Basics of Laue lens theory and simulations

or crystallography applied to high energy astrophysics …

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Coherent scattering in crystals

- What astrophysicists thought for a long time …

... the **inability to reflect or deflect individual photons** makes the **concentration of a gamma-ray beam impossible**.
A. J. Dean, *Nuclear Instruments and Methods in Physics Research* **221**, 1984

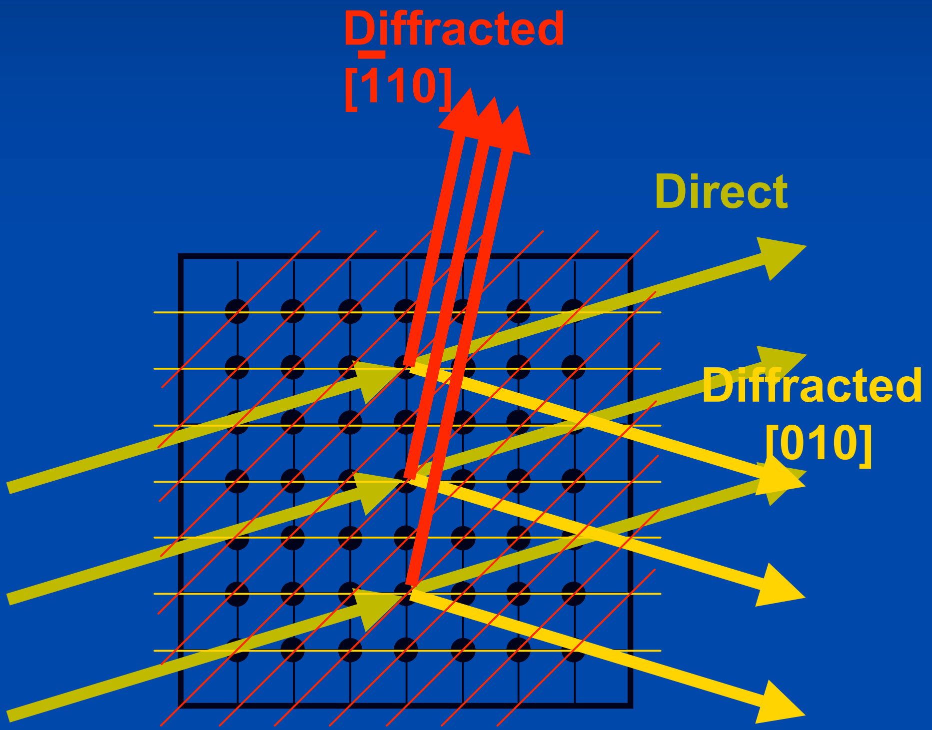
Focusing gamma rays seems out of the question since **their wavelengths** (less than 0.01 angstrom) **are smaller than the distance between atoms in solids**.
Giovanni F. Bignami, *Sky & Telescope*, October 1985

Higher-energy X-ray photons can pas through a lens, but since **they undergo no significant deflection**, **no focusing** can take place.
Gerald K. Skinner, *Scientific American*, August 1988

... **gamma-rays can not be focused**. **They are scattered incoherently** and the direction of the scattered electrons are lost.
von Ballmoos et al., *Astron. Astrophys.* **221**, 396, 1989

