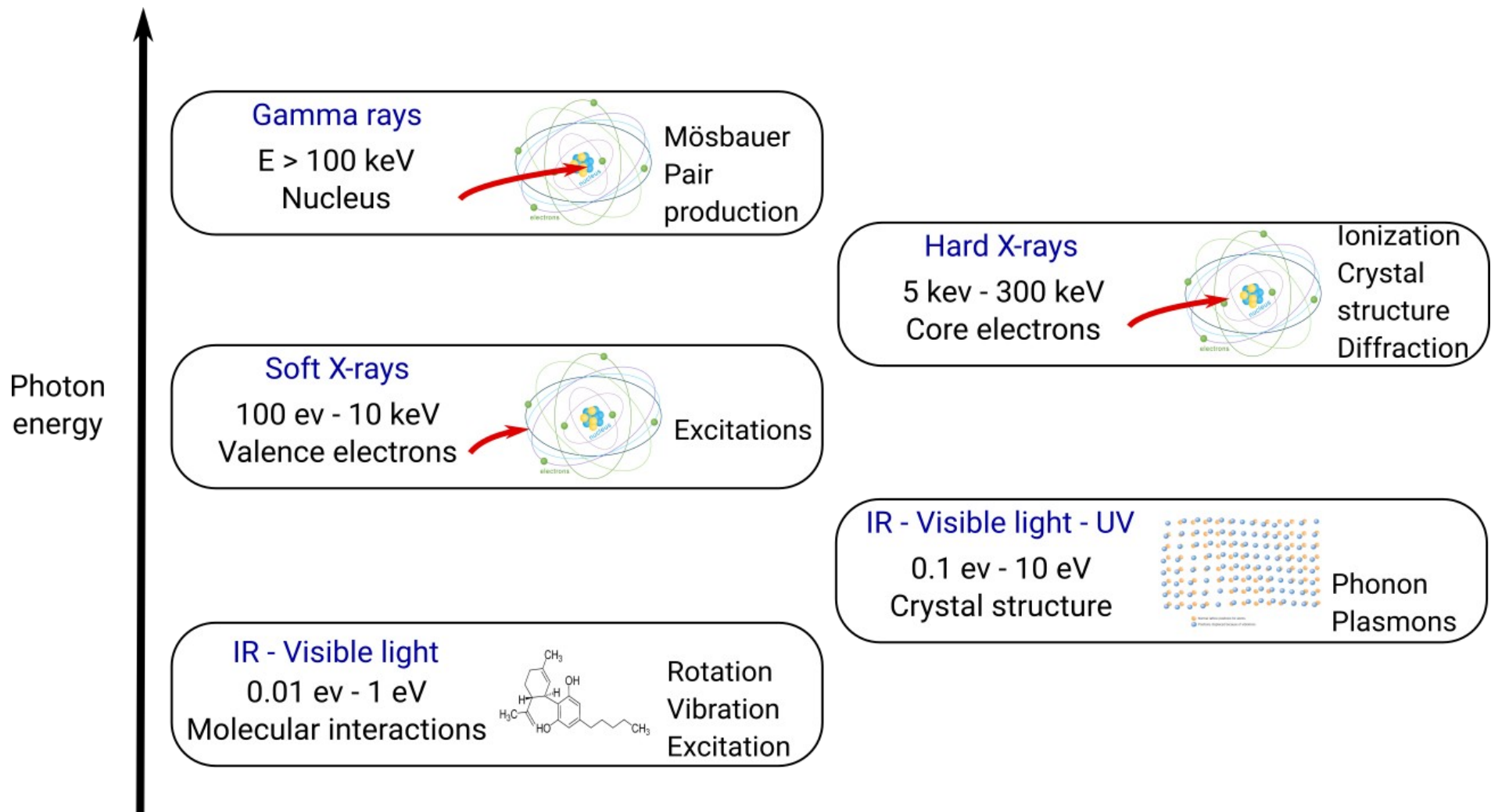
- 0.005 to 0.2 nm (0.05 to 2 $\text{\AA}$)
- 5 to 300 keV

Gamma-rays

- $E > 100 \text{ keV}$



Effect of photon energy



Atomic scale

- Thomson – Rayleigh diffusion
- Photo-electric effect
- Compton effect
- (materialization and nuclear reactions; high energy)

Crystalline scale (low energy)

- Molecular interactions (vibrations, rotations, etc)
- Phonons (collective oscillations of atoms)
- Plasmons (collective oscillations of electrons)

Crystalline scale (high energy)

- Diffraction

Incoming photon parameters

- Intensity I_0
- Wavelength / frequency λ_0 / ν_0
- Wave vector $\mathbf{k}_0$
- Energy $E_0 = h\nu_0$

After the interaction

- Transmission
 - Less intensity (absorption) $I < I_0$
 - Energy loss $E < E_0$, transmitted energy spectrum $I(E)$
- Change of wavevector $\mathbf{k}$: scattering
 - No energy loss: elastic scattering
 - With energy loss: inelastic scattering

4.1- Interactions of photons with matter

Atomic scale

Thomson/ Rayleigh scattering

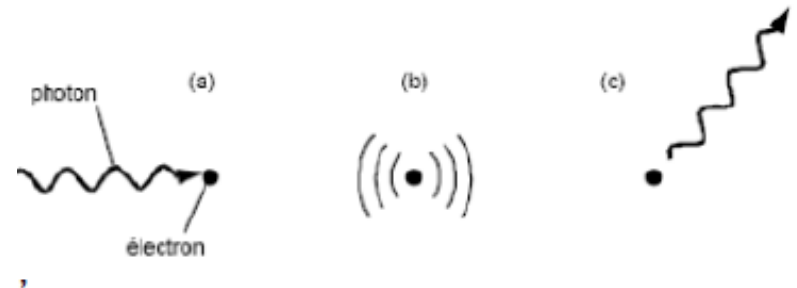
Low energy photons (IR, visible)

Photon absorbed and re-emitted in another direction → scattering

No change in energy → elastic scattering

Thomson scattering

- Photon absorbed by a single electron
- Excited state for the electron
- Emission of a new photon, same E, but $\neq$ direction



Rayleigh scattering

- Photon interacts with the whole electron cloud
- Excited state
- Emission of a new photon, same E, but $\neq$ direction

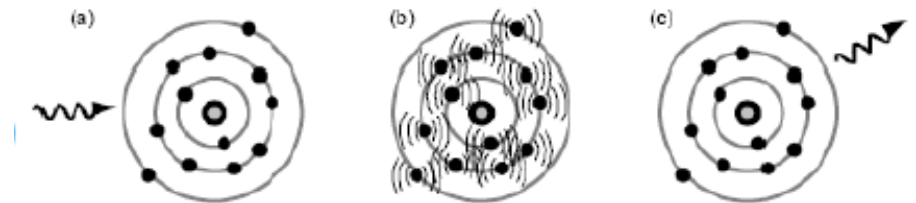


Photo-electric effect (50 eV – 50 keV)

Interaction between a photon and electrons

- Incoming photon $E = h \nu$
- Ionization and absorption of the photon
- Kinetic energy of the electron
 $E_c = h \nu - E_i$
- Excited electronic state in the atom
- Emission of multiple X-ray photons to return to the atomic ground state

