Reunion IMNC/SHFJ
9 Mars 2012

Luminescence

- emission of light by a substance

- Bioluminescence, emission by a living organism
- Chemiluminescence, a result of a chemical reaction
  - Electrochemiluminescence, a result of an electrochemical reaction
- Crystalloluminescence, produced during crystallization
- Electroluminescence, a result of an electric current passed through a substance
  - Cathodoluminescence, a result of being struck by an electron
- Mechanoluminescence, a result of a mechanical action on a solid
  - Triboluminescence, generated when bonds in a material are broken when that material is scratched, crushed, or rubbed
  - Fractoluminescence, generated when bonds in certain crystals are broken by fractures
  - Piezoluminescence, produced by the action of pressure on certain solids[2]
- Photoluminescence, a result of absorption of photons
  - Fluorescence, photoluminescence in which the emitted photons are of lower energy than those absorbed
  - Phosphorescence, fluorescence slightly delayed after initial absorption of radiation (on a scale of seconds to hours)
- Radioluminescence, a result of bombardment by ionizing radiation
- Sonoluminescence, a result of imploding bubbles in a liquid when excited by sound
- Thermoluminescence, the re-emission of absorbed light when a substance is heated

Fluorescence in Geant4

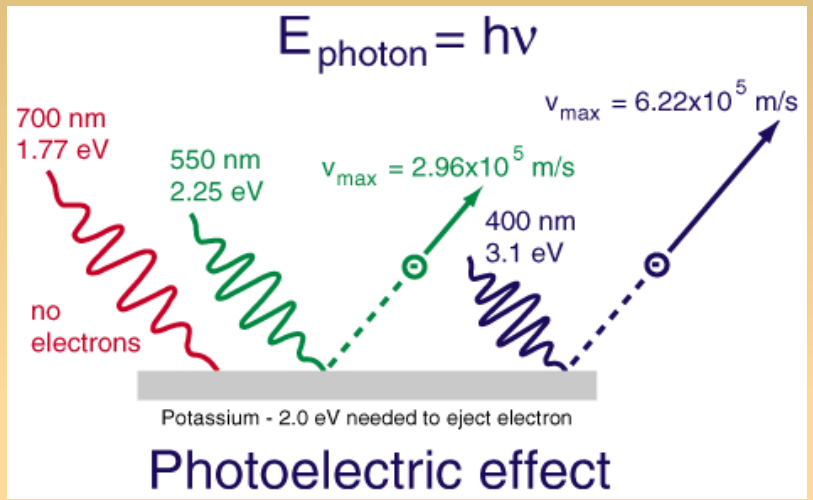
- X-ray fluorescence (GEANT4) This is what Geant4 provides!
  - The sample is exposed to x-rays and what is observed is x-ray fluorescence.
  - EM processes: PhotoElectric, Ionisation, Compton leaves atom in excited state.
  - Transition probabilities for Fluorescence taken from EADL (Evaluated Atomic Data Library) which describes the relaxation of ionized atoms back to neutrality, during which photons (fluorescence x-rays) and electrons (Auger and Coster-Kronig) are emitted.
  - Fluorescence is activated by Default

