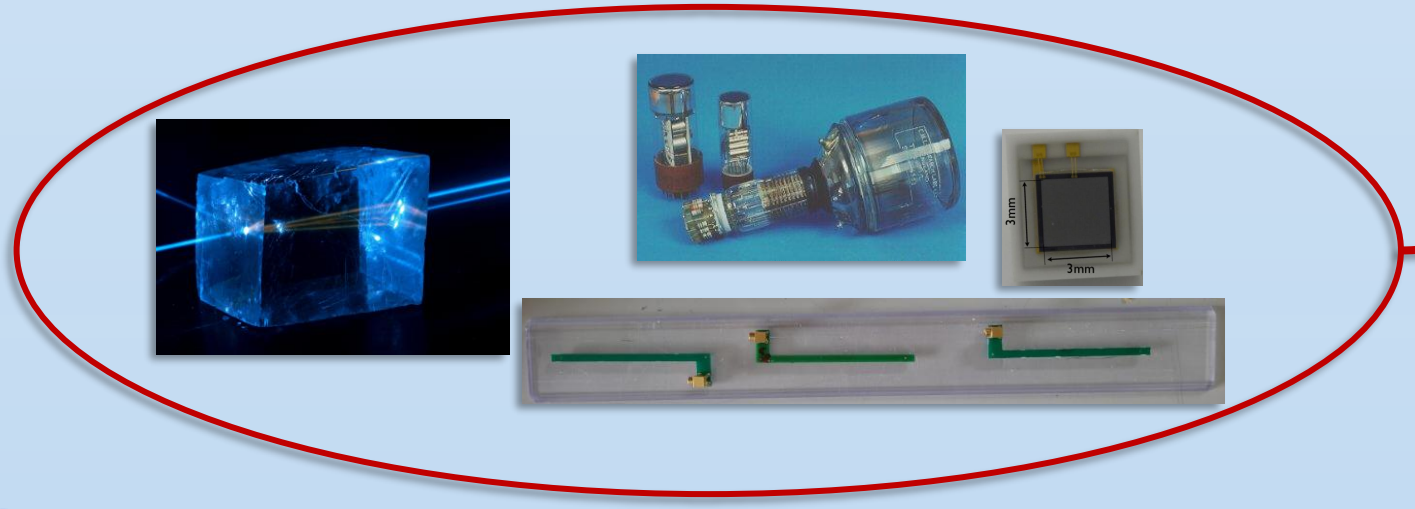
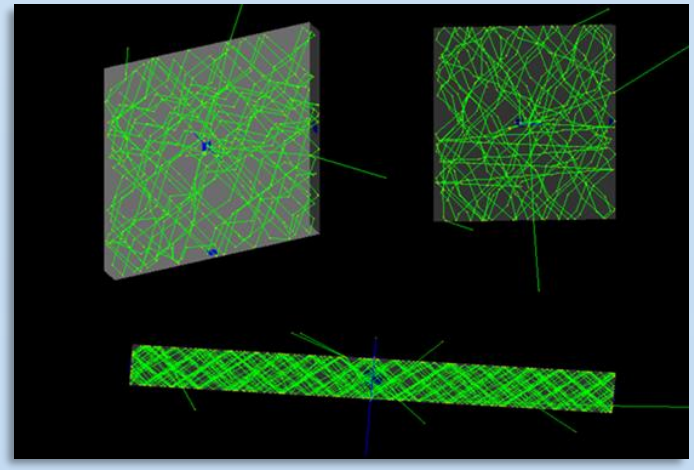
Simulation of optical photon propagation for generic scintillator-based detectors

Lecture 1

Scintillator and Photosensors





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Contents

- Interaction of particles with matter
- Scintillators:
  - Materials and Properties
- Silicon Photomultipliers (SiPMs)

Interaction of fast charged particles with matter

- Fast charged particles can interact electromagnetically with matter leading to ionization or collective excitations
- The mean energy loss rate ("stopping power") is given by Bethe's formula:

$$-\left\langle \frac{dE}{dx} \right\rangle = Kz^2 \frac{Z}{A} \rho \frac{1}{\beta^2} \left[\frac{1}{2} \ln \frac{2m_e c^2 \beta^2 \gamma^2 W_{max}}{I^2} - \beta^2 - \frac{\delta(\beta\gamma)}{2} \right]$$

where:

- W_{max} is the maximum energy transfer in a single collision (knock-on):

$$W_{max} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + 2\gamma\, m_e/M + (m_e/M)^2}$$

- z is the charge of the radiating particle (in unit of e)
- ρ, Z and A are the density, atomic number and mass number of the medium
- $K = 4\pi N_A r_e^2 m_e c^2 = 0.307 \mathrm{MeV} cm^2 g^{-1}$
- I is the mean excitation energy of the medium

- The term $\delta(\beta\gamma)$ is usually negligible in gases because of the low density

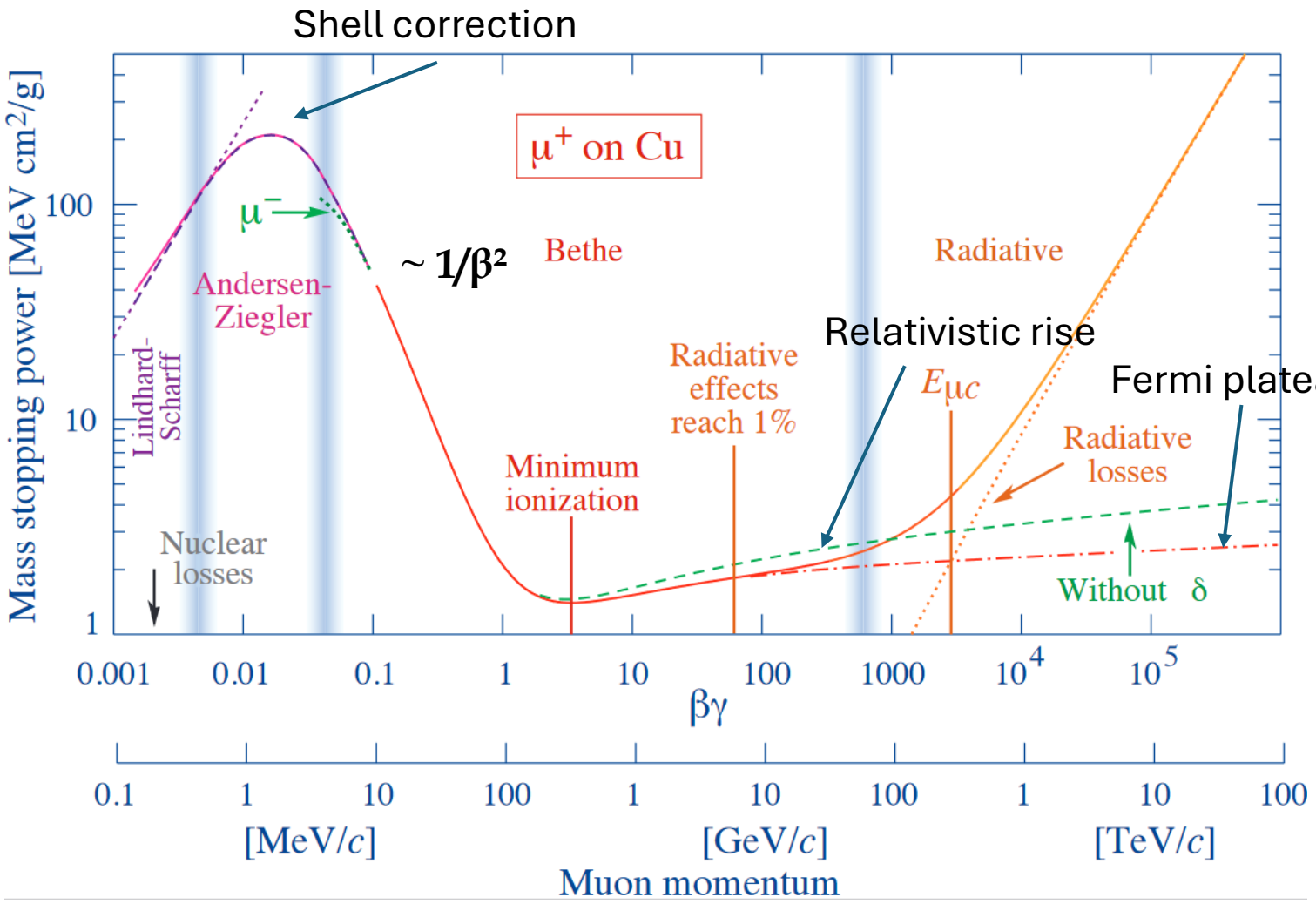
Interaction of fast charged particles with matter

- Bethe's formula is accurate at 1% level in the range $0.1 < \beta\gamma < 10^3$
- The average ionization energy can be evaluated with the formula

$$I(eV) = 16Z^{0.9}$$

  - The formula is accurate at 10% level for $Z > 1$
- The function $\delta(\beta\gamma)$ is the contribution from the density effect, which is relevant for particles with $\gamma > 10^3$ in high-density media
  - The particle electric fields induces a polarization in the medium, which screens the atoms, resulting in a reduced stopping power
- No theoretical models available for particles in the range $0.01 < \beta\gamma < 0.05$
  - Phenomenological formulas used in this range
- Particles with $\beta\gamma > 10^3$ can lose energy via bremsstrahlung
  - Bremsstrahlung becomes dominant above the critical energy
  - For electrons $E_c = 600MeV/(Z+1)$