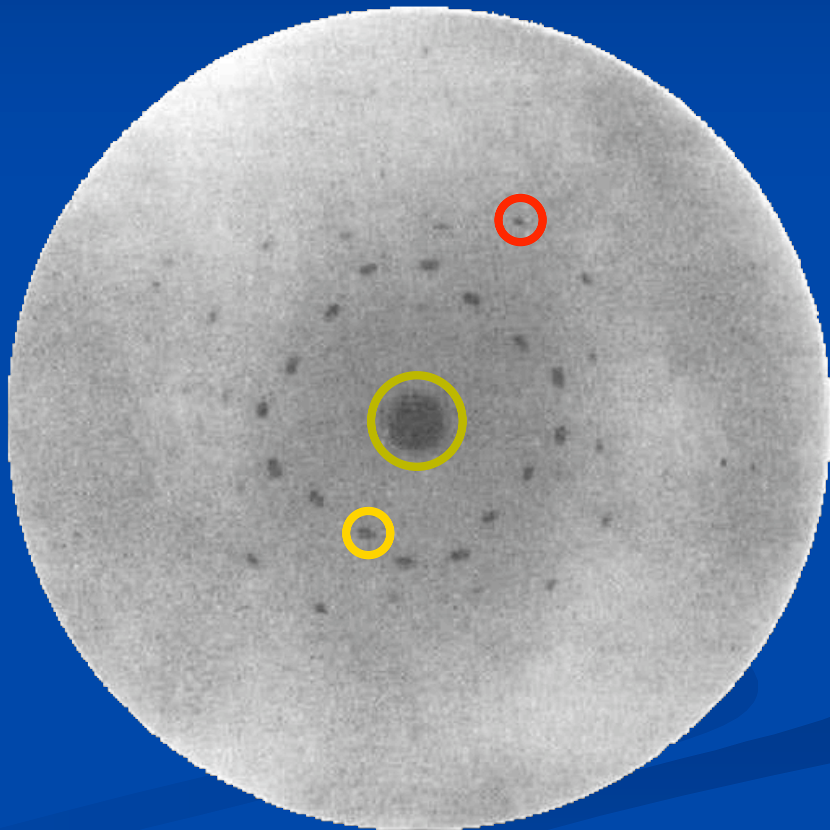
Coherent scattering in crystals

- But 93 years ago …



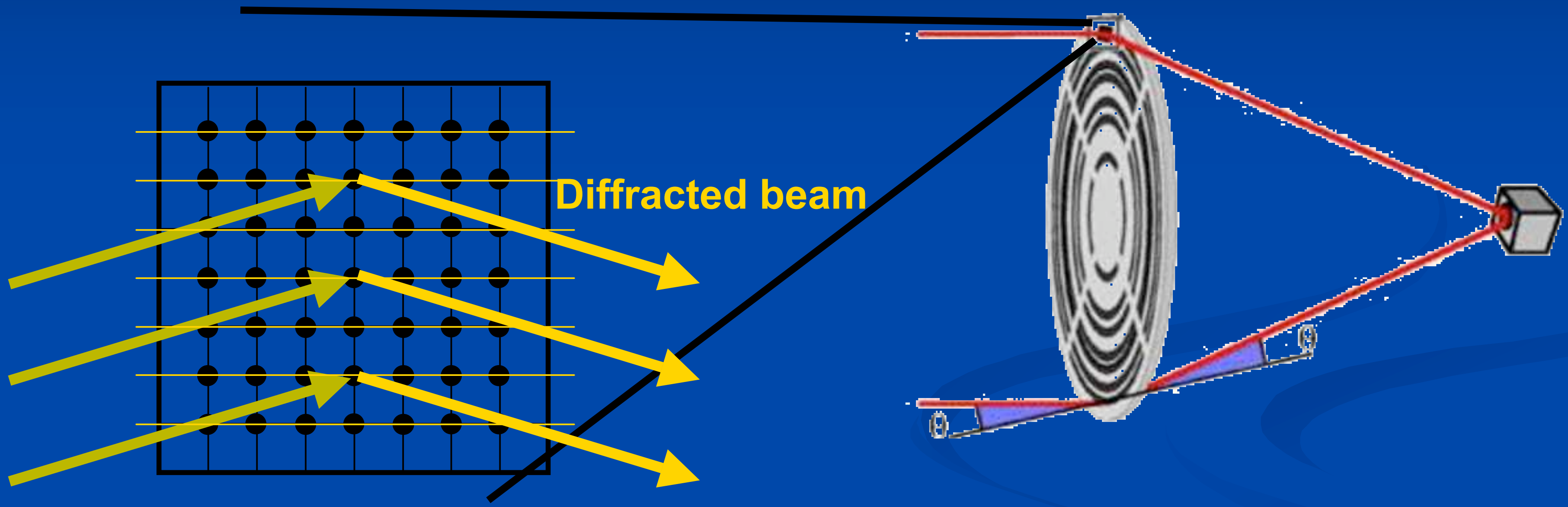
$2d_{hkl} \sin \theta = n\lambda$

Laue, Friedrich and Knipping, 1912



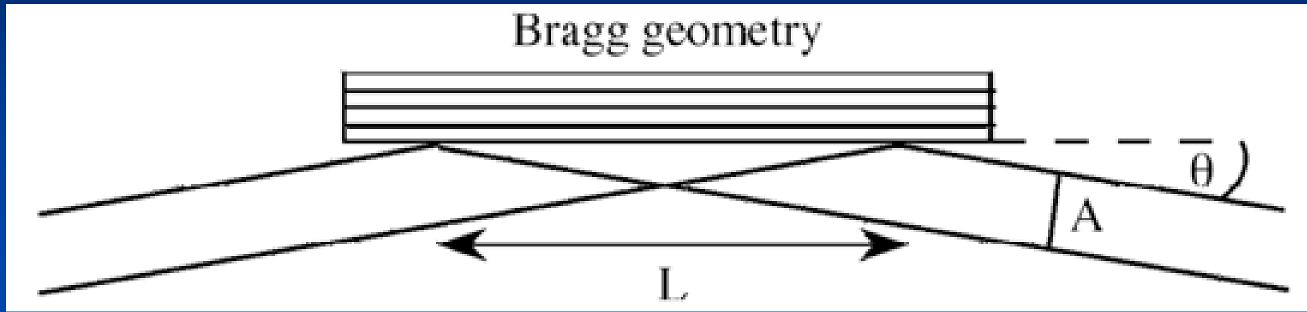
Bragg diffraction in a crystal
also valid for gamma-rays (small d_{hkl} and θ) !

Focusing gamma-rays - principle

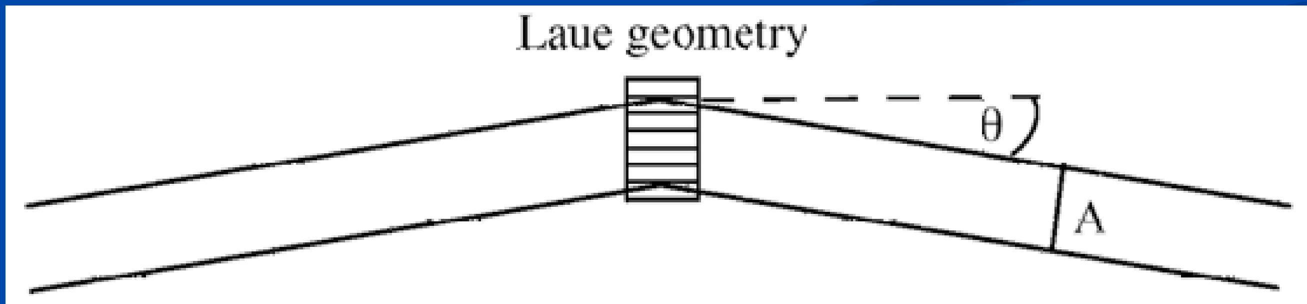


Crystals on concentric rings with varying materials, diffraction planes, etc…

Laue vs. Bragg geometry

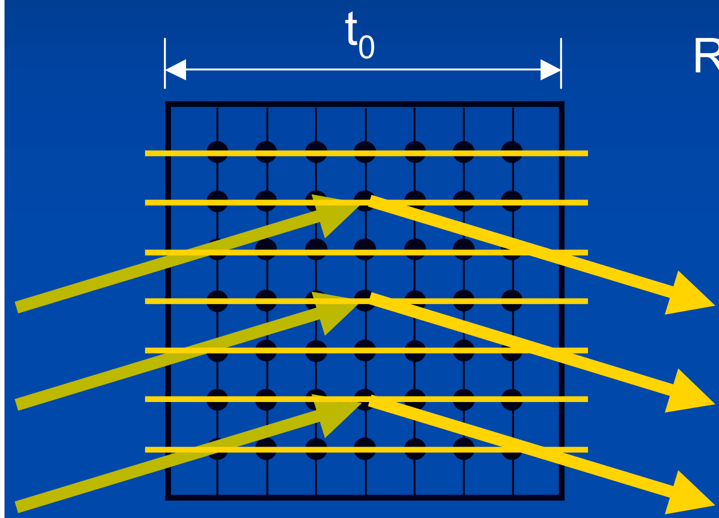


- Bragg geometry : like X-ray "supermirrors" (multilayer mirrors)
- For γ-rays : a 1-cm beam and an diffracted energy of 511 keV in Ge_{111} ⇒ L~2.8 m !



- At high energy, mean free path >~ "diffraction length" ⇒ Laue geometry possible (beam passing through the crystal).
- Requires to get homogeneous crystals (in volume not only surfaces).

Laue diffraction in crystals



Reflectivity :

$$R_m = \frac{d_{hkl}}{t_{ext}^2}\, t_0\, f\left(\frac{t_0}{t_{ext}}\right) e^{-\mu t_0}$$

planes distance

thickness

absorption

$1/\mu >> t_{ext}$

extinction length

« Pendellösung » effect

$f(x<<1)\sim 1$, $f(x>>1)\sim 1/(2x)$

$$t_{ext} \propto \frac{E\, V_c}{e^{-M}\,|F_s|}$$

energy

cell volume

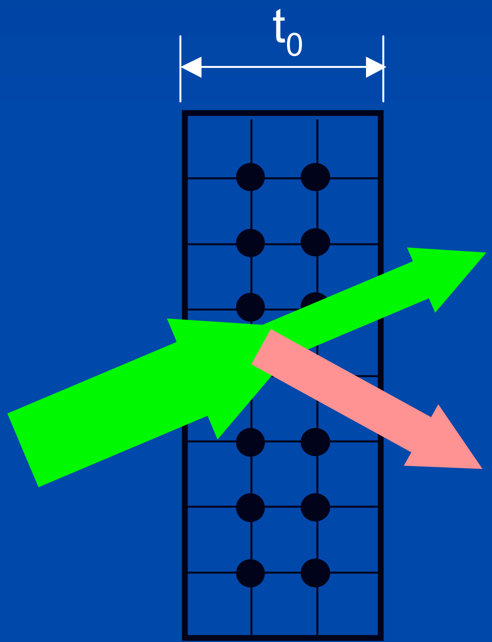
structure factor (Z, Geom)