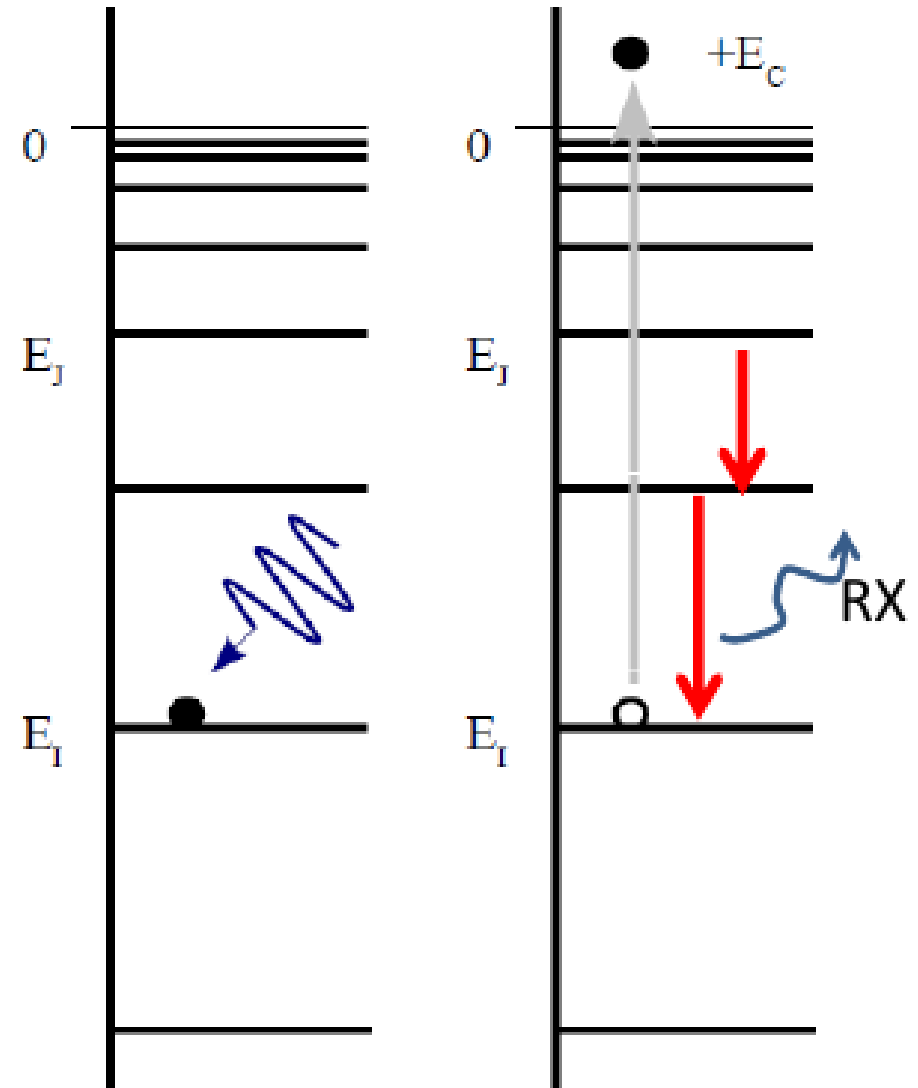
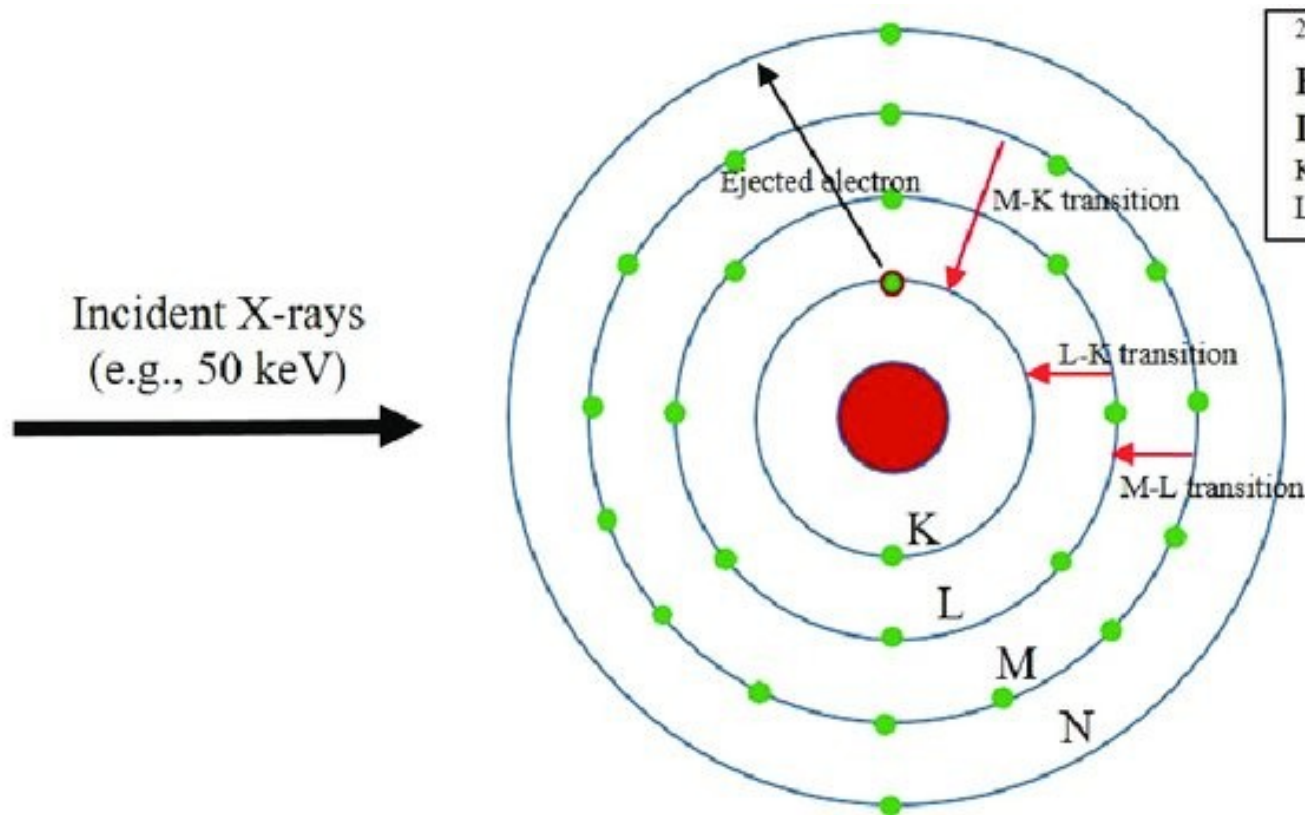


Illustration : Iron



26
Fe
Iron
$K\alpha = 6.405$
$L\alpha = 0.705$

$K\alpha$ (K-alpha) :

- L to K transition
- Emission of a photon with 6.4 keV

$K\beta$ (K-beta) :

- M to K transition
- Emission of a photon with 7.1 keV

$L\alpha$ (L-alpha) :