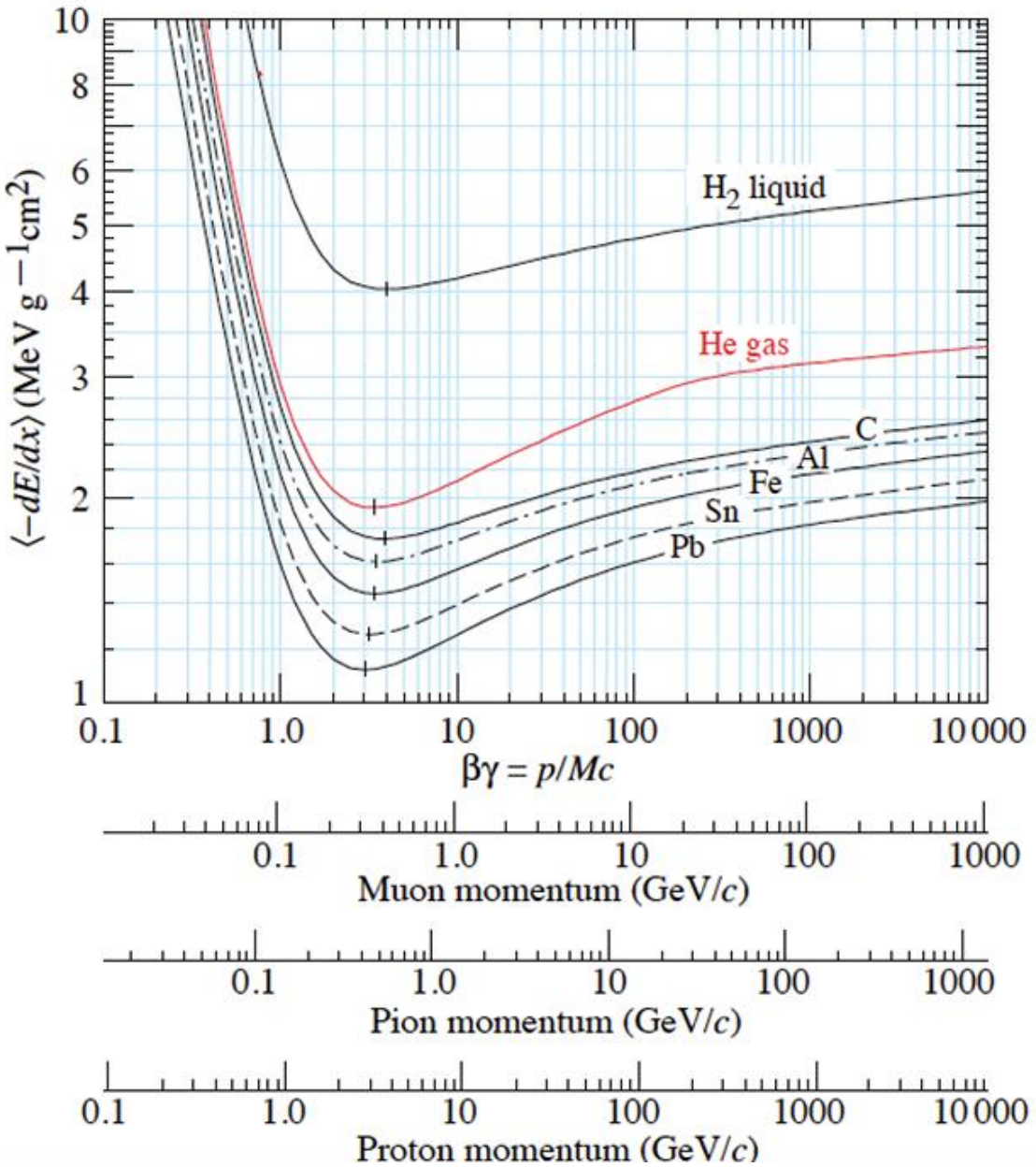
Bethe-Bloch

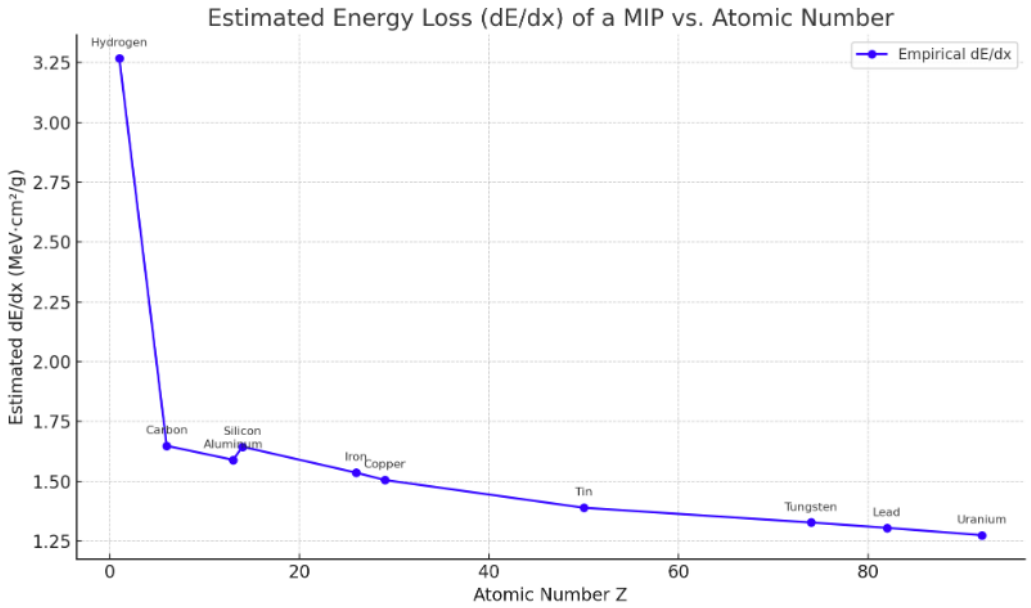


- **dE/dx ~ 1/β²** in the non-relativistic region, before the minimum ionization.
  - The **minimum ionization** occurs around **βγ ~ 3.5** (β ≈ 0.96), where **dE/dx ~ 1–2 MeV cm²/g**.
- In the **relativistic region**, **dE/dx ~ constant** (Fermi plateau), because the logarithmic rise is limited by the **density effect**. The rise is at most a factor of 2 (in gases).
- For **βγ < 0.05**, **shell corrections** become significant. The particle tends to **capture electrons**, reducing the electric field losing less energy.

It is convenient to express the traversed thickness **dx** as **ρ · dx** (mass thickness, in g/cm²):
in this way dE/dx becomes almost independent of the material type (Z/A ≈ 1/2 and the dependence of I on Z in the logarithm is small): $-dE/\rho dx \propto Z/A$ [MeV cm²/g]

Bethe-Bloch





Emphirical values :

$$\frac{dE}{dx} = C \cdot \frac{Z}{A}$$

where C is an emphirical term:

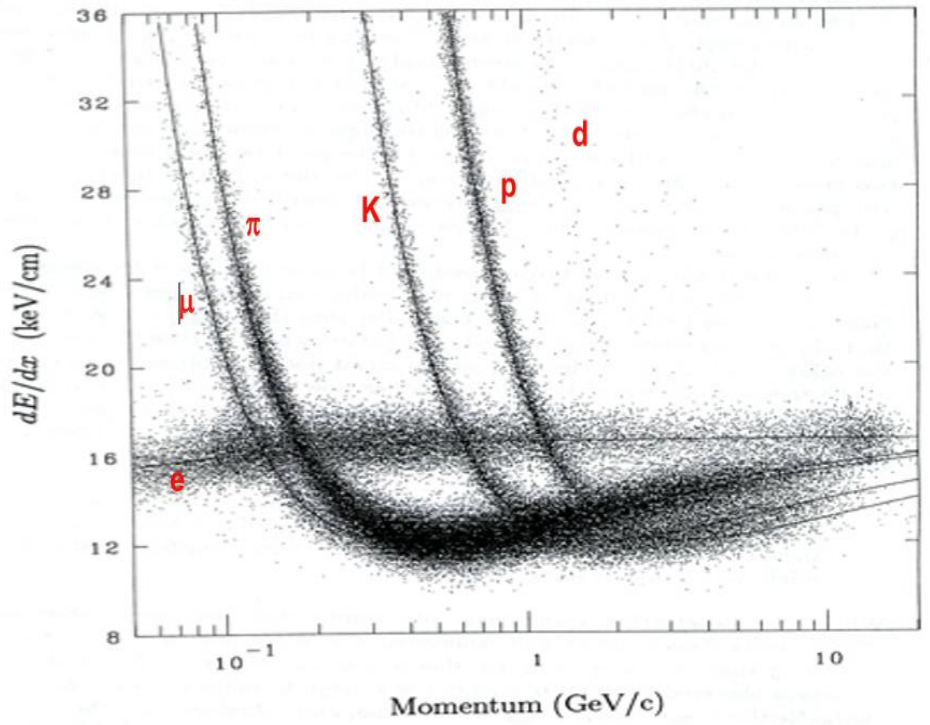
- C~1.5 MeV ·cm²/g for solid materials
- C~2.0 MeV ·cm²/g for lighter materials

Interaction of fast charged particles with matter

Particle identification

- At a given kinetic energy, heavier particles exhibit greater energy loss. Below the minimum ionization point, distinct energy loss curves are observed for different particle.