Debye factor (T)

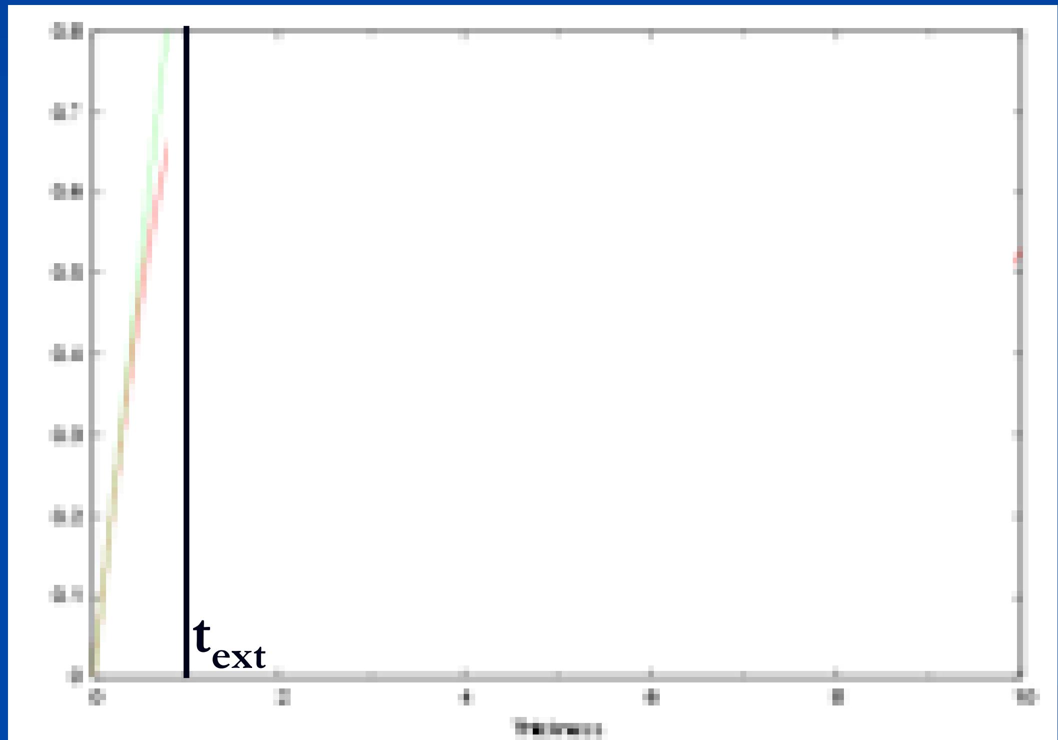
⇒ **Small efficiency**

⇒ **Monochromatic**

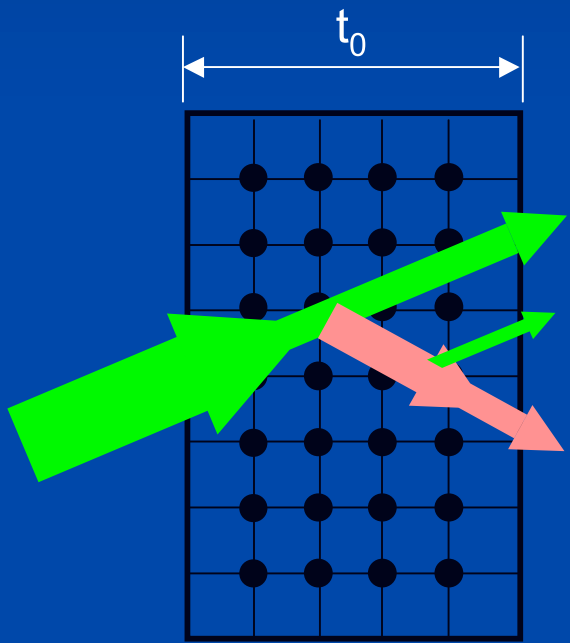
“Pendellösung” (extinction) effect



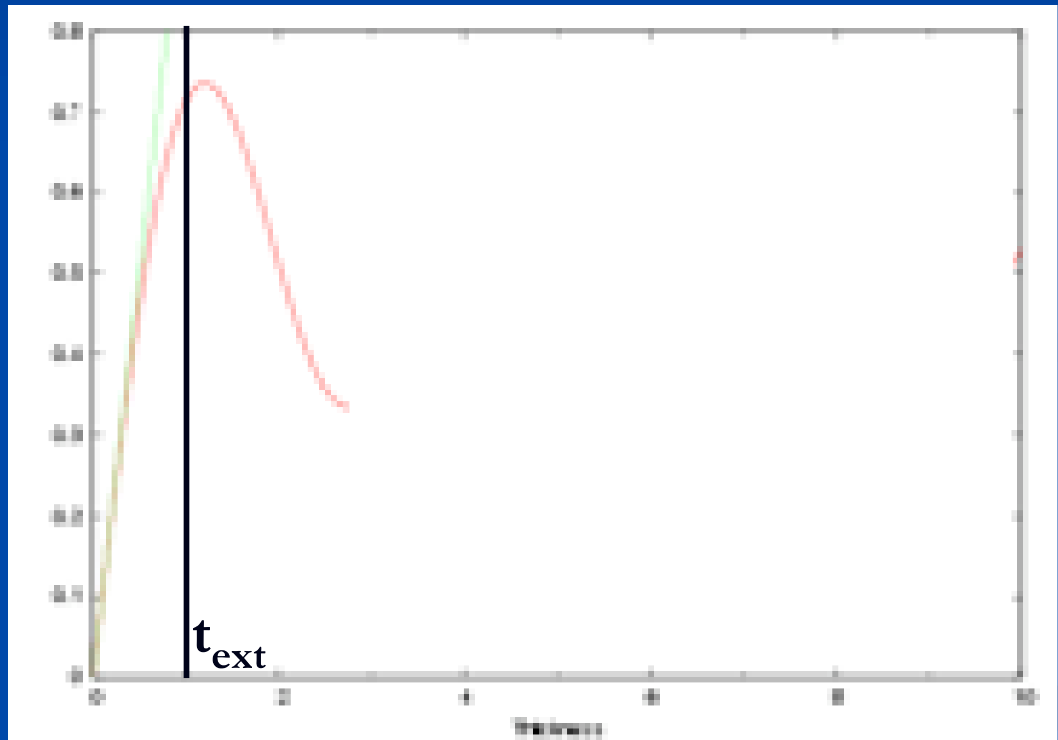
Diffracted fraction



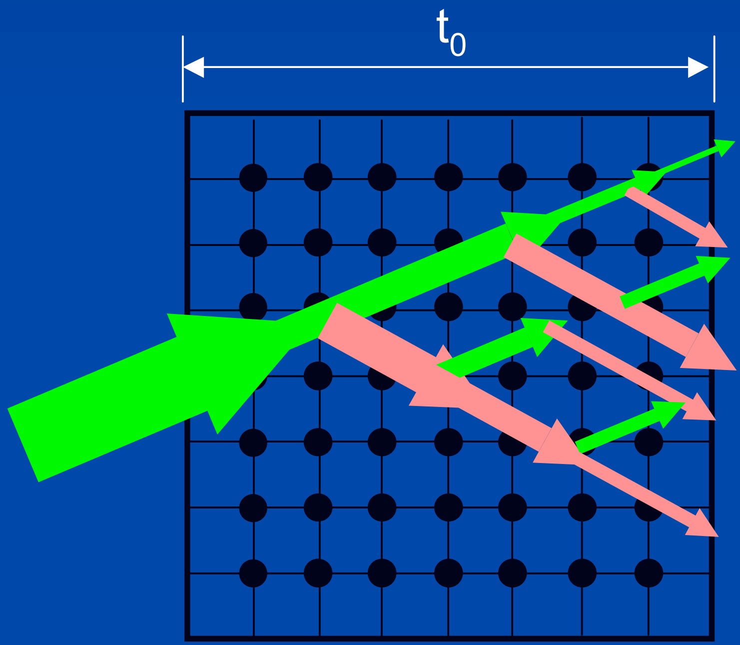
"Pendellösung" (extinction) effect



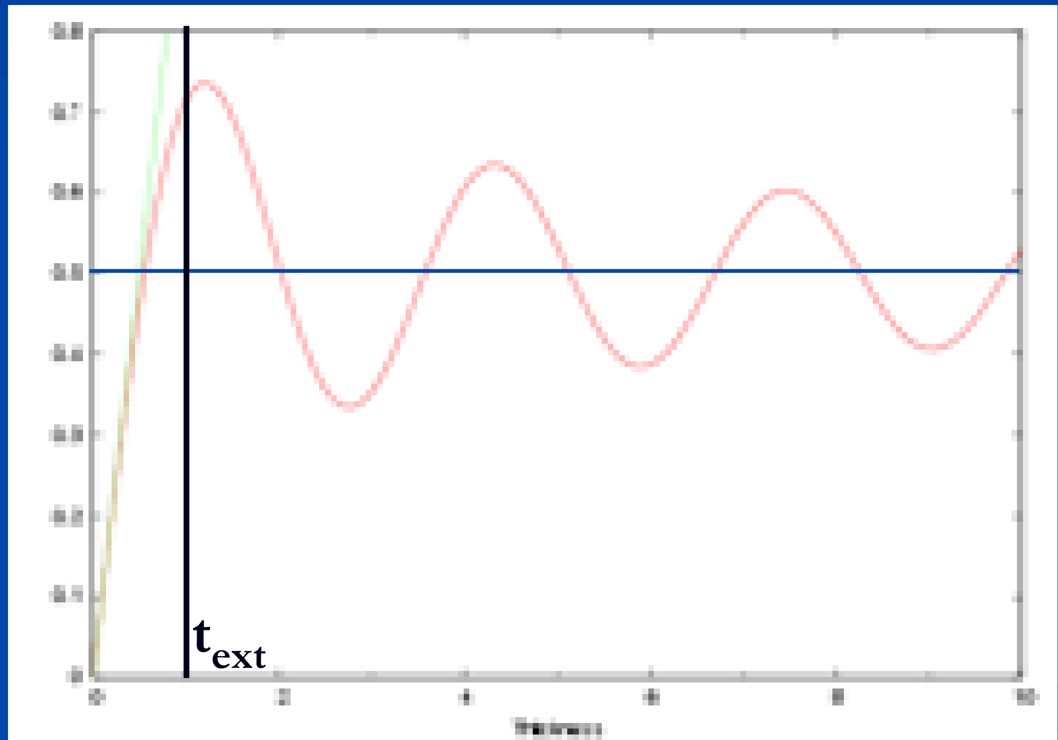
Diffracted fraction



“Pendellösung” (extinction) effect



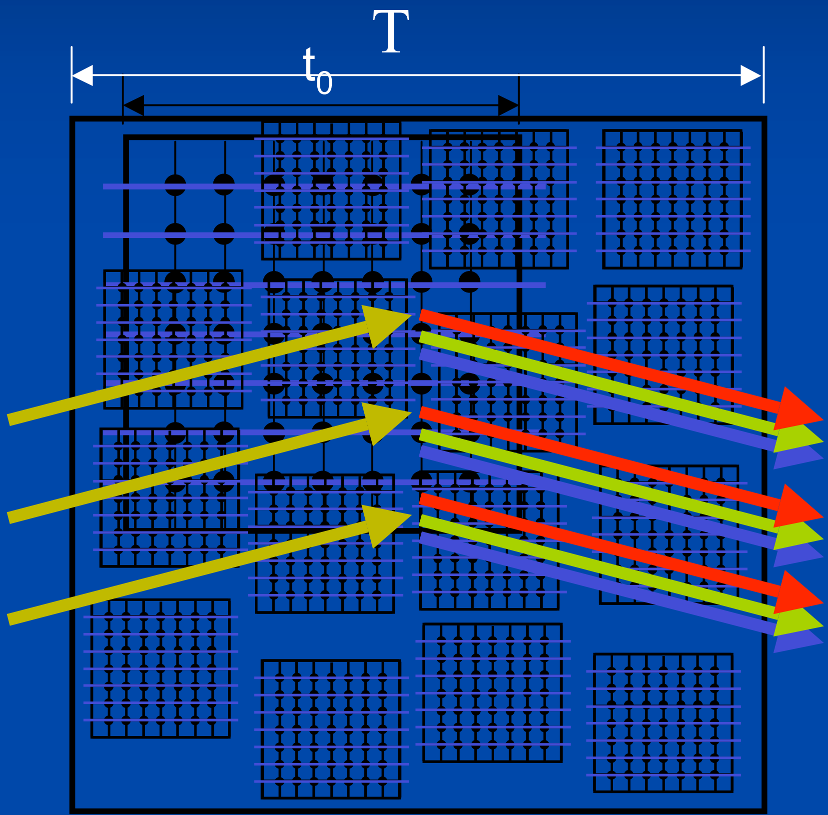
Diffracted fraction



$t_{ext} \propto E \Rightarrow$ A thick (“bad”) crystal at low energy can be thin (“good”) at high energy

Killing the coherence …

Darwin model of mosaic crystals :



- Aggregate of small « perfect » crystals
- Angular spread of the crystallites (increases the bandwidth/efficiency)
- Incoherent scattering ⇒ sum of diffracted intensities
- $t_0 << t_{ext}$ ⇒ “perfectly imperfect” crystal

$$\mathbf{r = 0.5*(1 - e^{-2\_T}) e^{-\mu T}}$$

$$\_ = \frac{d_{hkl}}{t_{ext}^2} W_m\left(\theta - \frac{hc}{2 d_{hkl} E}\right) f\left(\frac{t_0}{t_{ext}}\right)$$