- M to L transition
- Emission of a photon with 0.7 keV

Illustration : Teixeira Ribeiro, Ciência e Agrotecnologia, 2017

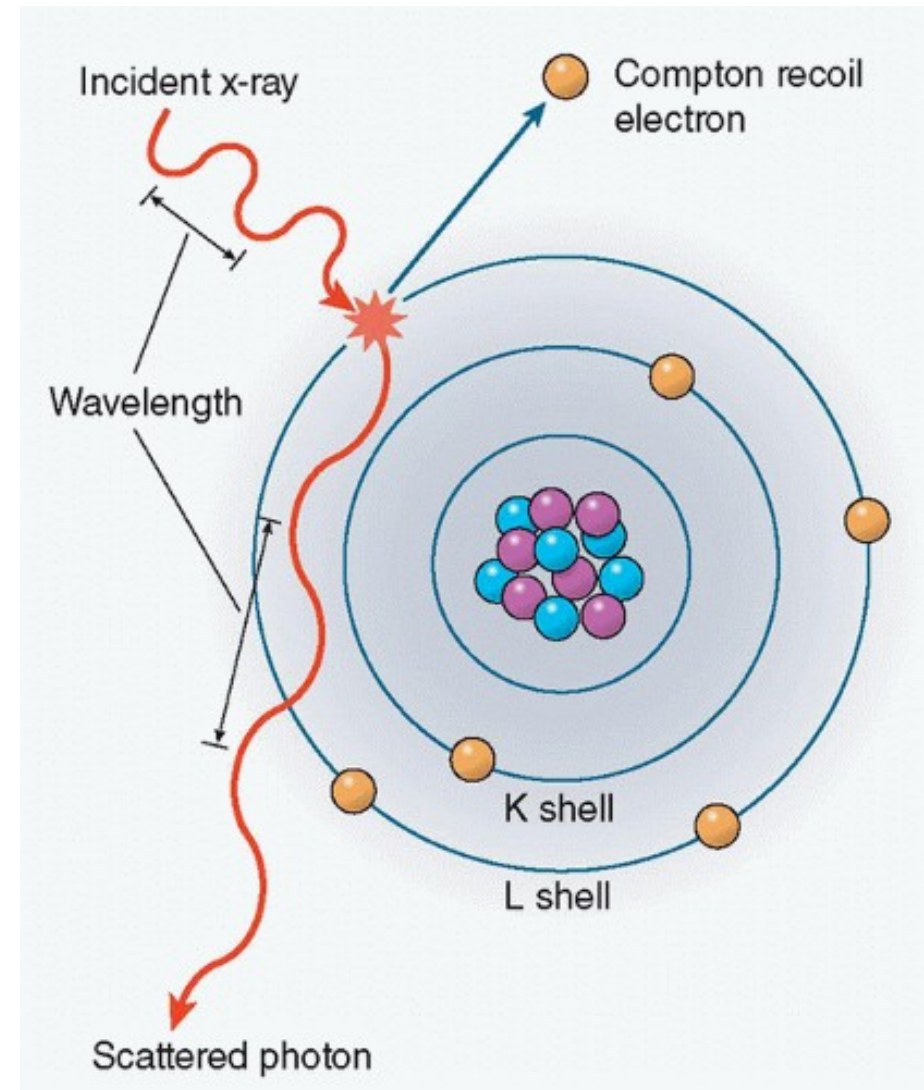
Compton scattering

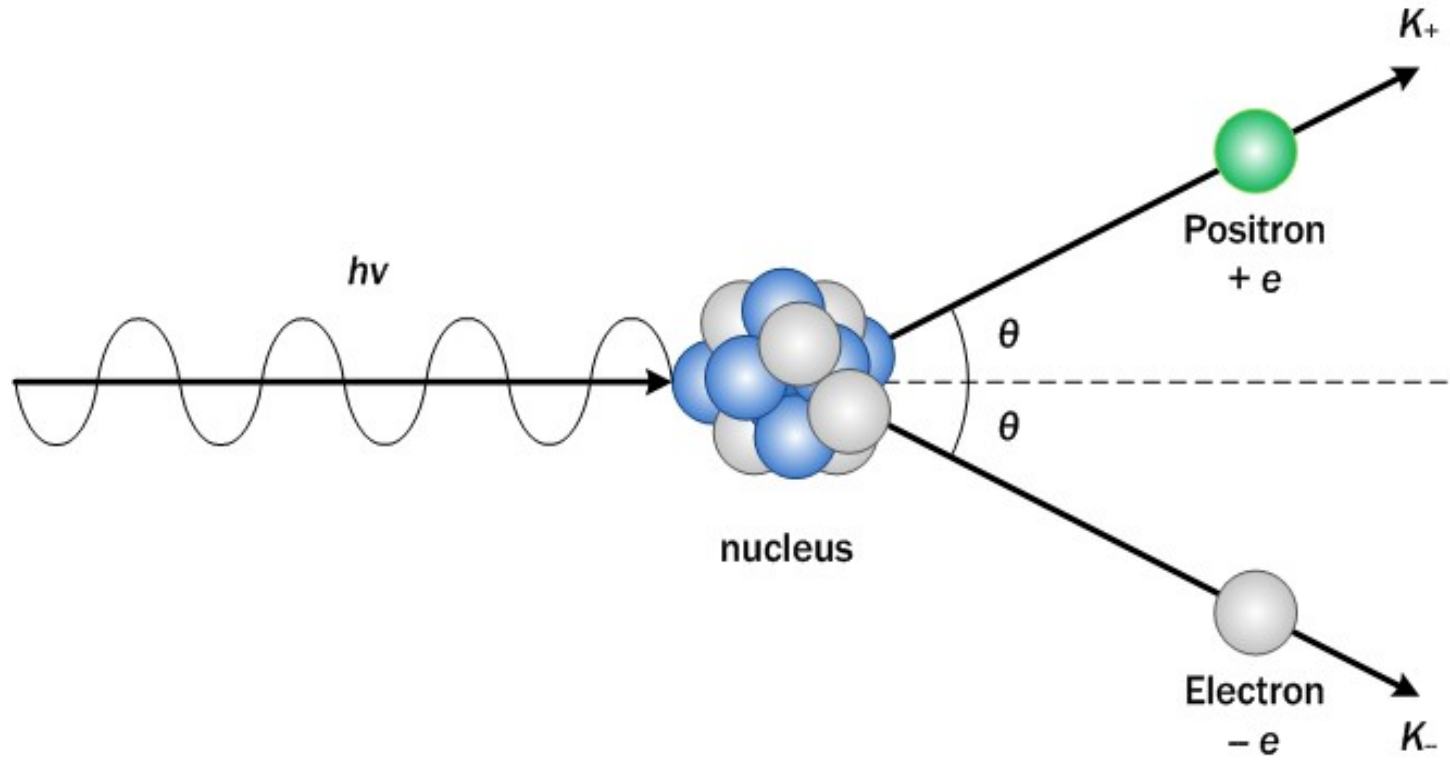
Interaction between incoming photon and electrons in the electron cloud

Ionization + creation of a new photon

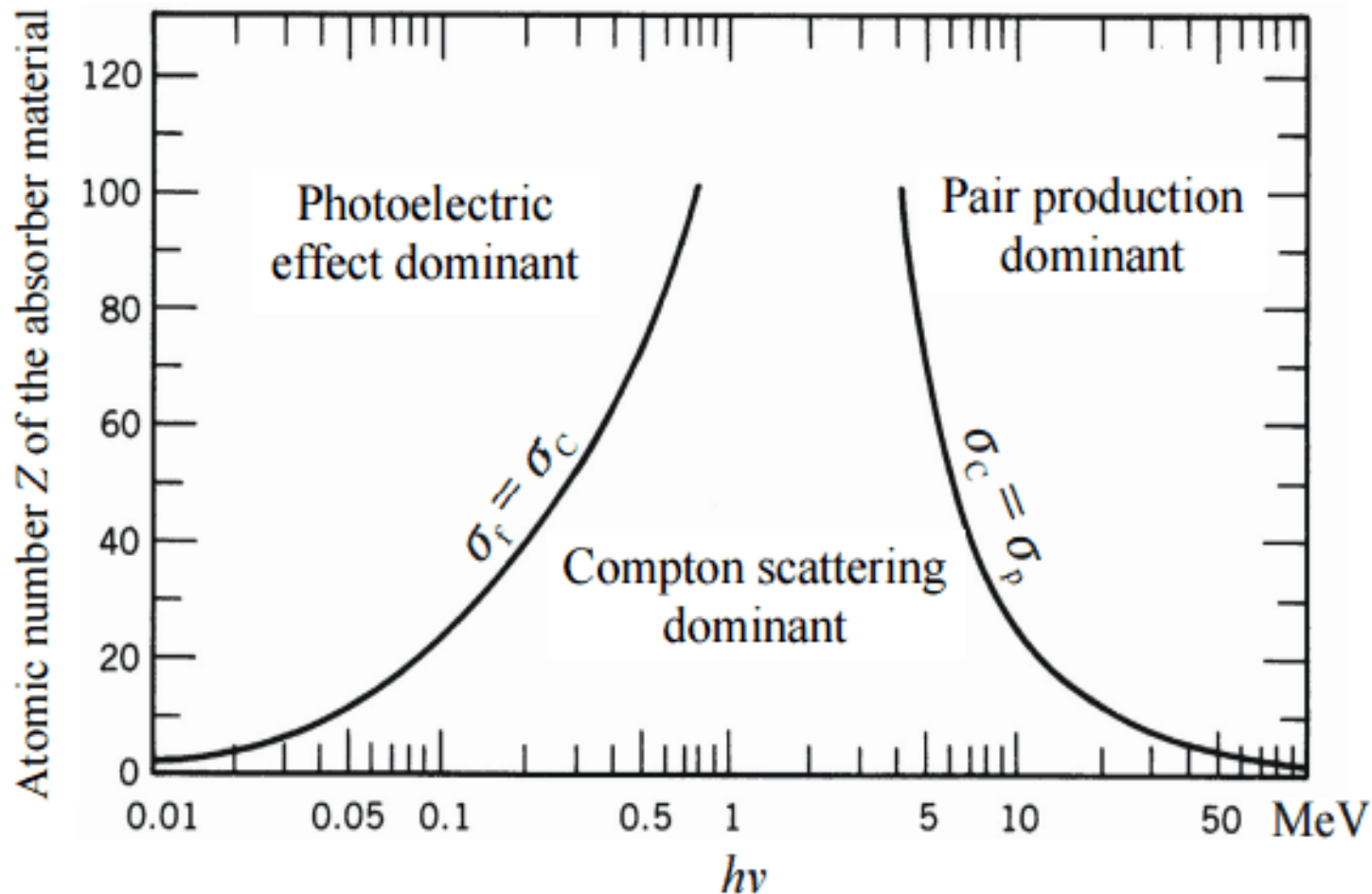
Energy conservation:

incoming photon energy =
scattered photon energy +
scattered electron energy +
ionization energy