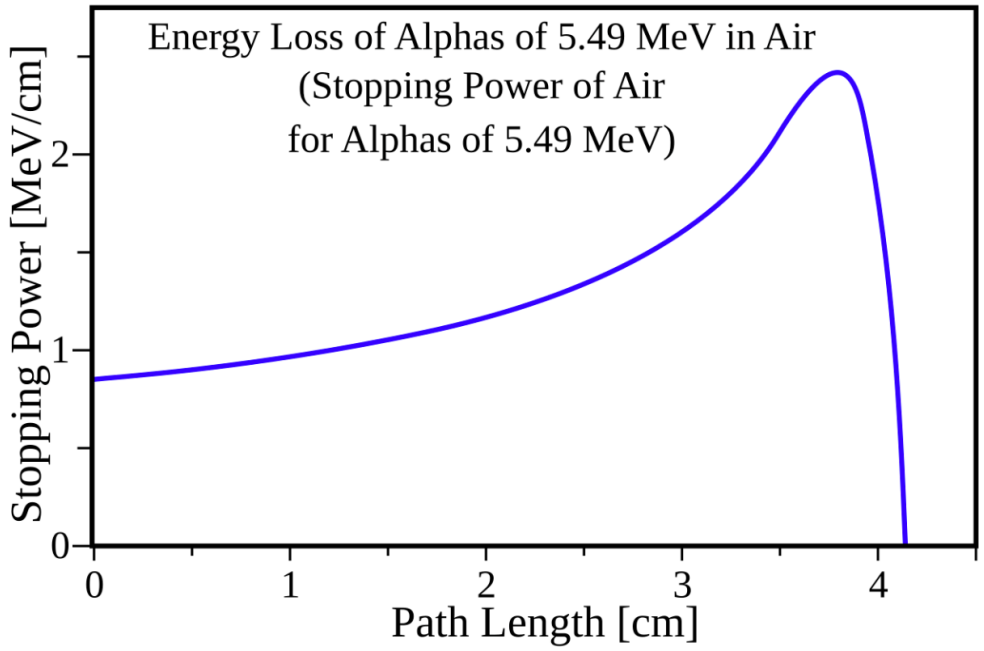
This characteristic can be used for charged particle identification when both momentum and energy loss measurements are available.



Bragg curve

- dE/dx increases as the particle's kinetic energy decreases. A particle deposits more energy in the material as it slows down and approaches the end of its range.

This characteristic is used in hadron therapy to deliver a high radiation dose to malignant tissue while sparing the surrounding healthy tissue.

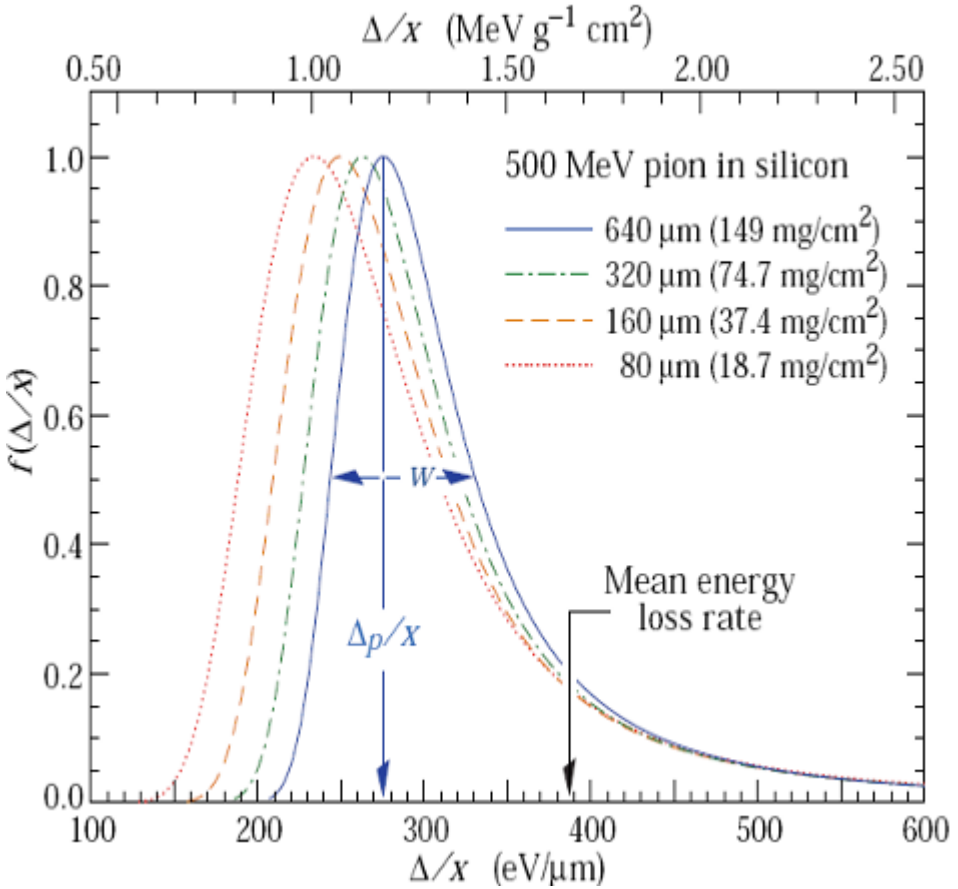


Energy loss

- A charged particle crossing a thin slab of matter will deposit an energy ΔE:
  - The average energy loss $\langle \Delta E \rangle$ can be calculated from the Bethe formula, taking the thickness into account
  - The energy losses will be distributed obeying the **Landau probability distribution function**
- For thin layers or low density materials:
  - Few collisions, some with high energy transfer.

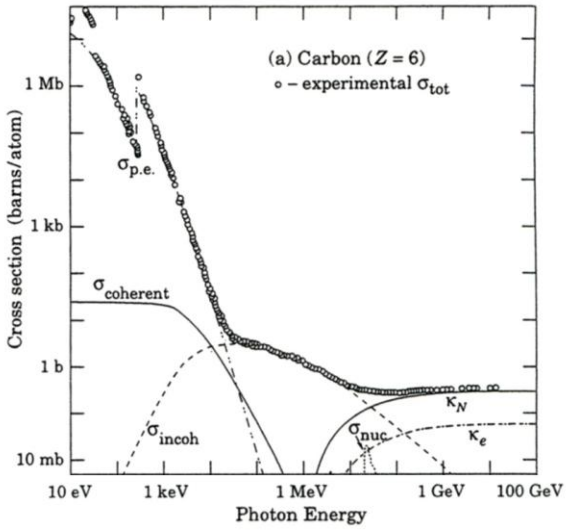
  ⇒ Energy loss distributions show large fluctuations towards high losses

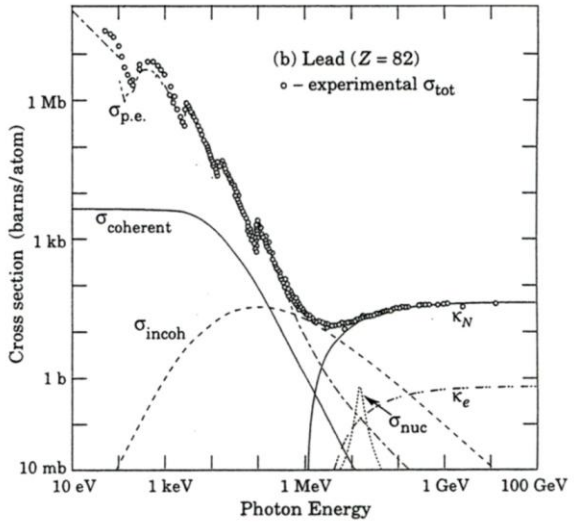
  ⇒ Long Landau tails

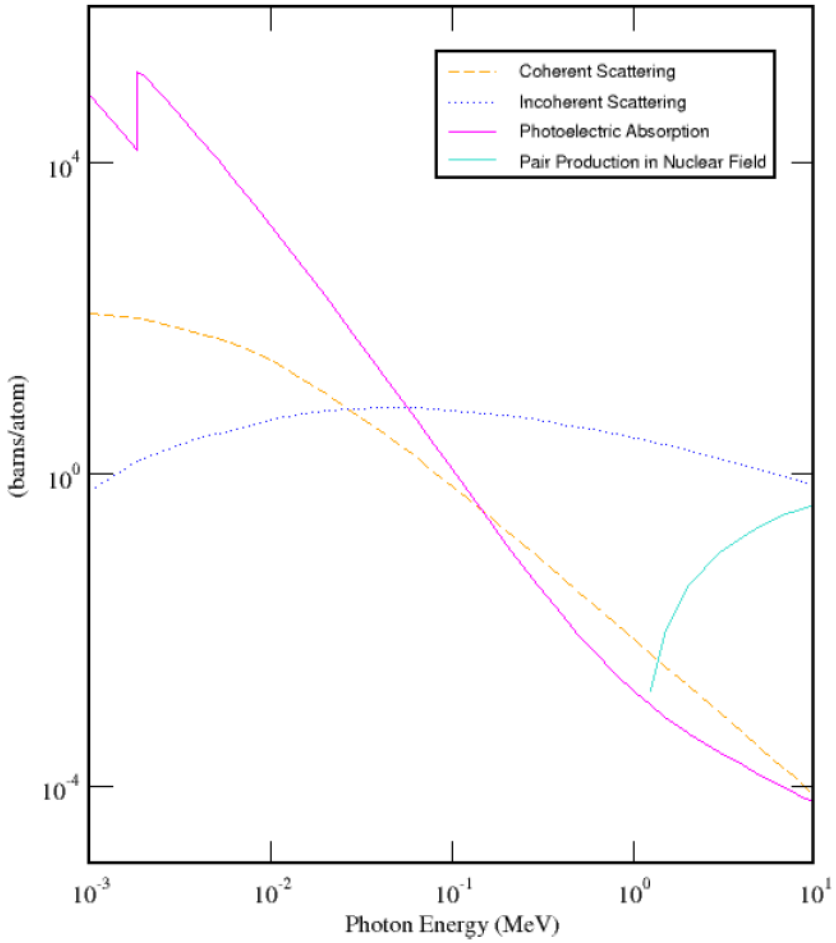


Interactions of photons

- Interaction processes:
  - Rayleigh scattering (coherent scattering)
  - Photoelectric effect
  - Compton effect (incoherent scattering)
  - Pair production
    - *Nuclear field*
    - *Electronic field*
  - Photonuclear interactions
    - *The target nucleus can be destroyed*