Angular dist. of crystallites (typ. gauss.)
m = FWHM = mosaicity

θ_{Bragg} (E)

Pendellösung
$f \propto 1, \quad t_0 << t_{ext}$
$f \propto 1/t_0, \quad t_0 >> t_{ext}$

Properties of the reflectivity curve

$$r = 0.5*(1 - e^{-2\_T}) e^{-\mu T}$$

$$\_ = \frac{d_{hkl}}{t_{ext}^2} W_m\left(\theta - \frac{hc}{2 d_{hkl} E}\right)$$

- Variation in θ (same E) ⇒ "rocking curve"
  Variation in E (same θ) ⇒ spectral curve

  } ~equivalent if ΔE<<E $\theta - \frac{hc}{2d_{hkl}E} = \Delta\theta$

- If $\frac{T}{m} << \frac{t_{ext}^2}{2d_{hkl}}$: $r \approx 2\_Te^{-\mu T} \Rightarrow \Delta\theta_{FWHM} \approx m$

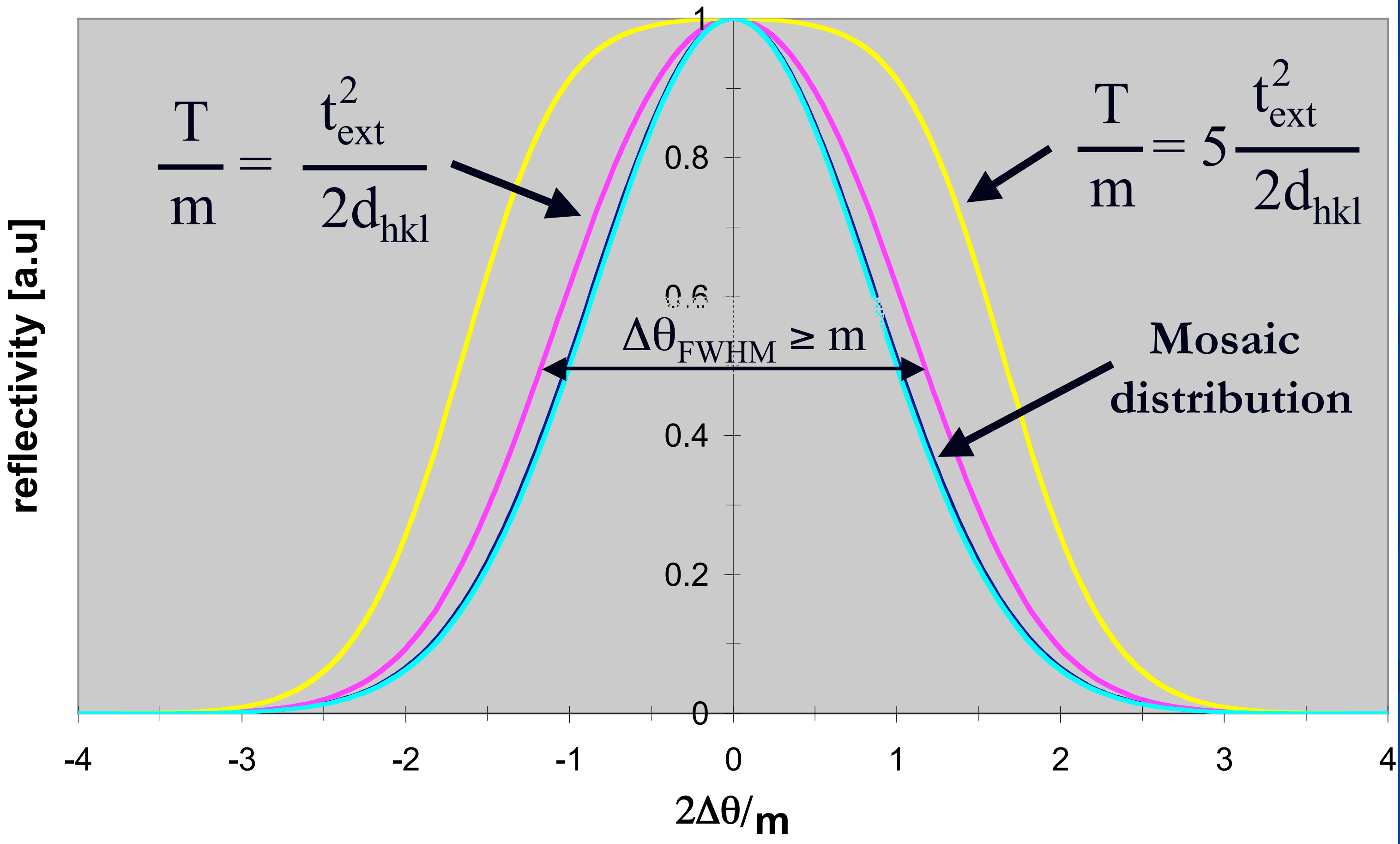
  examples at 500 keV :

  13.2 mm.arcmin^{-1} for Ge_{111}

  4.5 mm.arcmin^{-1} for Cu_{111}

Properties of the reflectivity curve

- Example for W_m gaussian (w/o absorption):



Optimization of crystal properties

- Peak efficiency optimization for a given mosaicity (m):
  - mosaicity from crystal growth constraints, expected bandwidth, …
  - maximization of peak efficiency (could be slightly different from the *integrated intensity* optimization..)
  - optimal thickness for a Gaussian distribution :

$$T_{opt} = \frac{\ln\left(1 + 0.939\,\frac{2d_{hkl}}{m t_{ext}^{2}\mu}\right)}{0.939\,\frac{2d_{hkl}}{m t_{ext}^{2}}}$$

- $T_{opt} < 1/\mu$ (mean free path) $\forall$ m
- $T_{opt} \rightarrow 1/\mu$ for $m\mu >> t^{2}_{ext}/2d_{hkl}$
- $T_{opt} \rightarrow 0$ for $m\mu << t^{2}_{ext}/2d_{hkl}$