Effect of atomic number and photon energy



Atom – photon interactions: summary

Thomson-Rayleigh scattering

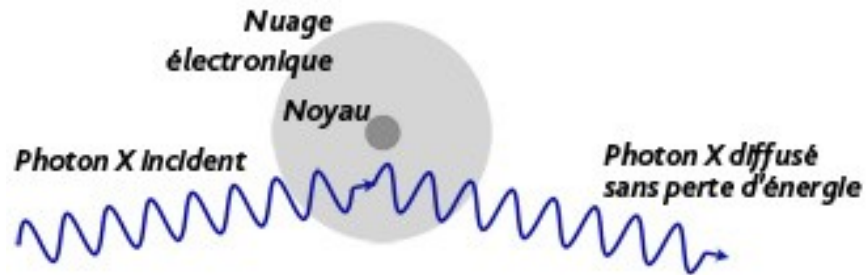
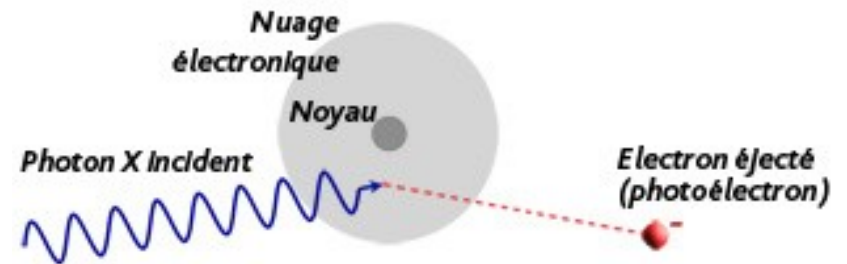
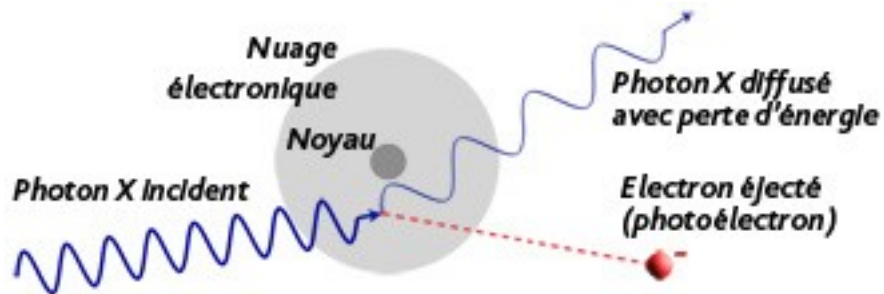


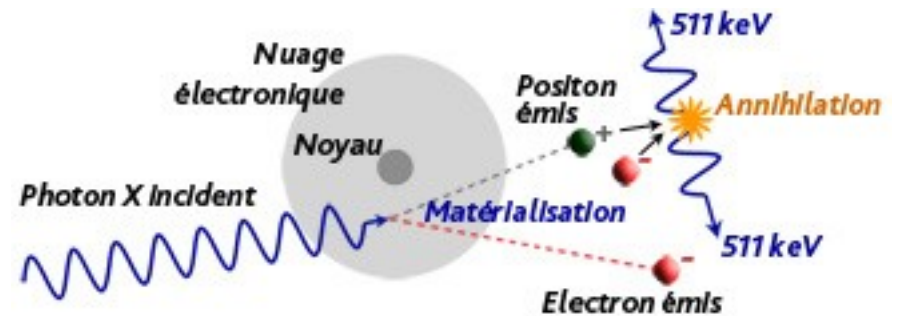
Photo-electric effect



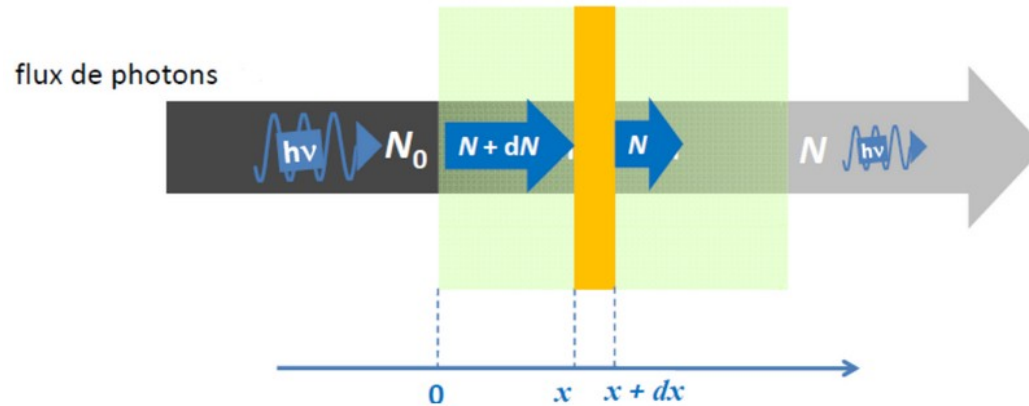
Compton scattering



Pair creation



X-ray absorption by matter



$$N = N_0 e^{-\mu x}$$

N : number or flux of photons

x : sample thickness

μ : linear attenuation coefficient

Table on side: 50% attenuation
length, $L = \ln(2)/\mu$

ordre de grandeur *CDA*:

CDA = couche de demi-atténuation

	30 keV	100 keV	500 keV
air	25 m	35 m	60 m
eau (<i>liquide</i>)	2 cm	4 cm	7 cm
béton	3 mm	2 cm	4 cm
plomb	0,02 mm	0,1 mm	4 mm

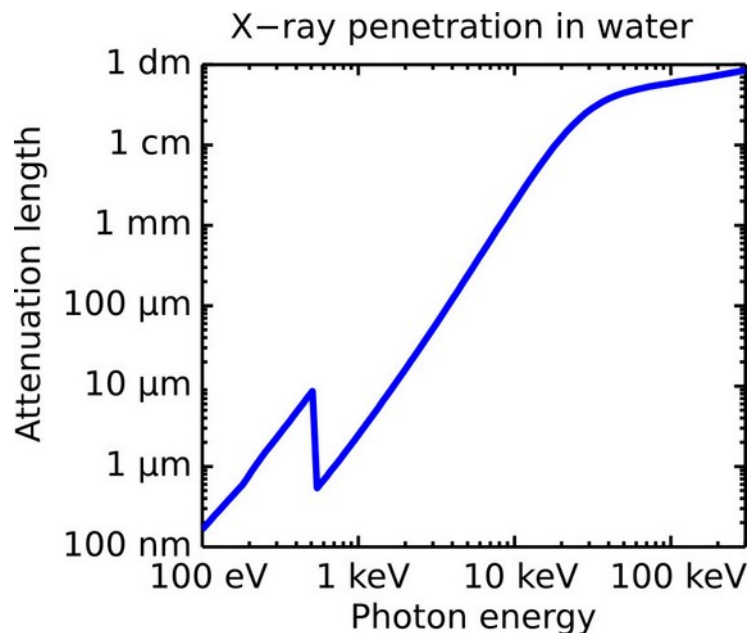
Attenuation is an effect of the different scattering mechanisms

Linear attenuation coefficient μ depends on

- Material composition
- Photon energy

Attenuation length in water

- $E = 100 \text{ eV}$ ($\lambda \sim 120 \text{ \AA}$) : $\sim 100 \text{ nm}$
- $E = 30 \text{ keV}$ ($\lambda \sim 0.5 \text{ \AA}$) : $\sim 10 \text{ cm}$



Peak at 930 eV

- Ionisation E of oxygen (threshold for photo-electric effect)
- Possible above 930 eV $\rightarrow$ absorption increases at 930 eV

Saturation at 20 keV

- Compton effect kicks in

Image wikipedia

X-ray scattering
databases at NIST
(National Institute of
Standards) :

- <http://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html>
- <http://physics.nist.gov/PhysRefData/FFast/html/form.html>



X-Ray Form Factor, Attenuation, and Scattering Tables

Element:*

23. Vanadium, V
24. Chromium, Cr
25. Manganese, Mn
26. Iron, Fe
27. Cobalt, Co
28. Nickel, Ni

- OR -

Compound* formula or element symbol:
(e.g., H2O for water)

Type of Data: ([Database Holdings](#))

f1 (e/atom) vs E (keV) Graph

Energy Range:

☐ Energy Range 0.001 - 2.00 keV

☐ Energy Range 2.00 - 433 keV

☐ Sub Range - keV

ρ (g cm⁻³) (optional, only used for the linear attenuation coefficient μ):

☐ No frames.

☐ Data in HTML tables.

***High uncertainties at low x-ray energy (<1 keV):**

See [estimated uncertainties for elements](#) in Table II of the JPCRD 2000 article.
At low energy, uncertainties may be greater for compounds than elements.