Cross sections of the main interaction processes of photons with silicon as a function of photon energy [2]
The photoelectric cross section exhibits an edge at energy $E \sim 1.838\,\mathrm{keV}$ (silicon *K-edge*)

Interactions of high-energy photons and electrons

- Dominant processes at high energies ($E > few\ MeV$):
  - Electrons and positrons: bremsstrahlung
  - Photons: production of e^+e^- pairs

- The length scale which describes both processes is the radiation length X_0
  - Is measured in units of g/cm^2
  - Corresponds to the average distance traveled by an electron (positron) before losing a fraction $1 - 1/e$ of its initial energy by bremsstrahlung
  - Corresponds to 7/9 of the mean free path of a photon relative to the pair production process
- A simple parameterization for X_0 is the following:

$$X_0(g/cm^2) = 180\frac{A}{Z^2}$$

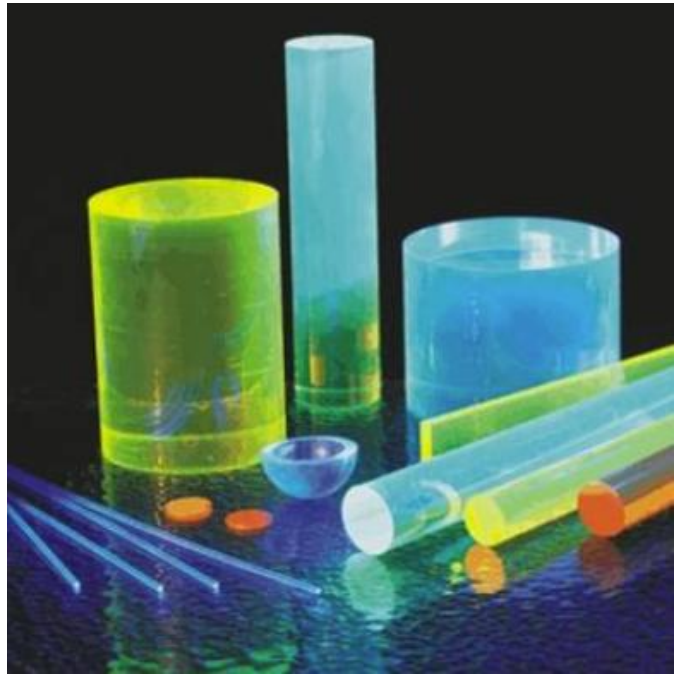
- For mixtures and compounds:

$$\frac{1}{X_0} = \sum_i \frac{w_i}{X_{0,i}}$$

  - Here $X_{0,i}$ and w_i are the radiation length and the weight fraction of the i-th element

Scintillators

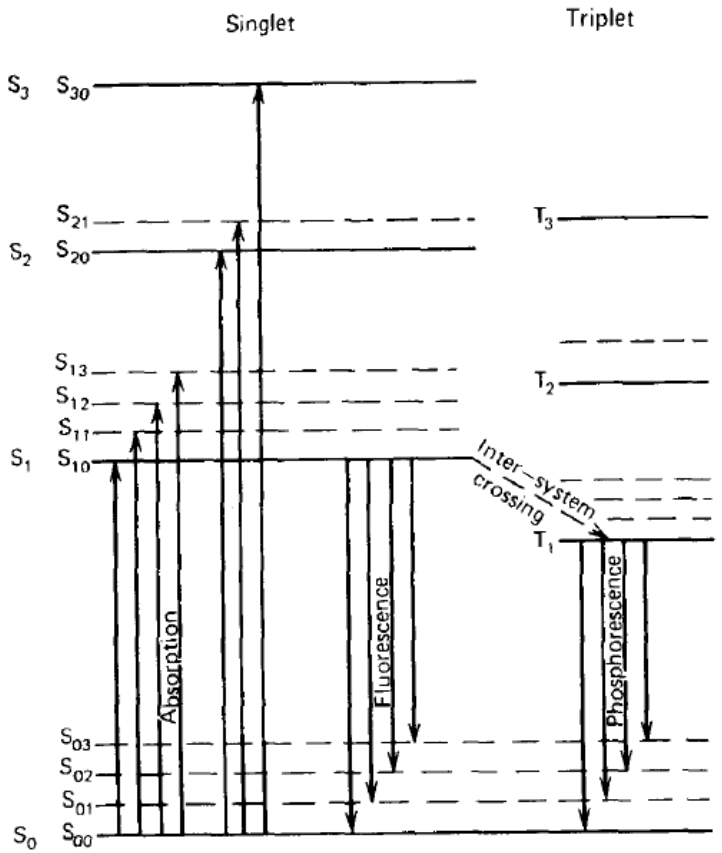
- The energy deposited by ionizing particles in a scintillator is converted into visible light, which is then collected by a photodetector
- Scintillator properties:
  - High scintillation efficiency
    - *A large fraction of the deposited energy should be converted into scintillation light*
  - Linearity
    - *The light yield should be proportional to the deposited energy*
  - Transparency
    - *The scintillator should not re-absorb the scintillation light*
  - Short decay time
    - *The light pulse should be fast to provide fast signals*



Scintillating materials

- Organic scintillators (liquid or plastic)
  - Low light yield and fast decay time of scintillation light
  - Scintillation light is emitted in the transitions between the energy levels of individual molecules
- Inorganic scintillators (Crystals)
  - High light yield but slow decay time of scintillation light
  - Scintillation light is emitted in the transitions between the energy levels of the lattice
- Light emission mechanisms:
  - Fluorescence (and delayed fluorescence)
  - Phosphorescence
    - *Phosphorescence light is emitted with longer wavelengths that fluorescence light*

Organic scintillators



- At room temperature all molecules are in the ground state S_{00}
  - Excited vibrational levels S_{0j} are not populated since $\Delta E_{vib} \approx 0.15eV \gg kT \approx 25meV$
- When a particle deposits its energy in the scintillators, electrons are excited in the higher energy singlet levels S_{ij}
- De-excitations from high-energy levels to S_{10} happen without photon emission
  - Decay times are extremely fast ($\sim 1ps$)
- Fluorescence photons are emitted in the de-excitations from S_{10} to any of the states S_{0j}
  - Typical decay times are in the range $1 - 10ns$
- Electrons in S_{10} may migrate in the level T_{10} (intersystem crossing process) and vice versa
- Phosphorescence photons are emitted in the de-excitations from T_{10} to any of the states S_{0j}
- Delayed fluorescence photons are emitted in the de-excitations from S_{10} to any of the states S_{0j} following the transitions $S_1 \leftrightarrow T_1$

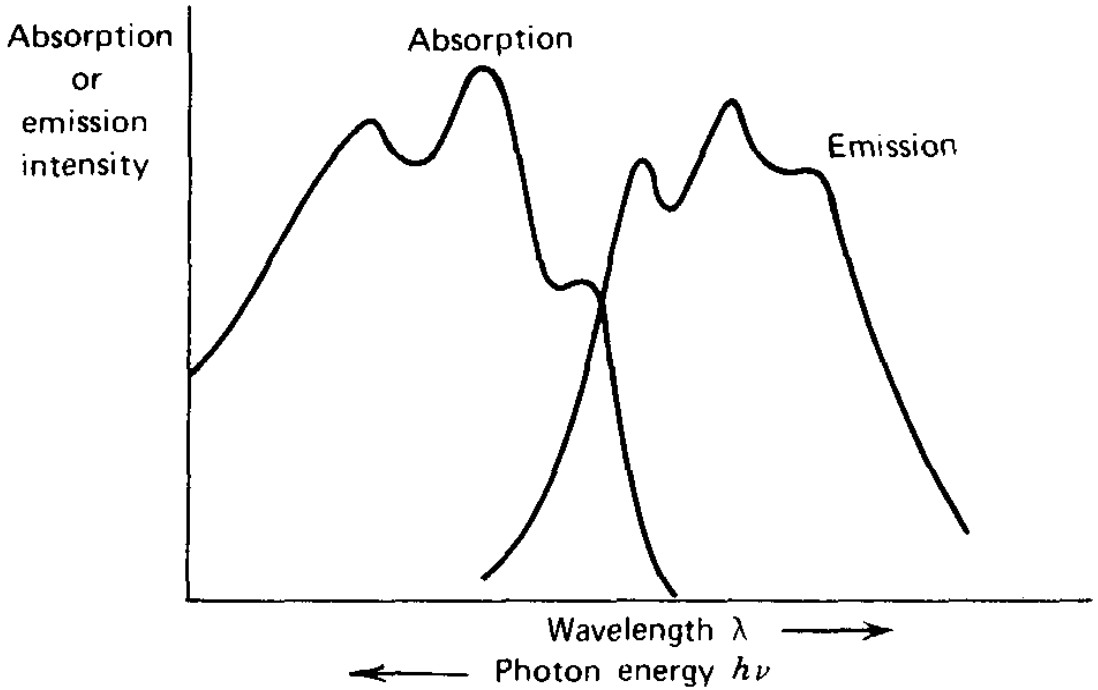
Organic scintillators

- Excited states S_2,S_3,S_4... decay into S_1 state without radiation emmision → non radiative decay
- Decay time ~ ps
- Prompt fluorescence light intensity expressed as $I = I_0 e^{-t/\tau}$

  with τ being the time constant (~ ns) → prompt scintillation component is relatively fast
- Lifetime of T_1 of the order of ms → time constant for phosphorences and delayed fluorescence is longer than fluorescence
  - Wavelength of phosphorescence spectrum longer than fluorescence spectrum (T_1 lower than S_1)