Optimization of crystal properties

- Significance optimization in the diffracted bandwidth
  - total diffracted flux : $S \propto r_{peak} * \Delta E_{FWHM}$
  - background noise : $N \propto \Delta E_{FWHM}$
  - significance : _ $\propto S/\sqrt{N} \propto r_{peak} * \sqrt{\Delta E_{FWHM}}$
  - maximization of _ w.r.t m (mosaicity) and T (thickness)
  - optimum for a Gaussian distribution :

$$m_{opt} = 0.2871 \frac{2d_{hkl}}{t_{ext}^2 \mu}$$

$$T_{opt} = \frac{1}{2\mu}$$

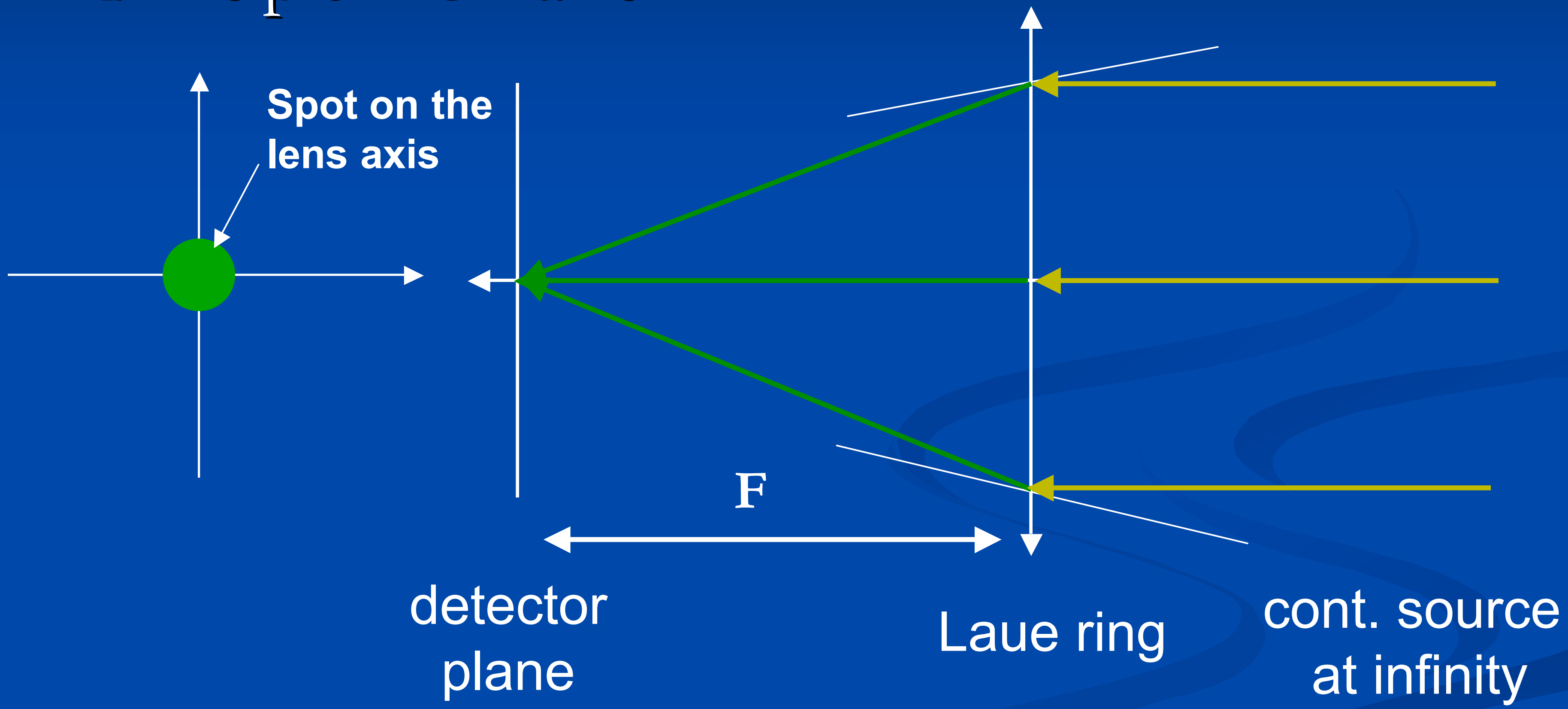
- **T_{opt} independent of crystal properties (half of the mean free path)**
- **$T_{opt}/m_{opt} = 1.74\ t^2_{ext}/2d_{hkl}$**
- **Crystals thinner than peak maximization**

Optimization of crystal properties

- The real world is more complex … :
  - Unable to separate photons from different rings with different materials/diffracting planes
  - The Darwin model is only an approximation
  - Constraints from crystal growth (homogeneity, quality, …)
  - The E bandwith(s) should be driven by the scientific objectives
  - Pointing accuracy ⇒ spectral broadening
  - mosaicity ⇒ beam divergence => loss of detectability and angular resolution on the detector plane
  - …
- Global optimization required