Example: mass attenuation coefficient for Fe

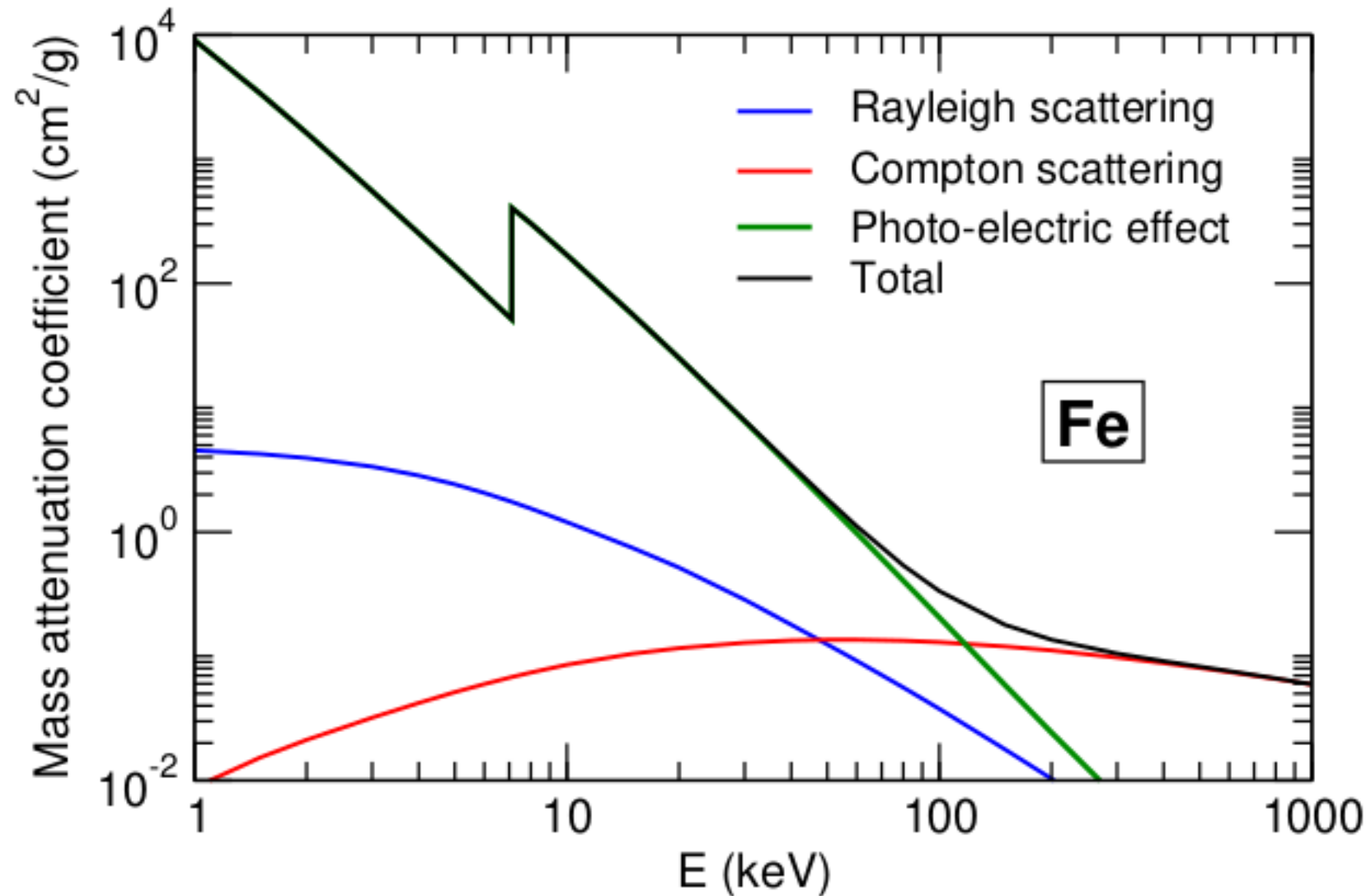


Figure generated from data on the NIST databases

4.2- Interactions of photons with matter

Crystal and molecular scale

Vibrons, rotons, phonons, plasmons

Photons can interact with

- vibrons: vibration modes in a molecule or a structure
- rotons: rotation modes in a molecule or a structure
- phonons: collective oscillations of atomic cores, acoustic waves in a solid
- plasmons : collective oscillations of atom electrons

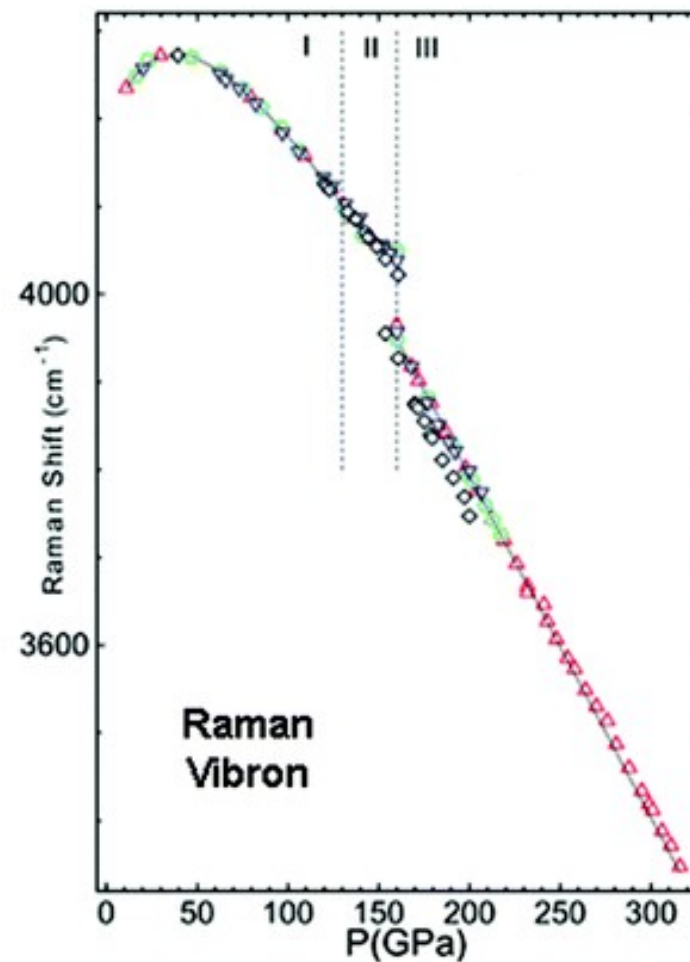
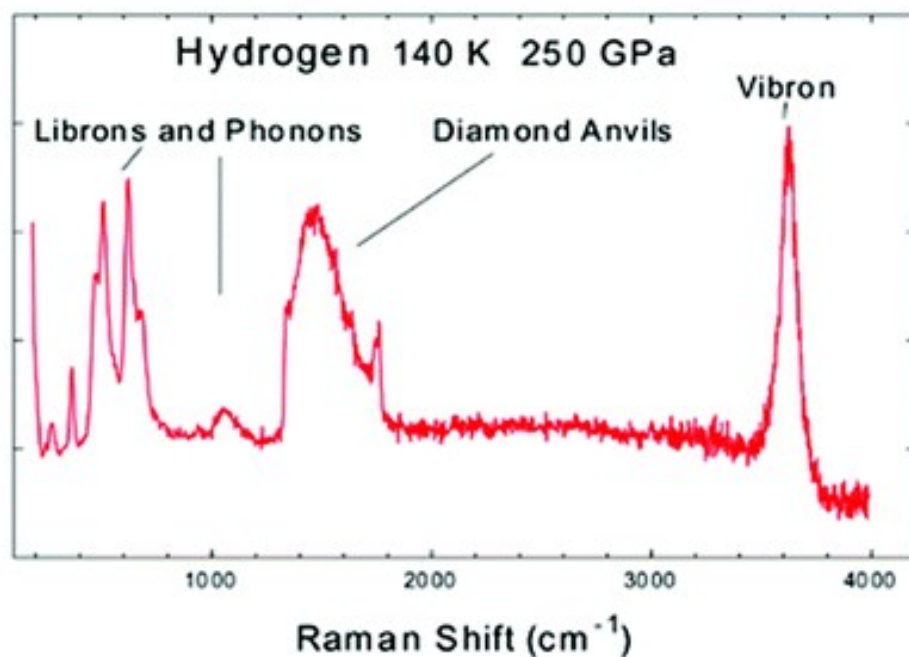
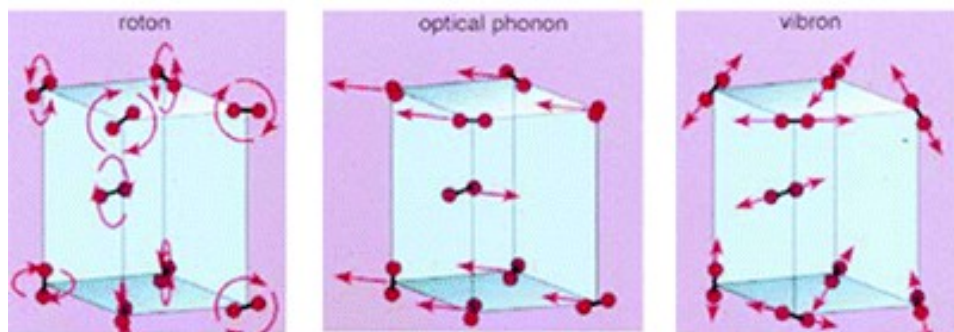
Spectroscopy techniques : infra-red, Raman, Brillouin, etc