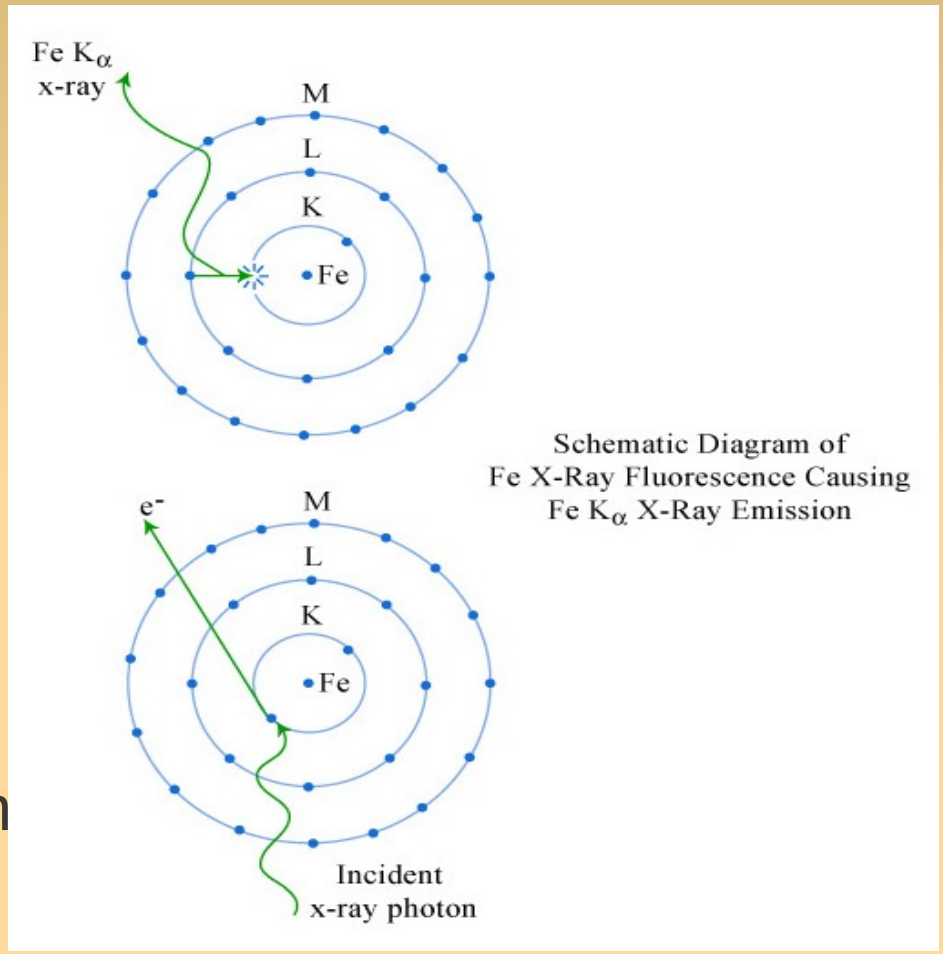
    in Livermore and Penelope PB.

Energy range (keV)	Wavelength range	Name
$< 10^{-7}$	cm to km	Radio waves (short, medium, long waves)
$< 10^{-3}$	µm to cm	Microwaves
$< 10^{-3}$	µm to mm	Infra-red
0.0017 - 0.0033	380 to 750 nm	Visible light
0.0033 - 0.1	10 to 380 nm	Ultra-violet
0.11 - 100	0.01 to 12 nm	X-rays
10 - 5000	0.0002 to 0.12 nm	Gamma radiation

- Visible light fluorescence This is what we need!
  - Absorption of UV rays causes low energy e^- to be ejected from the atom shells. Holes are then populated by other e^- which causes emission of light (color) in the visible. Optical photons energy [1-4]eV or wavelength [800-300]nm.

Geant4 PhotoElectric Effect + fluorescence



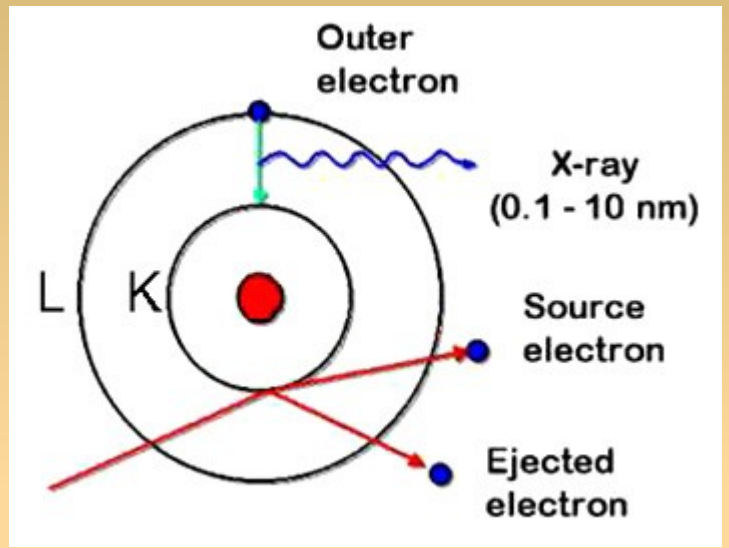


Default particle: gamma

e- emitted from matter after absorption of a x-ray photon
- creation of vacancies in atom shells
- unstable atom
- electron from outer shell are transferred to Inner shells + x-ray emission