Absorption and emission spectra

- Emission spectra peaked on longer wavelengths than absorption
  - $S_0 \rightarrow S_1, S_2, S_3 \ldots$ transition require higher energies than $S_1 \rightarrow S_0$ or $T_1 \rightarrow S_0$
- Fluorescence emission: less energetic than the energy needed to excite the molelcules → small overlapping between absorption and emission spectra



Quenching

- Scintillation efficiency: fraction of all incident particle energy that is converted into visible light
  - Should be as large as possible
- Unfortunately there are alternate de-excitation modes available to the excited molecules that do not involve the emission of light (non-radiative modes) → mainly heat
- All such radiationless de-excitation processes are grouped together under the term quenching and reduce efficiency
- Quenching can be addressed to:
  - Transfer of energy from molecule to molecule before de-excitation occurs
    - *Important for organic scintillators that involves more than one species of molecules*
  - Impurities
    - *Dissolved oxygen in liquid scintillators*
  - Wavelength shifter: component added to the scintillating material to absorb the light produced by the primary scintillant and reradiate it at a longer wavelength → used to match photodetector spectral sensitivity

Common organic scintillators

- Liquid scintillators
  - An organic scintillator is dissolved in a solvent
    - *Sometimes a wavelength shifter is added to the mixture*
  - Are used in large volume detectors
- Plastic scintillators
  - An organic scintillator is dissolved in a solvent, which is then polymerized
  - Typical materials are the polystyrene and the polyvinyltoluene
  - Can be fabricated in any size and shape
    - *Fibers, ribbons, tiles, bars, …*
  - Commonly used in space applications

Scintillator	Type	Light Yield (photons/MeV/cm)	Decay Time (ns)	Emission Wavelength (nm)
BC-408	Plastic	10000	2.1	425
EJ-200	Plastic	10000	2.1	425
EJ-204	Plastic	10000	1.8	408
EJ-301	Liquid	12000	3.2	420
NE-213	Liquid	12000	3.5	420

Light yield

- A small fraction of the energy deposited in the material is converted in fluorescence light
  - Most of the energy is lost via reticular vibrations and heat dissipation
- A relation between the fluorescent energy emitted per unit path length (light yield) and the energy loss by the particle is given by the Birks law:

$$\frac{dL}{dx} = \frac{S\frac{dE}{dx}}{1 + kB\frac{dE}{dx}}$$

dL/dx = fluorescent energy emitted per unit path length

dE/dx = specific energy loss

S = scintillation efficiency

kB = adjustable parameter for a specific scintillator to take quenching effect into account

Electrons and α particles

- For electrons dE/dx is small:

$$\left.\frac{dL}{dx}\right|_e = S\frac{dE}{dx} \Rightarrow \left.\frac{dL}{dE}\right|_e = S$$

- For α particles dE/dx is large:

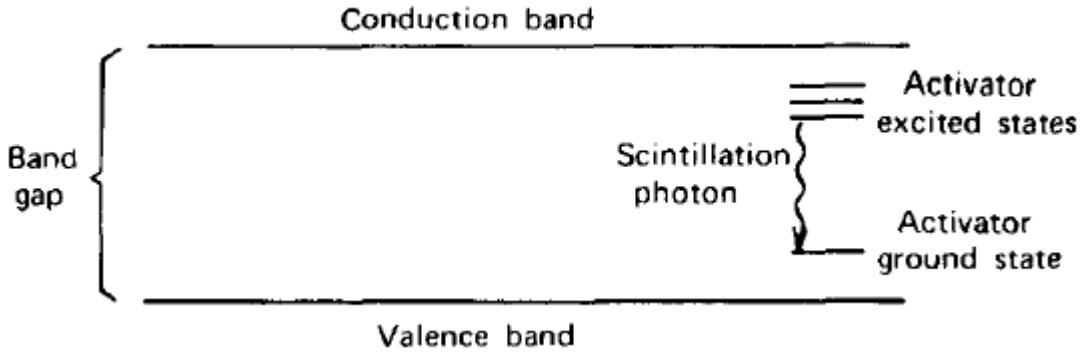
$$\left.\frac{dL}{dx}\right|_\alpha = \frac{S}{kB}$$

- The factor kB can be determined from response of the scintillator to electrons and α particles:

$$kB = \left.\frac{dL}{dE}\right|_e \Big/ \left.\frac{dL}{dx}\right|_\alpha$$

Inorganic scintillators

- An inorganic scintillator consists of a pure crystal doped with small amounts of impurities (activators)
  - The activator energy levels lie within the forbidden band of the crystal
- Ionizing particle deposits its energy in the scintillator → e-h pairs are created



- Holes moving in the valence band reach the activator sites and ionize activator atoms
- Electrons migrate in the conduction band until they reach ionized activator atoms
- The activator is then left in an excited state, and de-excites with the emission of a scintillation photon (fluorescence)
  - Live times of excited states are in the range $50 - 500ns$
- If the transition to the ground state is forbidden, further energy must be supplied (usually from thermal excitation) to raise the activator in a state from which de-excitation to ground state is allowed
  - In this case, de-excitations result into phosphorescence photons

Common inorganic scintillators

- NaI(Tl)
  - High light yield, 230ns decay time
  - Good linearity
  - Hygroscopic, fragile, can easily be damaged by mechanical or thermal shock
- CsI(Tl) and CsI(Na)
  - High light yield, 680ns and 460ns decay times for CsI(Tl) and CsI(Na)
  - Efficient gamma-ray absorption → good for calorimetry
  - Robust → widely used for space applications

Material	Dopant	Radiation Type	Light Yield (photons/keV)	Emission Wavelength (nm)	Decay Time (ns)	Density (g/cm^3)	Hygroscopic
NaI(Tl)	Thallium (Tl)	γ, X-rays	~38–40	~415	~230	3.67	Yes
NaI(Li)	Lithium (Li)	γ, thermal neutrons	~10–15	~410	~230	3.67	Yes
CsI(Tl)	Thallium (Tl)	γ, X-rays	~54	~550	~1000	4.51	Slightly
CsI(Na)	Sodium (Na)	γ, X-rays	~40	~420	~630	4.51	Slightly
BGO	-	γ	~8–10	~480	~300	7.13	No
LYSO(Ce)	Cerium (Ce)	γ, PET	~32–38	~420	~40	7.1	No
$LaBr_3$(Ce)	Cerium (Ce)	γ	~63	~380	~16	5.08	Slightly

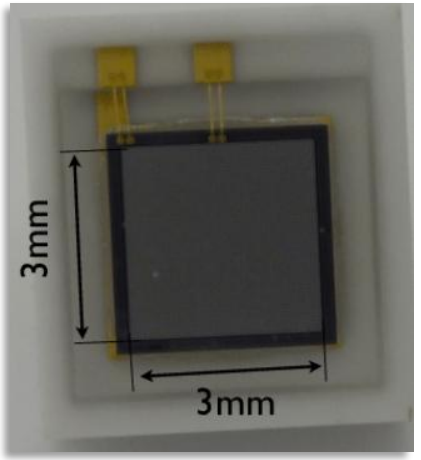
Light Collection

- Largest possible fraction of the emitted scintillation light to be collected
- The uniformity of light collection depends on the interface between the scintillator and the container holding it
- Ideally: uniform collection to ensure that all events depositing the same energy, regardless of where they occur in the scintillator, would give rise to the same mean pulse amplitude
  - The scintillation light is emitted in all directions → a limited fraction will be directly collected by the photosensor, the rest has to be reflected one or more times with possible losses → techniques to maximize reflection → **WRAPPING**
  - Optical coupling between the scintillator and the photosensor (optical grease) to avoid internal trapping due to total reflection

Silicon photomultipliers (SIPM)

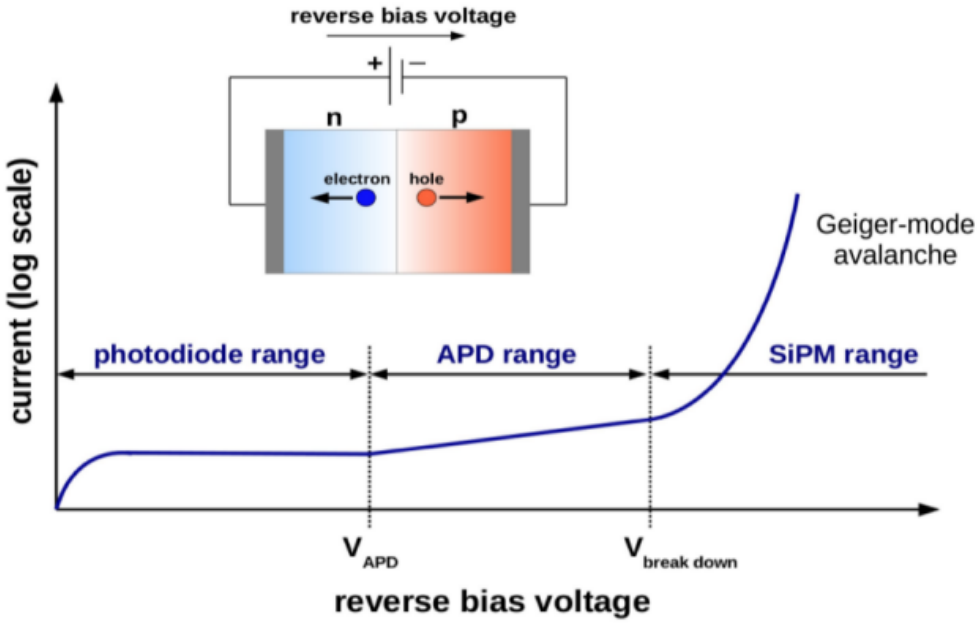
SiPM

- PMTs are the most widely used: Silicon Photomultipliers SiPMs provide similar or even better performances to the standard photomultiplier tubes (PMTs) with lower power consumption
  - SiPMs are interesting sensor that are used for many high energy physics applications
- Solid state (silicon) alternative to traditional PMTs
- Higher Quantum Efficiency (QE) and potential better energy resolution
- Lower power consumption, small dimension
- Typical peak frequency about 500 – 600 nm
- Based on avalanche photodiodes → pn junction biased reversed
  - In photodiodes: light creates e-h in the material, which are collected and proportional to light intensity → good for bright sources