More details in Advanced Characterization I

Remember that it works on solids as well

Many possibilities for photons / molecules interactions

Example: Solid H₂ – 140 K – 250 GPa



Goncharov and Hemley, *Chem. Soc. Rev.*, 2006, **35**, 899-907

Cf next
class

X-rays diffraction

- Effect on electronic cloud
- Rayleigh scattering by the electronic cloud
- Constructive interference between scattered photons

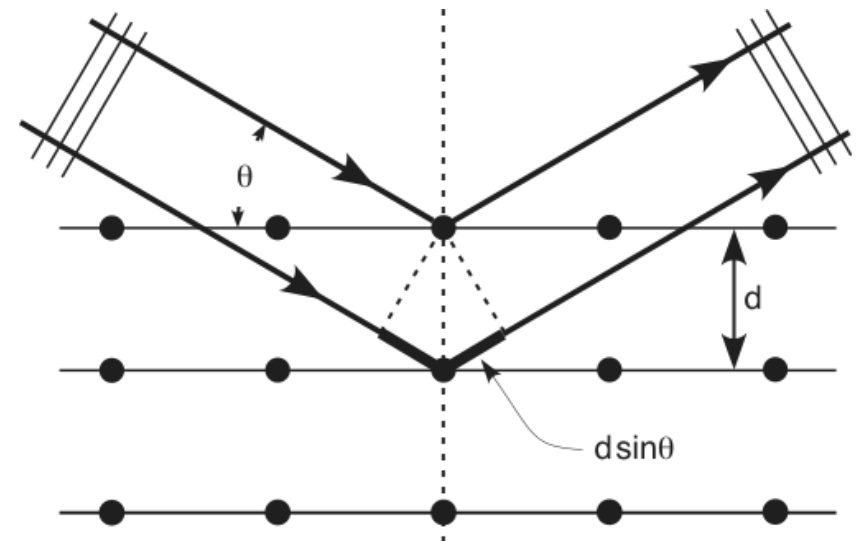
$$n \lambda = 2 d_{hkl} \sin \theta$$

λ : incident wavelength

d_{hkl} : distance between 2 crystal plane families

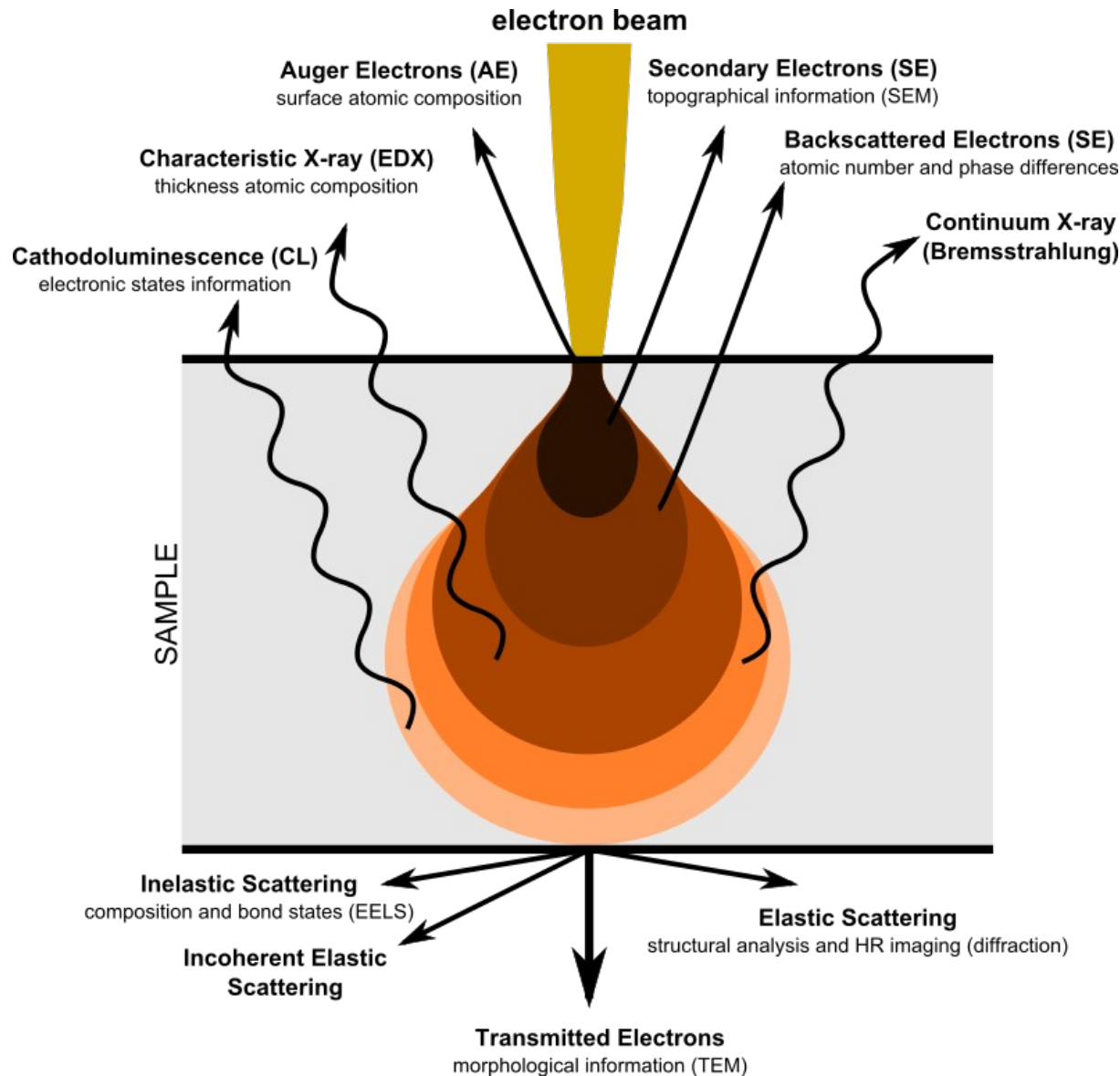
θ : Bragg angle

n : order of diffraction (integer)



5- Interactions of electrons with matter

Electron-matter interactions: a summary



SEM mostly use thick samples → no signal in transmission

TEM use thin samples → can work on both transmission and reflexion

Illustration Wikipedia

Elastic scattering by the atomic potentials

- Far from the atom

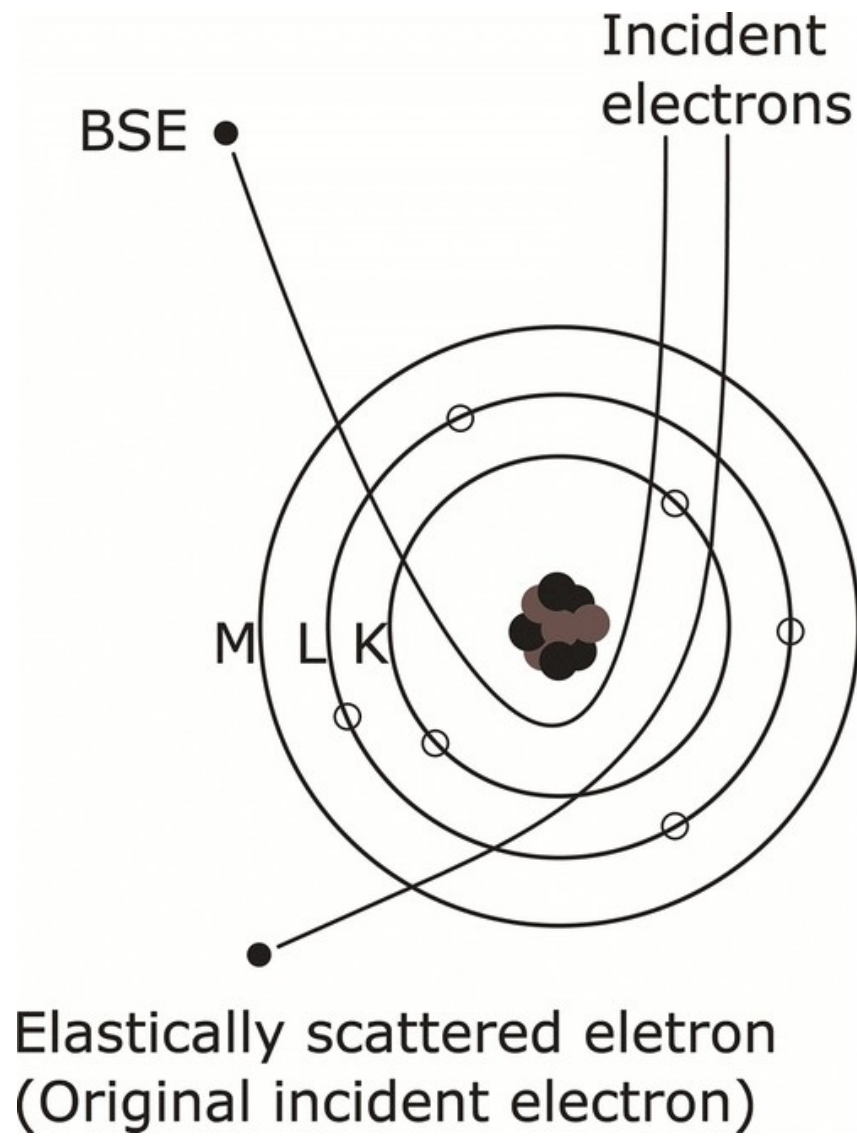
Inelastic scattering by electrons of the electronic cloud