No Optical Photons

Geant4 Electron Ionisation + fluorescence

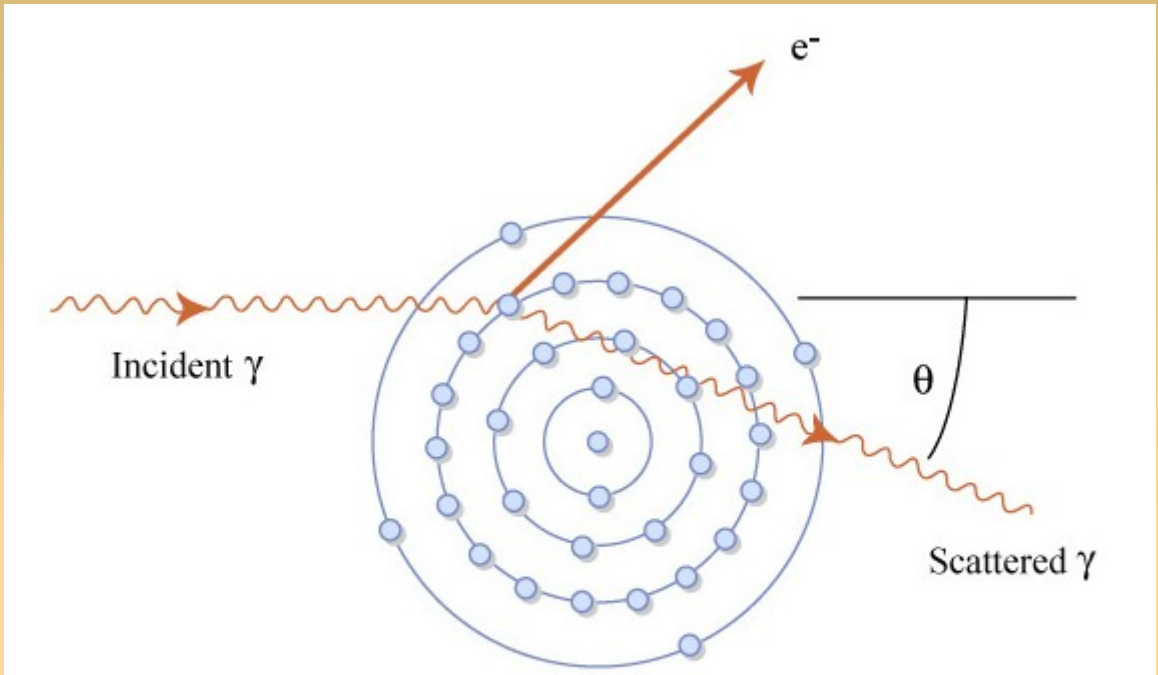


- Default particle: e-/e+
- e-/e+ interacts with gas phase atoms or molecules
- Unstable atom
- Electron from outer shell are transferred to inner shells