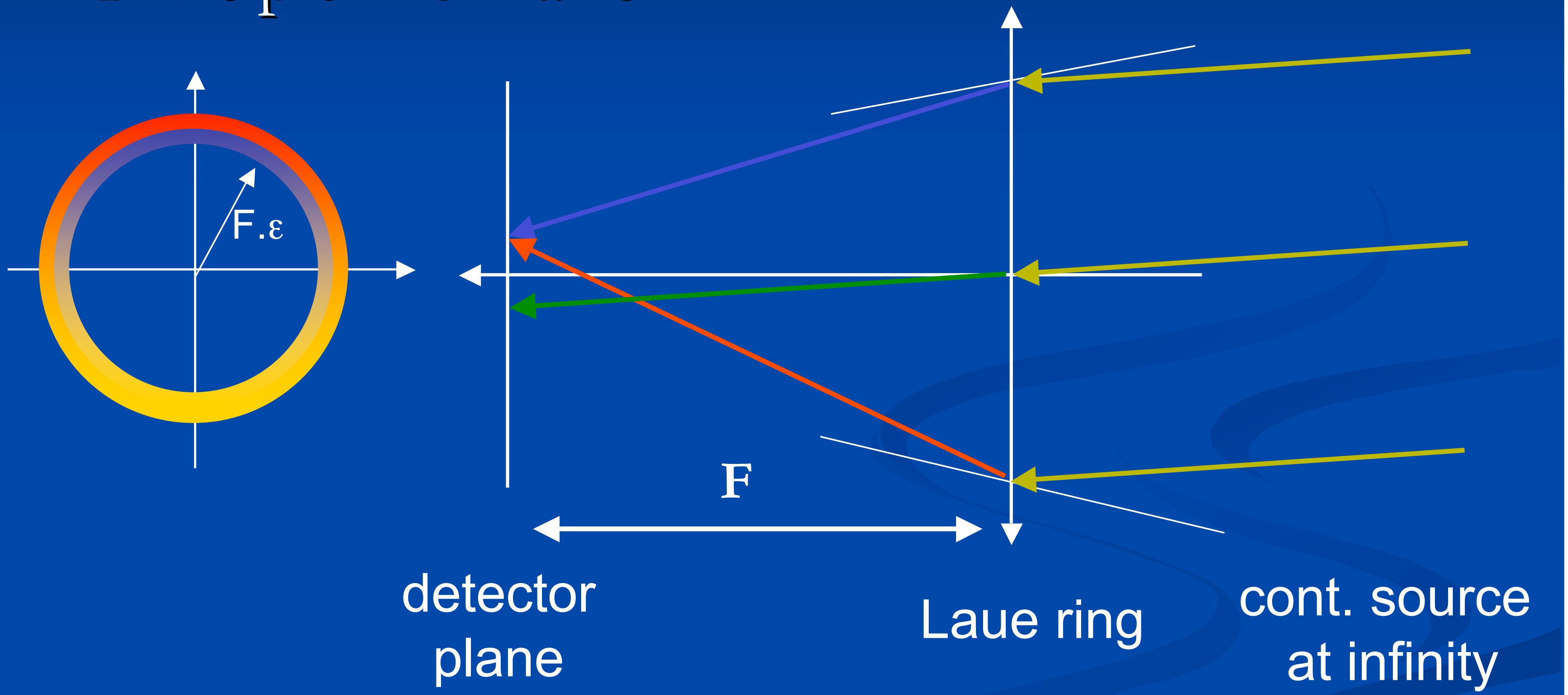
Off-axis response of a Laue ring

- Principle – On axis



Off-axis response of a Laue ring

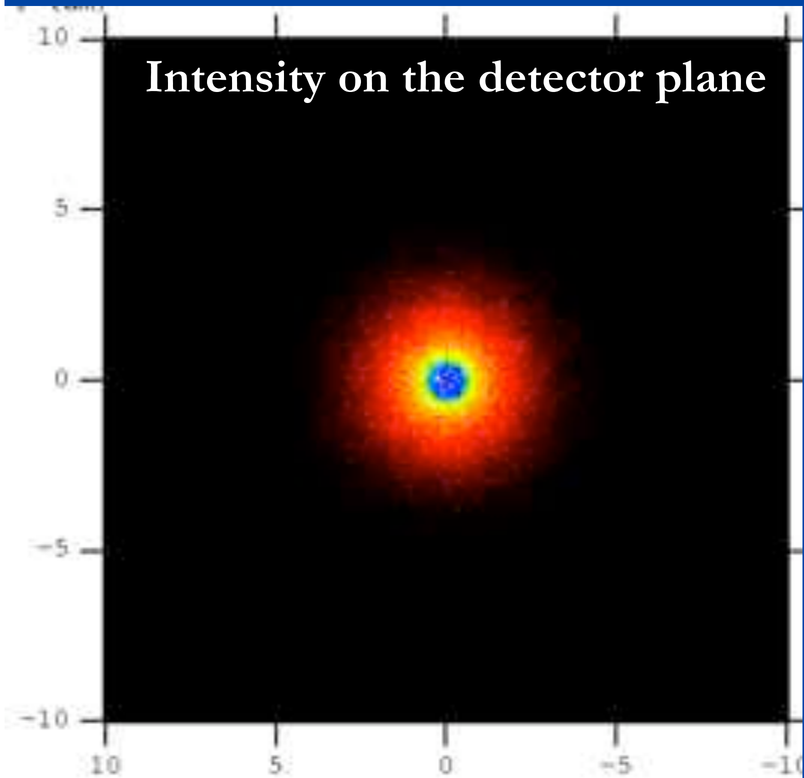
- Principle – Off axis

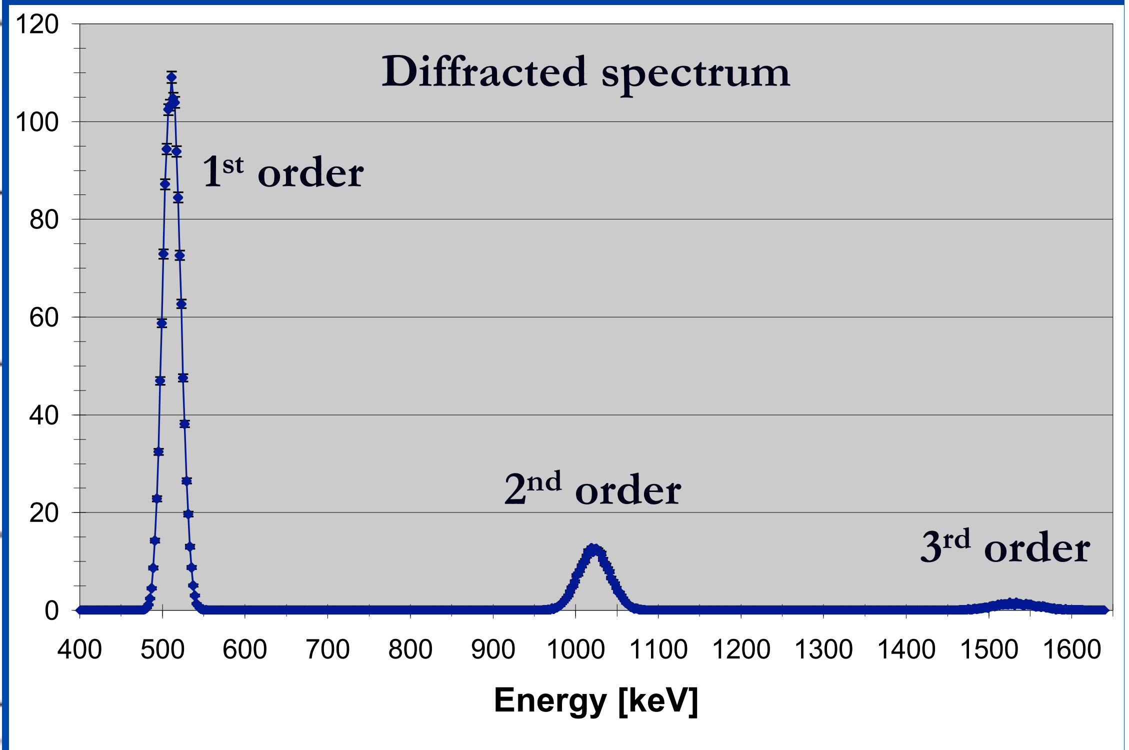


⇒ **Intensity ring on the detector plane with E_{diff} depending on the azimuth**