- Within the atomic radius

Deceleration radiation in the material

- Close to the atomic core

Electron elastic scattering



Coulomb forces between the incoming electron, the nucleus and the electronic cloud.

Most efficient for atoms with a high Z number

Forward scattering (that goes through the sample) is used to create diffraction images in the TEM.

Backwards scattering is used for imaging in the SEM.

Inelastic scattering

Incoming electron, interaction with electron in the electron cloud

→ scattered electron + ejected electron

Ejected electron = secondary electron

Relaxation of electronic cloud

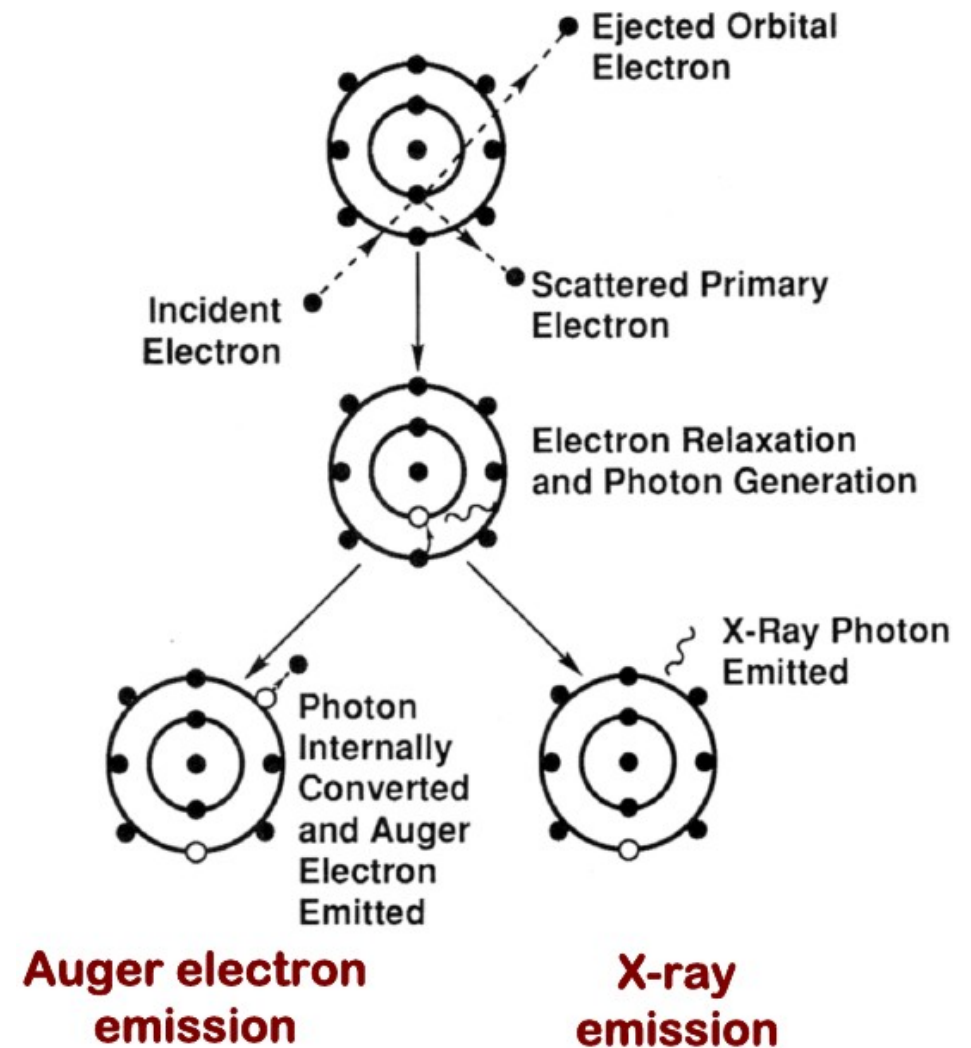
→ photon emission

Photon can be emitted directly, typically in the X-rays

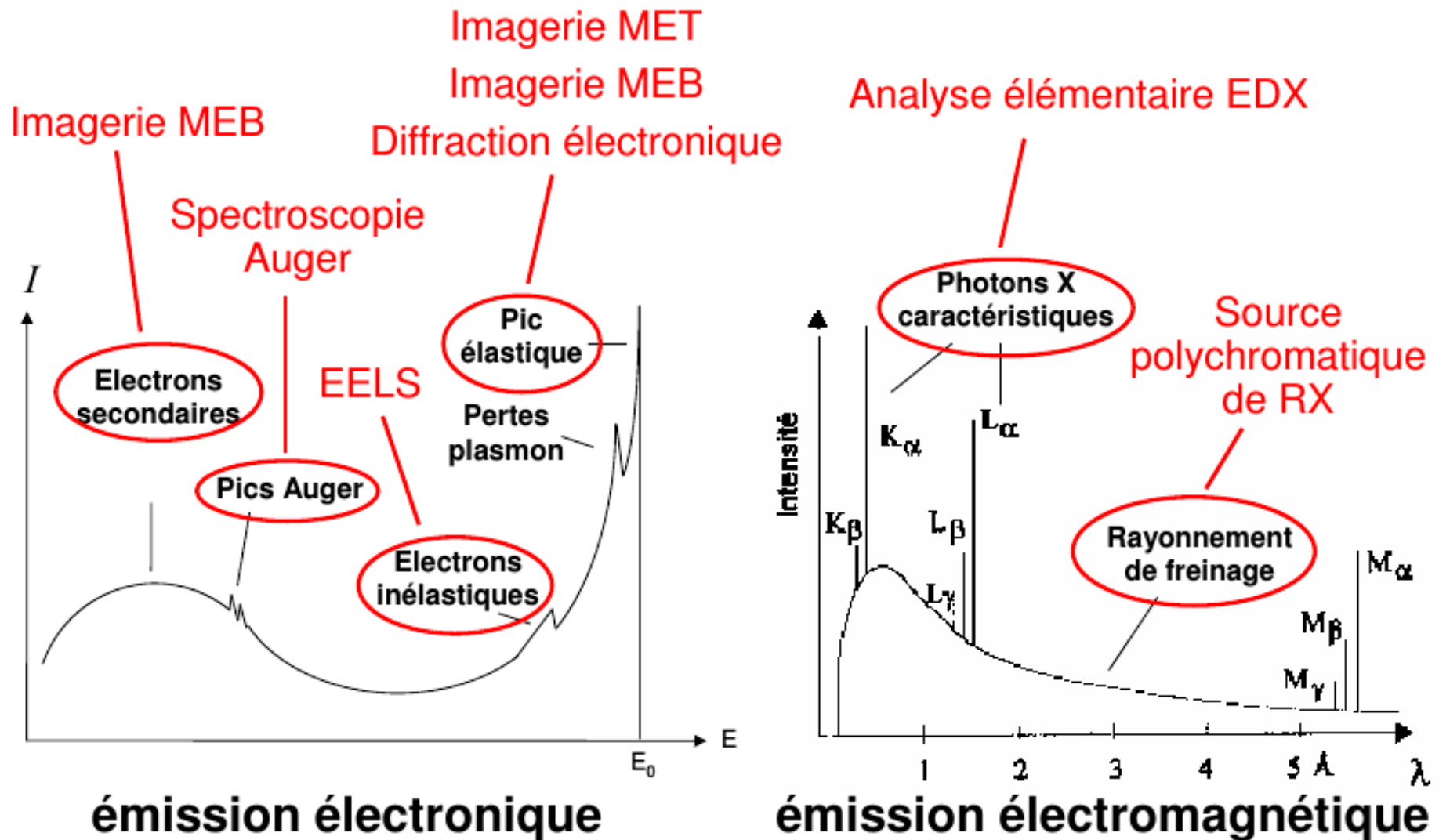
→ X-ray emission

Photon can be absorbed by the atom, with emission of another electron

→ Auger electrons



Electron-matter interactions: emission spectrum



Classes of Damien Jacob on electron microscopy

6- Interactions of neutrons with matter

“heavy” particles with no charge

- Nearly no interaction with electrons
- Interactions with the nucleus

Interaction depends on

- The target nucleus
- Incoming neutron energy

Classification of neutrons

- Slow (thermal) neutrons : $E_n < 0.5 \text{ eV}$
- Intermediate neutrons: $0.5 \text{ eV} < E_n < 10 \text{ keV}$
- Fast neutrons: $E_n > 10 \text{ keV}$