  + x-ray emission

No Optical Photons

Geant4 Compton scattering + fluorescence



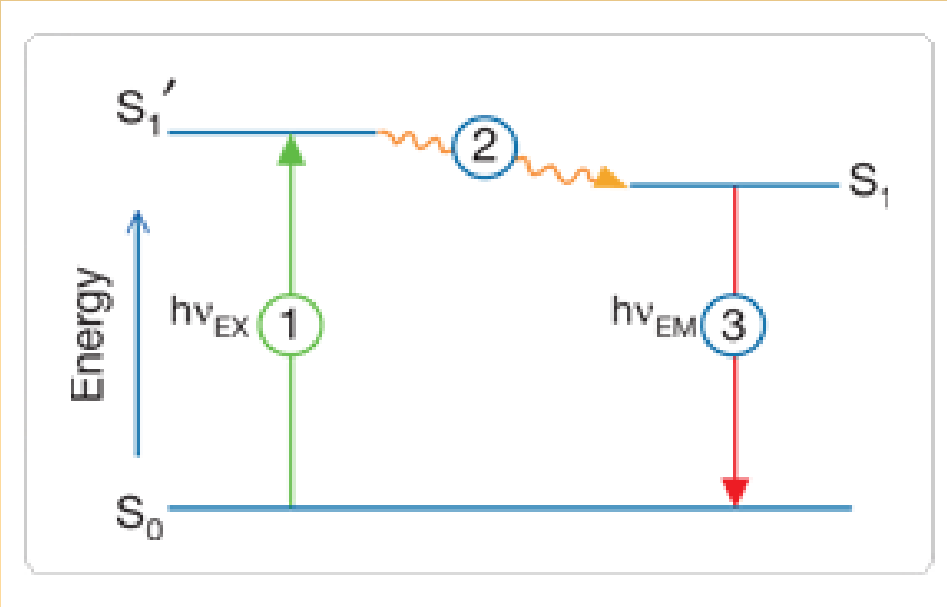
- The inelastic scattering of photons in matter
- Part of the energy of the x/gamma ray is transferred to a scattering electron, which recoils and is ejected from its atom (which becomes ionized)
- The rest of the energy is taken by the scattered x-gamma ray

No Optical Photons

Visible Light Fluorescence

Optical Photons

1) Photon supplied by external source (laser) is absorbed by the fluorophore: Excited state

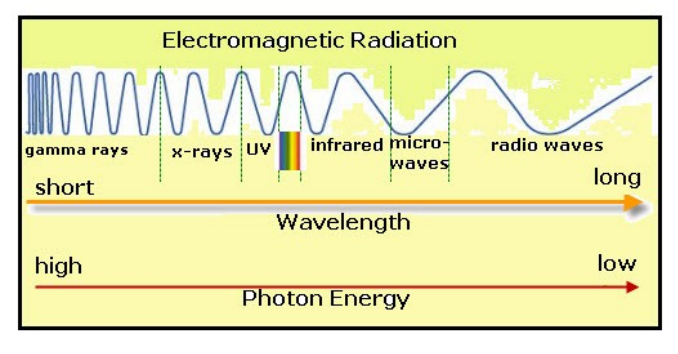


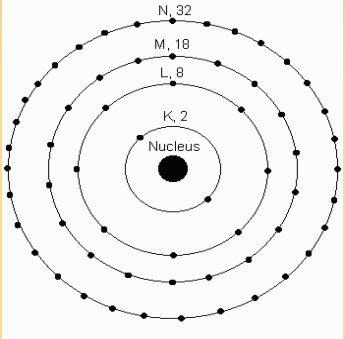
3) Photon is emitted (lower energy – longer λ than excitation photon)

2) Lifetime of the excited state is 1-10 ns – the fluorophore undergoes changes – interactions with environment: Relaxed excided state (Fluorescence quantum yield)

G4 Electromagnetic Processes HyperNews + offline discussion

- ”Fluorescence produces gamma and not optical photons - it is different scale in energy. Geant4 de-excitation module provides simulation of X-ray emission from K, L, and in some cases M atomic shells” (Vladimir.Ivantchenko@cern.ch)





- Conclusion (Peter):

  Geant4 does not produce fluorescent photons at optical photon's energy/wavelength.

Some Hope...
Wave Length Shifting

- Discussion with Peter G.
- There are only three processes in the present Geant4 that produce optical photons as secondaries: Cherenkov, Scintillation and WaveLengthShift.
- Maybe it is possible to use the wavelength shifting process to simulate the fluorescence in visible.
- WLS fibers are used in many HEP experiments.

CMS Hadronic EndCap calorimeter is made of scintillator tiles with WLS fibers embedded. These fibers collect light produced in tiles. They absorb blue from scintillator and re-emit green so that as much light reaches PMTs.