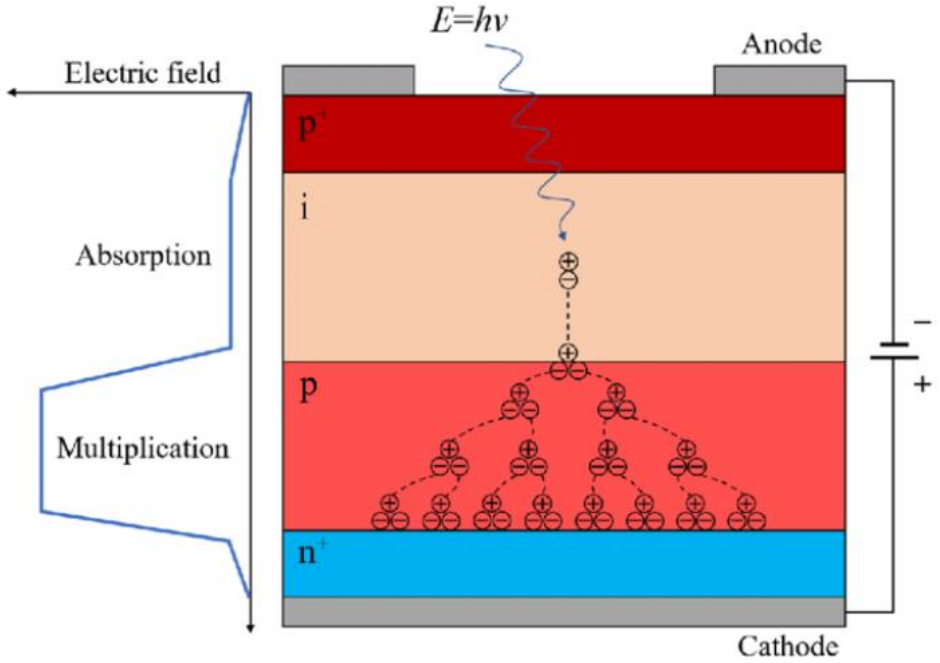
Operating voltage

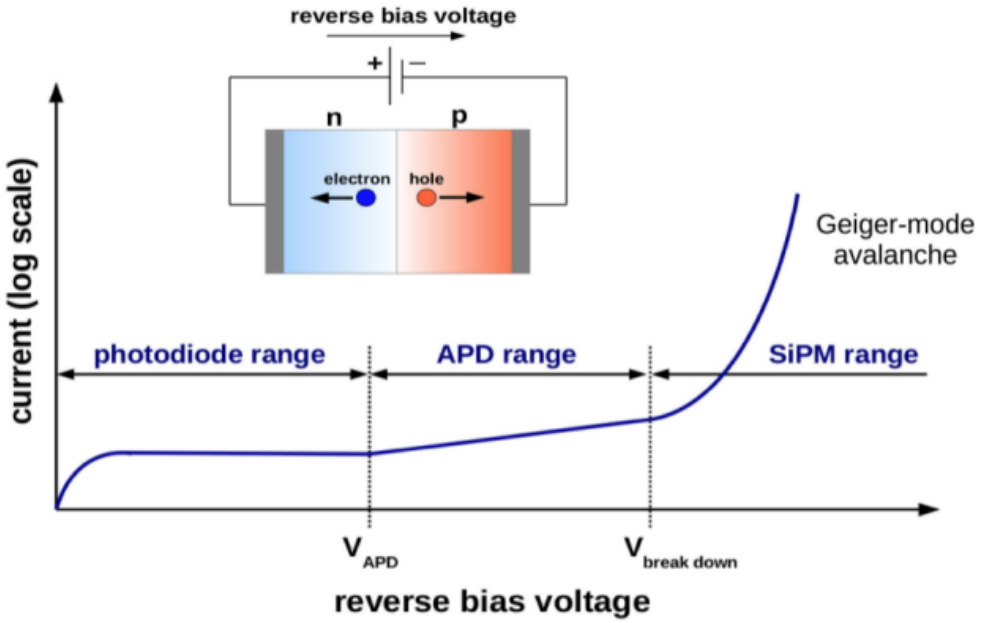
- Same device (p-n junction) depending on HV
  - Photodiode
    - *Low V and low E*
    - *Each photon created e-h pair*
    - *No multiplication of e-h*
  - Avalanche photodiode
    - *High E*
    - *Electrons gain energy and create secondary pairs*
    - *Avalanche is self-quenched*
  - Gaiger Mode – Avalance Photo Diode (GM – APD)
    - *Very high E*
    - *Also holes create secondary pairs*
    - *Need for quenchers*



Avalanche photodiodes (APD)

- Conventional photodiode: small amount of charge produced
- Operated below the breakdown voltage
  - Linearity: current signal prop to number of photons
- Avalanche process to increase the charge → high applied voltage needed
  - Charge carriers are accelerated by the electric field → more electron-hole pairs created along by collisions the path
- Gain is very sensitive to temperature and applied voltage
  - At the same voltage, gain decreased with temperature



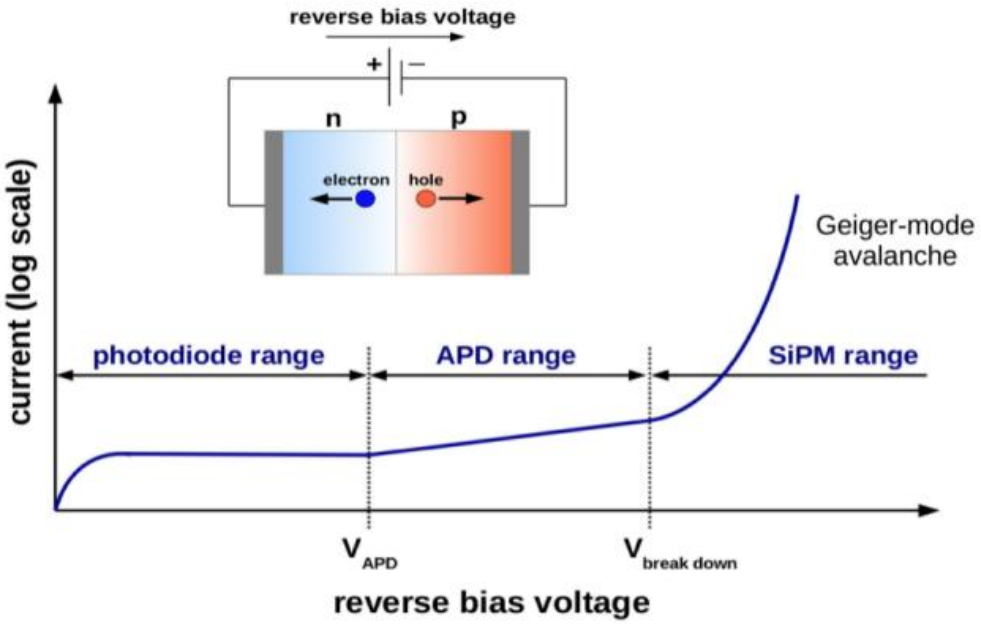


Geiger Mode APD (GM-APD)

- Diodes in which the voltage is raised high enough in order for the avalanche process to "run away" (high electric field > 5×10^5 V/cm)
- As V approches the breakdown voltage (BD), carriers will be accelerated until their kinetic energy is enough to create secondary charge pairs through the process of impact ionization → multiplication "without limit"
  - Large output pulse from a single absorbed photon
  - The silicon will break down and become conductive, effectively amplifying the original electron-hole pair into a macroscopic current flow

SPAD: single photon avalanche photodiode

Process called Geiger discharge, in analogy to the ionization discharge observed in a Geiger-Müller tube



Avalanche quenching

- Avalanche self-sustaining, unless it is stopped (quenched) by some passive or active external circuit
  - Passive quenching: introducing a large **series resistor R_Q** (kΩ) to limit the current leading to a voltage drop
    - *Reverse voltage is lowered below breakdown → further multiplication ceases*
    - *The device can return to quiescent state → ready for new detection*
    - *The time it takes for the GM-APD to recharge to the full operating voltage is called the recovery time*
      - *Tens of ns (R_Q x diode capacitance)*
  - Active quenching: fast integrated transistors to lower the applied voltage and reduce the avalanche