Possible neutron matter interactions

Elastic scattering

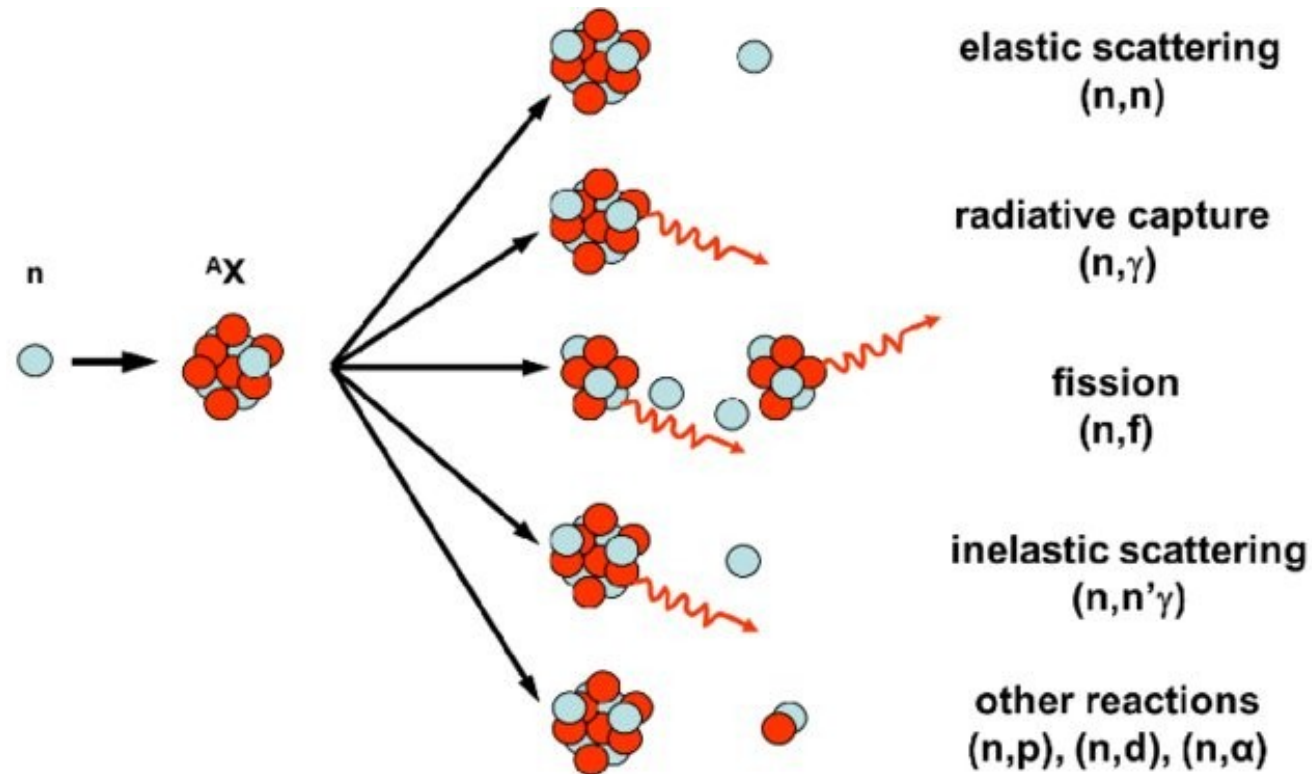
- No change in the target atom
- Some of the incoming energy transferred to the target

Inelastic scattering

- Emission of photons
- No change in the target atom
- Some of the incoming energy transferred to the target

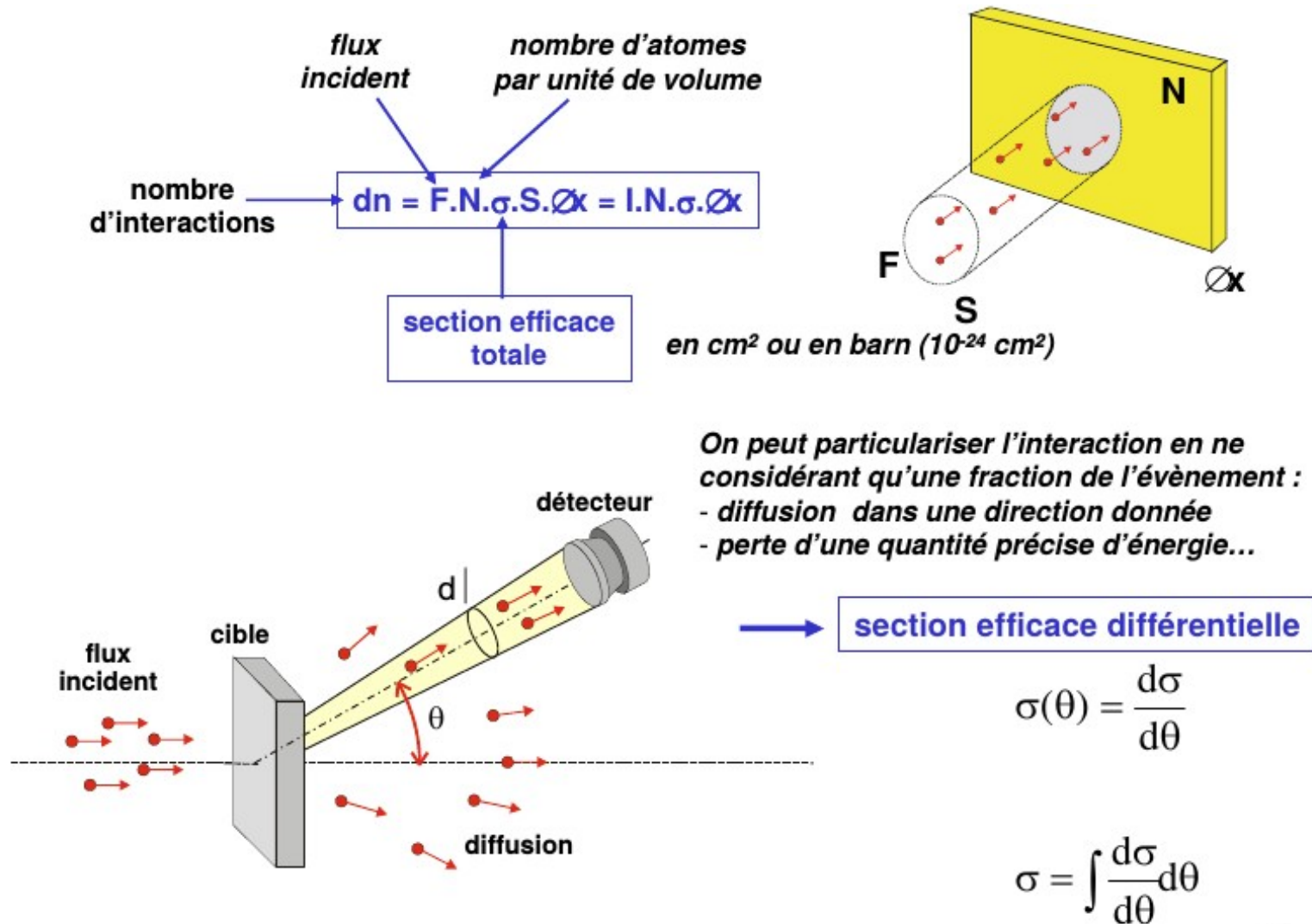
Nuclear reactions

- Changes in the target atom



Extra

Section efficace : caractérise l'efficacité d'une interaction



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