Plan/Needs

- Plan: I expose my biological sample to some uv/near visible rays (a few eV G4opticalphoton). If that sample has been marked by a fluorophore it will emit fluorescence photons at 510nm (green) if excited by optical photons (uv or blue light) at 488nm.
  - Specify the biological sample as a "wave length shifting material".
  - How do the photons get absorbed in the material? Provide the 'WLS absorption length' - the mean free path of the incoming 50eV optical photons in your material.
  - What other photons emerge? Specify the spectrum of your fluorescence, e.g. wave length shifted photons.

- There is nothing in G4 that would simulate this under exact physics principles. But it could be approximated by the existing WLS process if you provide the required empirical parameters.

GateOpticalWLS

- Created GateOpticalWLSPB with ProcessName ”OpticalWLS”
- Inherit from G4OpWLS class.

- Created a Gate macro OptImaging_Fluorescence.mac

```
/gate/physics/addProcess OpticalAbsorption
/gate/physics/addProcess OpticalRayleigh
/gate/physics/addProcess OpticalBoundary
/gate/physics/addProcess OpticalMie

/gate/physics/addProcess OpticalWLS
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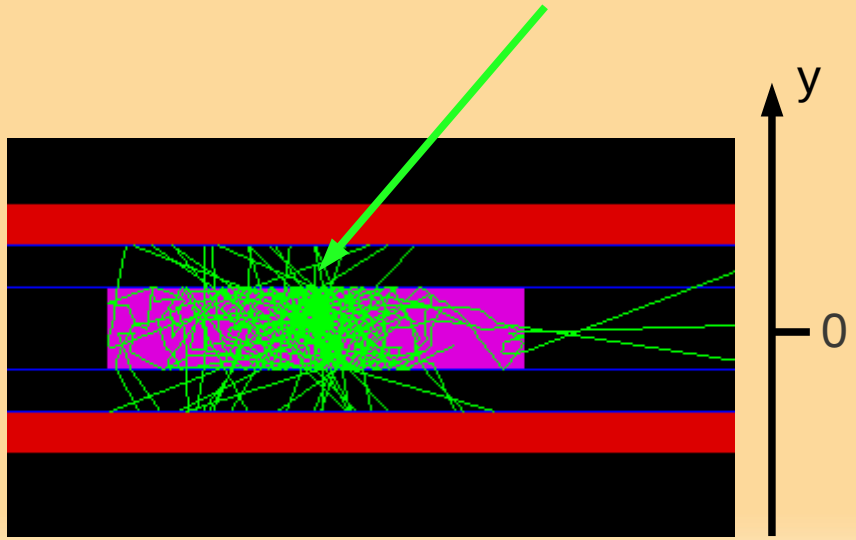
Source of optical photons is here: +0.75mm



Phantom is (5x5x1)mm^3
1mm thickness

Detectors (red layers) are 5cm long and large and 0.5mm thick.

Tests with *fake* material
(1000 generated optical photons)

Mie/Abs./Boundary

T	R	A
9%	6.3%	84.7%

Mie/Abs./Boundary/WLS

T	R	A
3.3%	10.7%	86%

Boundary/WLS

T	R	lost
56.5%	41%	2.5%

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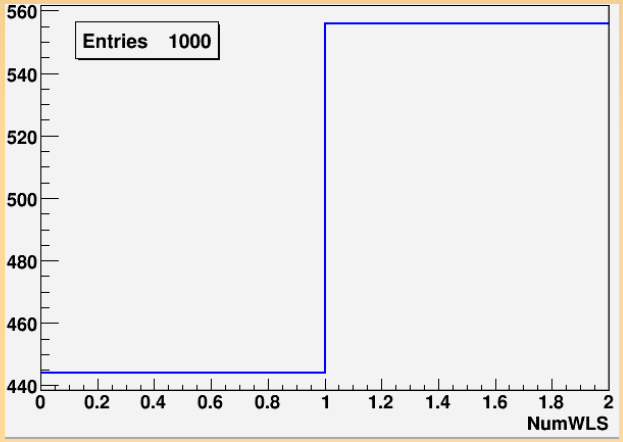
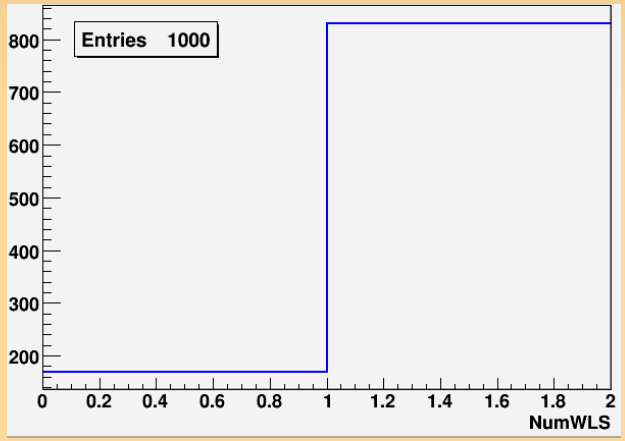
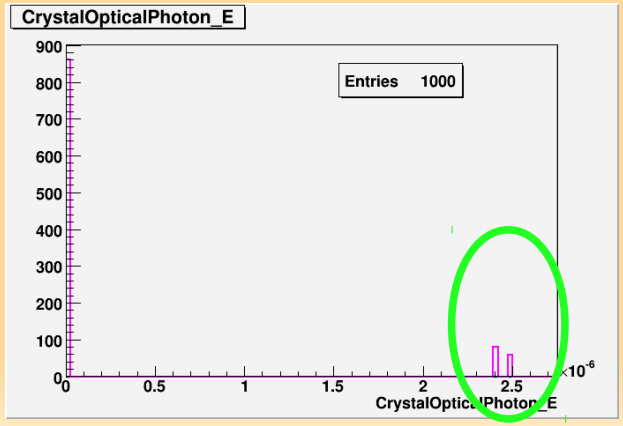
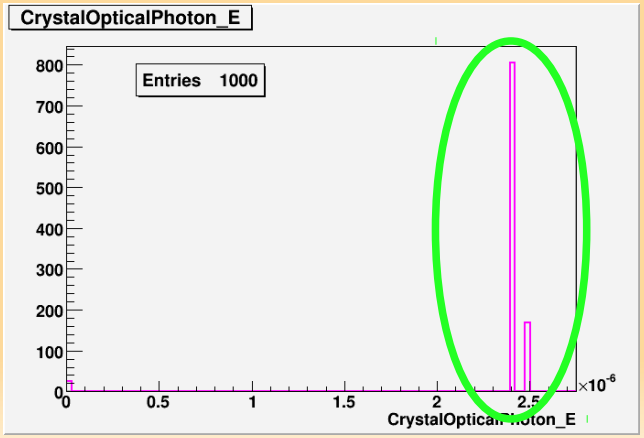
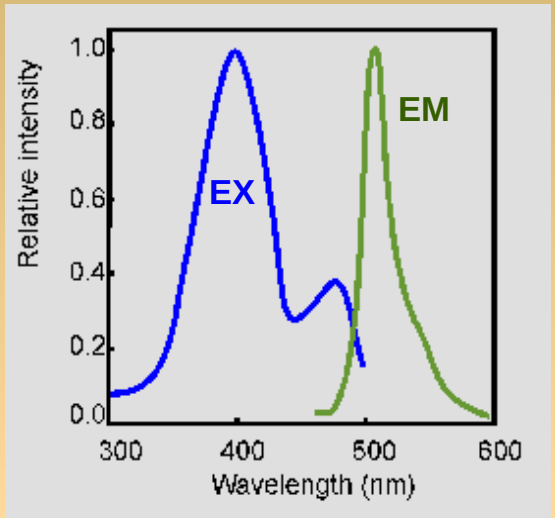








Simulation of the Green Fluorescence Protein (GFP)

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Time delay between absorption and re-emission