No information on the number of photons

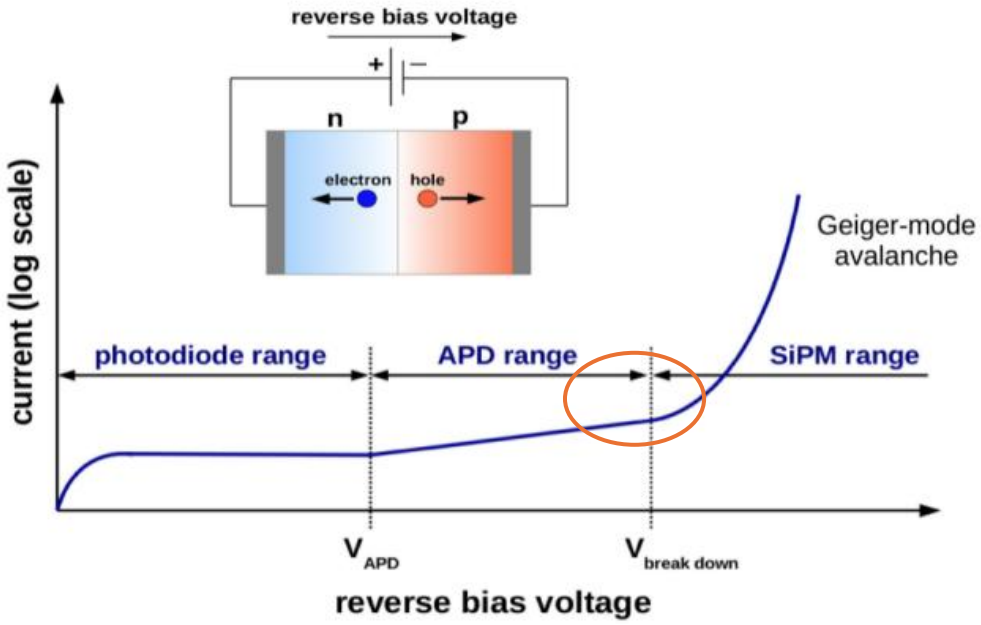
Breakdown voltage

- The reverse current-voltage curve shows a divergence at a certain bias voltage, the breakdown voltage (V_{BD})
- At this voltage the multiplication factor M diverges
- The value of V_{BD} depends on the internal structure of the diode (doping profiles) and on the temperature
- V_{BD} increases with the thickness of the depletion region and with the temperature
  - The temperature dependence of V_{BD} increases with the depletion region thickness

- The gain is the number of charge carriers collected per avalanche

$$G = \frac{avalanche\ charge}{q}$$

- Proportional to V_{OV}!
- Typically in the order of 10^5 to 10^7
- Single p.e. signals well above electronic noise → excellent single photon counting capabilities



The Silicon Photomultiplier

- For applications in which a signal proportional to the original number of photons is required, the single-cell Geiger-mode APD is not interesting
  - All the information on the number of photons is lost!
- In order to overcome this limitation → **Silicon Photomultiplier (or SiPM)**
  - Array of small APD cells, each with dimensions of only tens of μm, each operated in GM
  - Size of individual APD cell is small enough so that the probability that a cell is hit by a photon during a pulse or is hit by two photons is low
  - Single photon incident on a cell

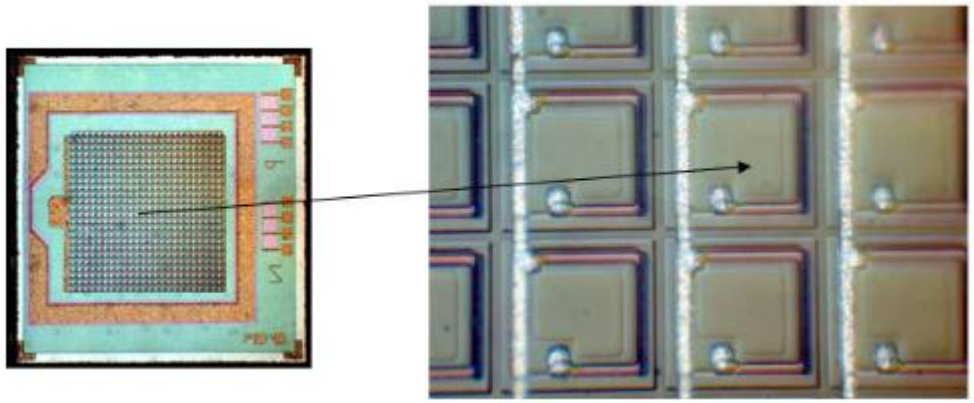
*The **number of cells** producing an avalanche is **proportional** to the **number of incident photons***

The Silicon Photomultiplier

- Arrays of many small-dimension GM-APD
- The SPAD or GM-APD is the smallest building block or microcell a SiPM
- SPADs are connected in parallel
  - One quenching resistor per SPAD
  - Common bias applied to all SPADs (a bit over breakdown voltage)
  - Each SPAD fires independently
  - The output signal is obtained by connecting in parallel all the outputs from individidual SPADs

→ analog pulse whose amplitude is proportional to the number of detected photons

Analog photon counter

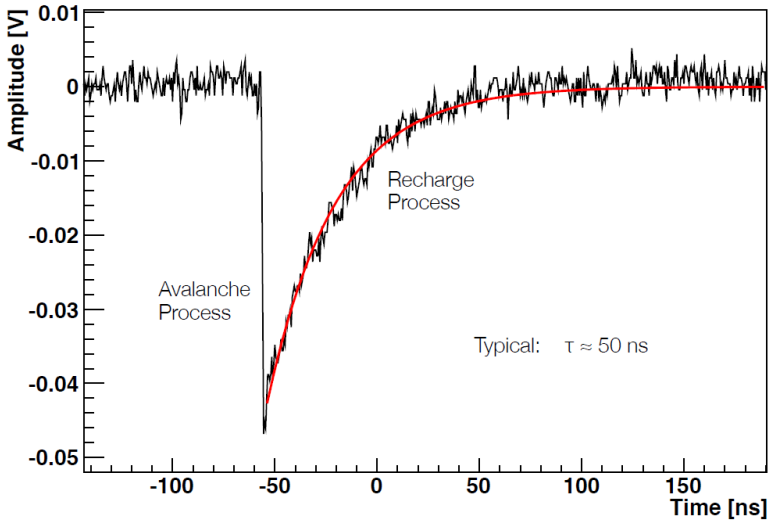


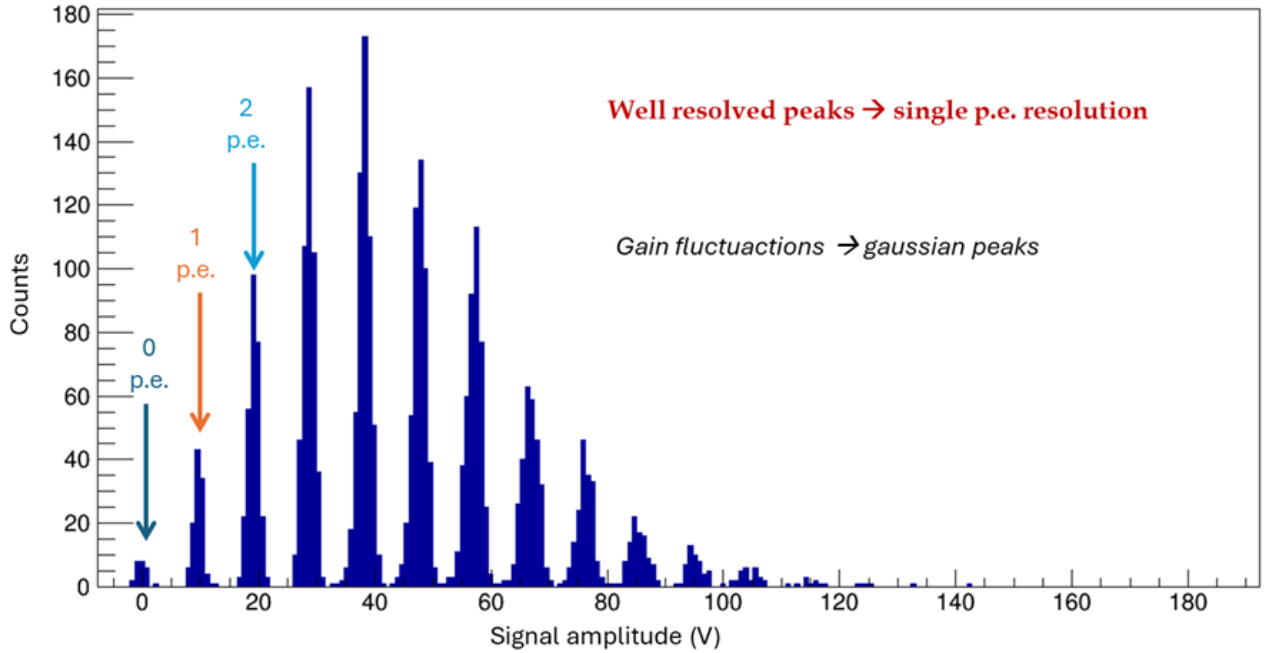
SiPM

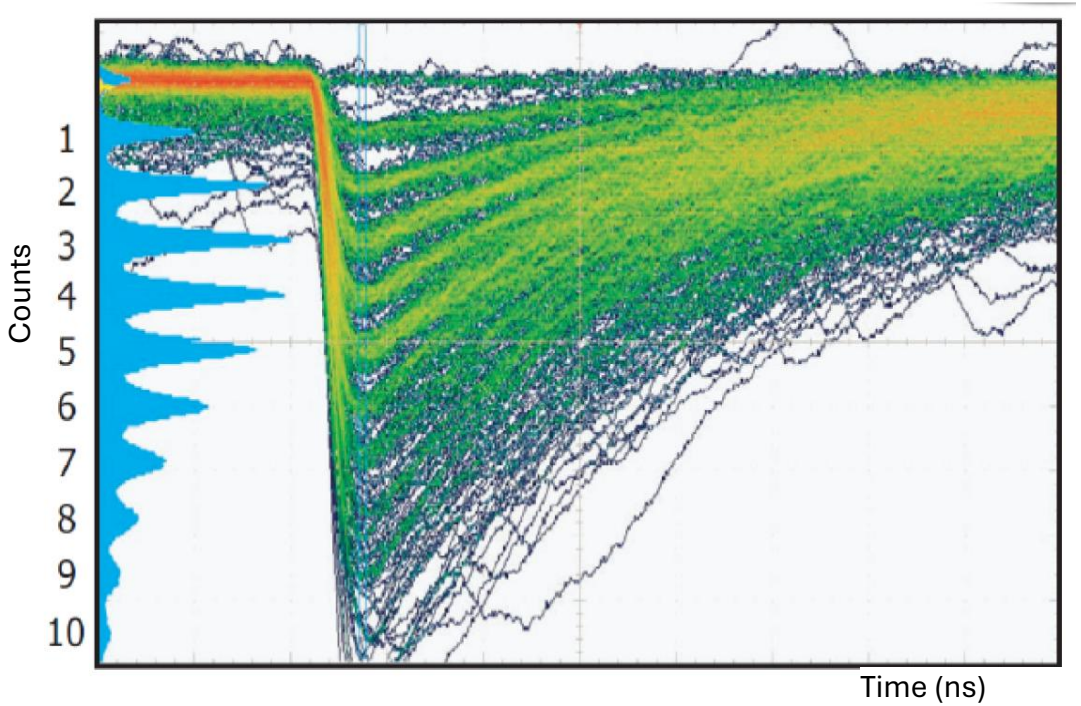
- Lack of proportionality in GM-APD → dense array of small GM-APDs to create a single detector
  - Each GM-APD + quenching resistor is a "microcell"
  - Very small size of each microcell → probability that a microcell absorbs two or more photons is very small
- 10^4 and more microcells
- When a microcell in the SiPM absorbs a photon, a Geiger avalanche is started → photocurrent flowing through the microcell

  → voltage drop across the quenching resistor as in GM-APD
- The Geiger avalanche will be confined to the single microcell
- During the avalanche process, all other microcells will remain fully charged

Response to low-level light pulses







Photon detection efficiency

- The photon detection efficiency (PDE) of the SiPM is a product of the geometric fill factor, the quantum efficiency, and the avalanche initiation probability:

$$PDE(V_{OV}, \lambda) = FF \cdot QE(\lambda) \cdot P_t(V_{OV}, \lambda)$$

- The Fill Factor (FF) depends on the dead spaces among microcells
  - Geometric factor ➔ defined as the activa area of all SPADs divided by the toal area of the SiPM
  - Smaller pixel size yields small FF
    - *Trade-off between dynamic range and PDE*
    - *Typical* $FF = 60 - 80\%$

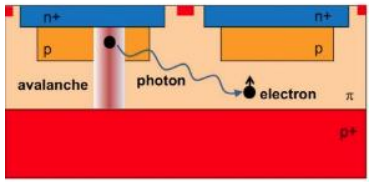
- The Quantum Efficiency (QE) is the probability that a photon that cross the device and create a p.e.
  - Strongly dependent on the wavelength and related to optical absorption coefficient of the semiconductor substrate

- The avalanche initiation probability (or trigger probability) is the probability that the p.e.* will give rise to the avalanche
  - Some p.e. may be generated in the low-E region and not gain enough energy

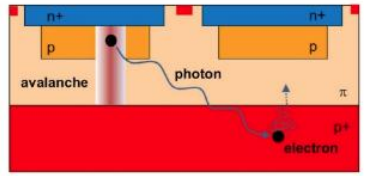
Commercial SiPMs are available with PDEs well above those of traditional PMT

Noise

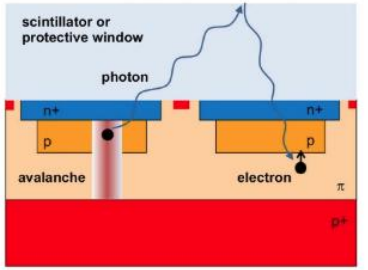
- SPADs are very sensitive to single p.e. but they are also very sensitive to thermally generated conduction-band electrons in the silicon
- These electrons lead to spurious events → dark noise (DCR)
- Strongly dependance on T → as large as 10^6 pulses/s per mm^2 @ room T
  - Higher thresholds (e.g. 5-6 p.e., depending on application) or lower T
- Impurities in the silicon lattice can traps electrons in the avalanche that are then released and can trigger a new avalanche → afterpulse (within same cell)
- Avalanche can emit a fluorescence photon that can trigger an avalanche in a neighboring cell → optical cross-talk (among different cells)
  - It increases if the fill factor increases → but high fill factor is good
  - Can be reduced using opaque trenches between microcells
- To keep the DCR low → single SPADs not bigger than ~ 100 μm
- Optical photons production increases with gain → noise strongly dependent on overvoltage



prompt or direct crosstalk



delayed crosstalk



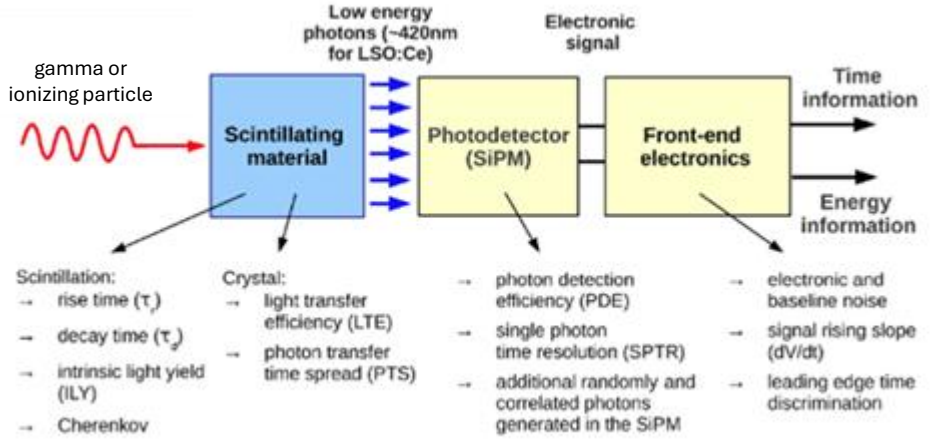
external crosstalk

Temperature dependance

- At higher T the mean free path of electrons decreases → a higher electric field is required to gain energy and start the avalanche
- Higher T → higher V_{BD}
- Typical dependence 20-60 mV/°C
- The gain depends on the overvoltage and the cell capacitance → by lowering the temperature the gain increases due to a BD shift (OV increases)
- Dark Count Rate (DCR) strongly depends on T
- PDE and crosstalk are more or less stable with T

Scintillation light and SiPM

- One application of SiPMs is to detect the produced optical, near-UV or VUV photons of scintillating materials
- Crystals like LYSO:Ce, BGO CsI(Tl) ...are commonly used
- Detector composed of three building blocks
  - Scintillating material
    - *Absorption of radiation and conversion into UV or visible photon*
  - Photodectector (SiPM)
    - *Detection of UV or visible photons*
  - Front-end electronics
    - *Readout of electric signal*



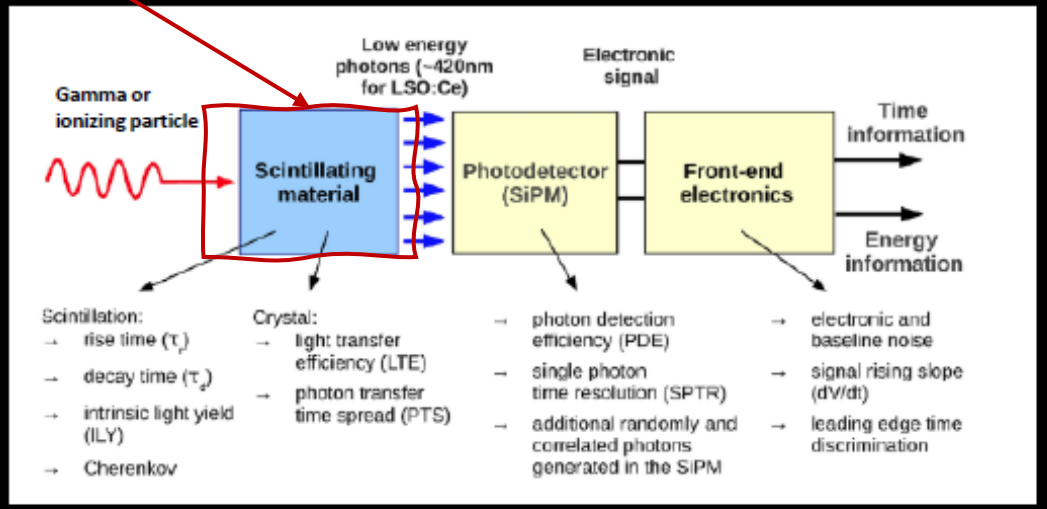
Gamma spectroscopy

- SiPMs successfully found their way into gamma spectroscopy with scintillators
- Many advantages:
  - Insensitive to magnetic fields
  - Low bias voltage
  - Adaptable for a variety of different scintillators emitting at different wavelengths
  - No burn-in effect due to input light saturation
- But also drawbacks:
  - Temperature dependance
  - Possible non-linearity due to light decay time longer than SiPM recovery time → microcells triggered multiple times within the same light pulse
  - Limited linearity and dynamic ranges
  - Crosstalk and afterpulsing

Simulation of optical photon propagation for generic scintillator-based detectors

- Geant4 (GEometry ANd Traking)

- Detector composed of three building blocks
  - Scintillating material
    - Absorption of radiation and conversion into UV or visible photon
  - Photodectector (SiPM)
    - Detection of UV or visible photons
  - Front-end electronics
    - Readout of electric signal



You must provide the necessary information to configure your simulation

References

- Knoll, Radiation detection and measurement, New York, John Wiley and Sons, Inc., 1979. 831 p.
- Gundacker, S., Heering, A., The silicon photomultiplier: fundamentals and applications of a modern solid-state photon detector, 2020 Phys. Med. Biol. 65 17TR01