Off-axis response of a Laue ring

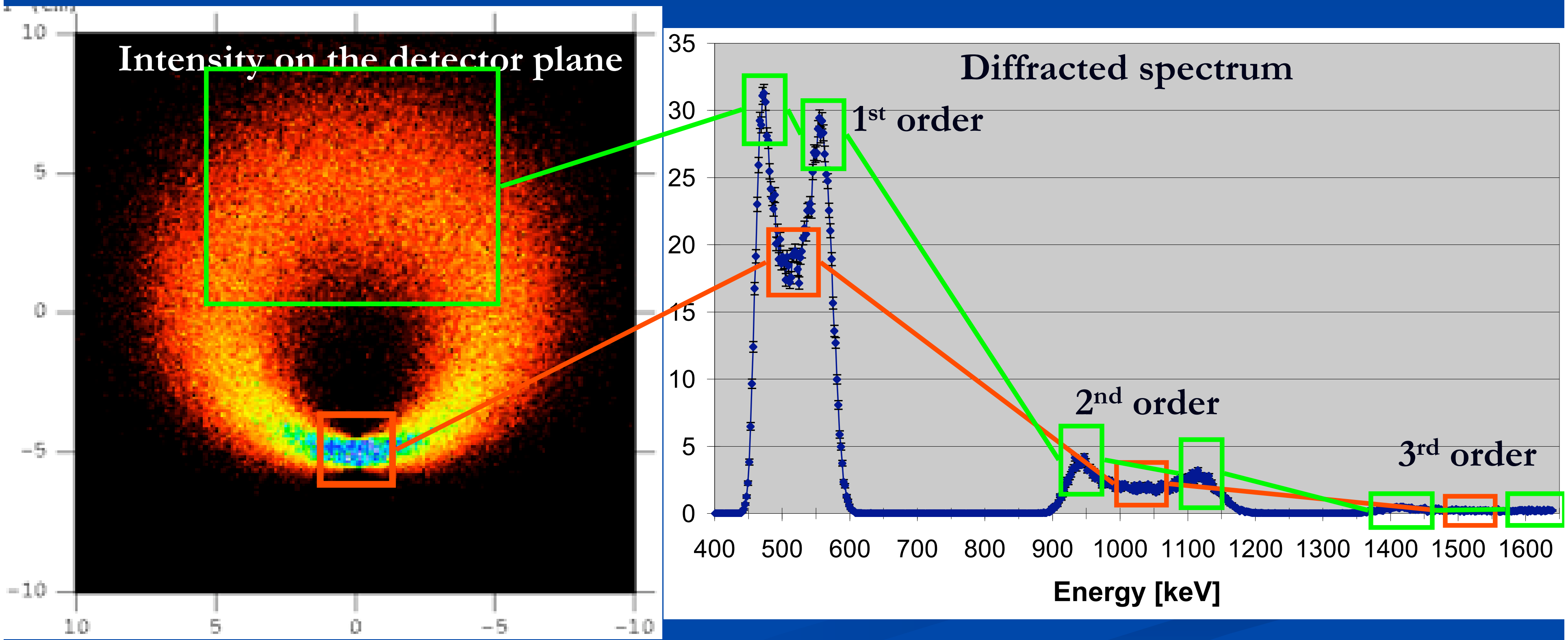
- Monte Carlo simulation – On axis
  1 Cu_{111} ring, R=1.00 m, ΔR=1.5 cm, f=86 m, E_∞=511 keV





Off-axis response of a Laue ring

- Monte Carlo simulation – Off axis (δ=1 arcmin)
  1 Cu_{111} ring, R=1.00 m, ΔR=1.5 cm, f=86 m, E_∞=511 keV



Short vs. long focal length

- Spectral response

$$E \propto \frac{F_\infty}{r.d_{hkl}} \Rightarrow \Delta E \propto \frac{d_{hkl}}{E^2.F_\infty}.\Delta r$$

Rings spacing

$$\theta_B \propto \frac{1}{E.d_{hkl}} \Rightarrow \Delta E \propto E^2.d_{hkl}.\Delta\theta$$

Mosaicity

Short focal length :

No energy overlap from one ring to another

⇒ superposition of diffracted energies (⇒ $r.d_{hkl}$ = cst)

⇒ monochromatic, low efficiency

Long focal length :

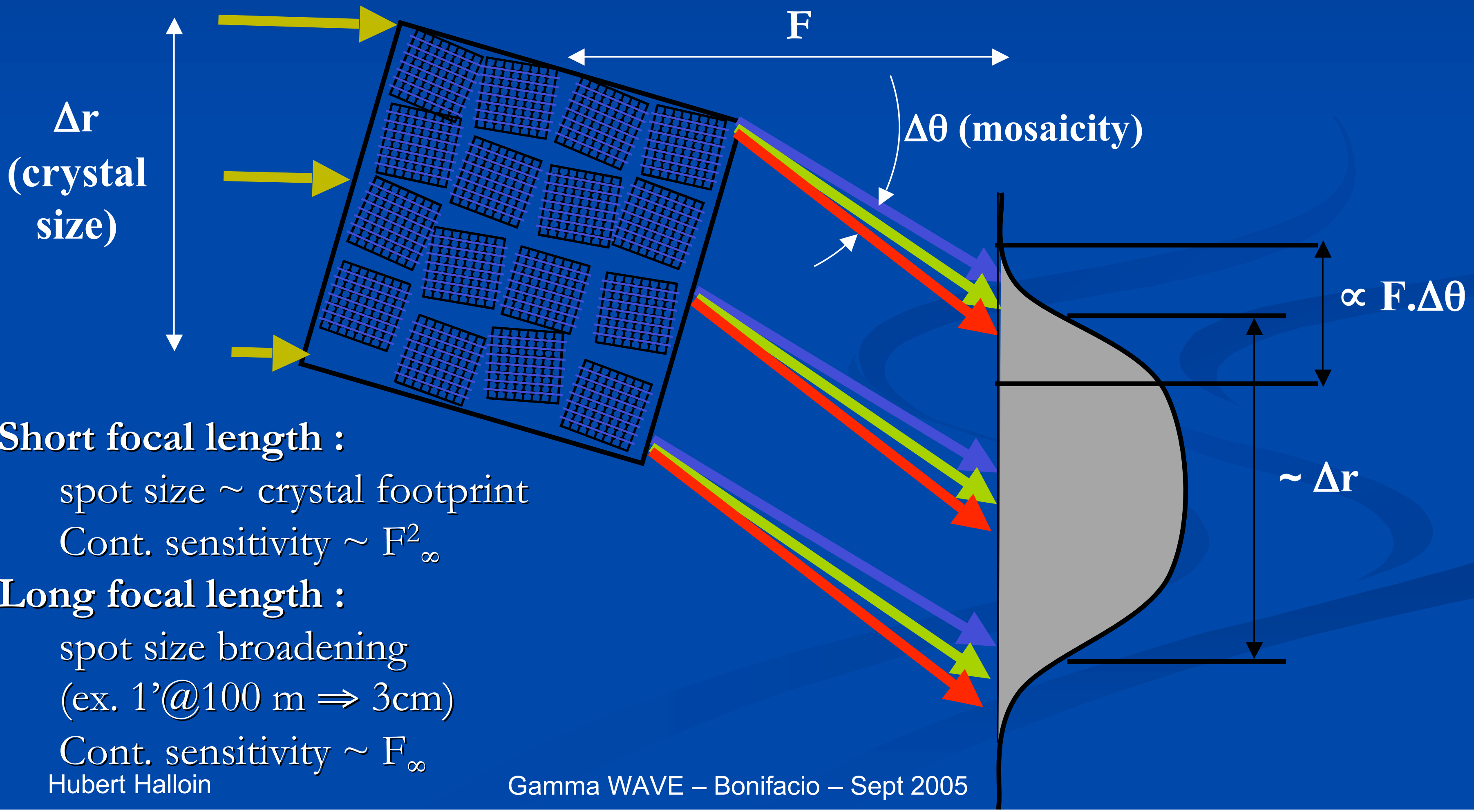
energy overlap possible between r and r+Δr

⇒ juxtaposition of diffracted energies

⇒ broad energy bandwidth for a given d_{hkl}, use of the most efficient orders

Short vs. long focal length

- Beam divergence / focal spot size



Short focal length :

spot size ~ crystal footprint

Cont. sensitivity ~ $F^2{}_{\infty}$

Long focal length :

spot size broadening

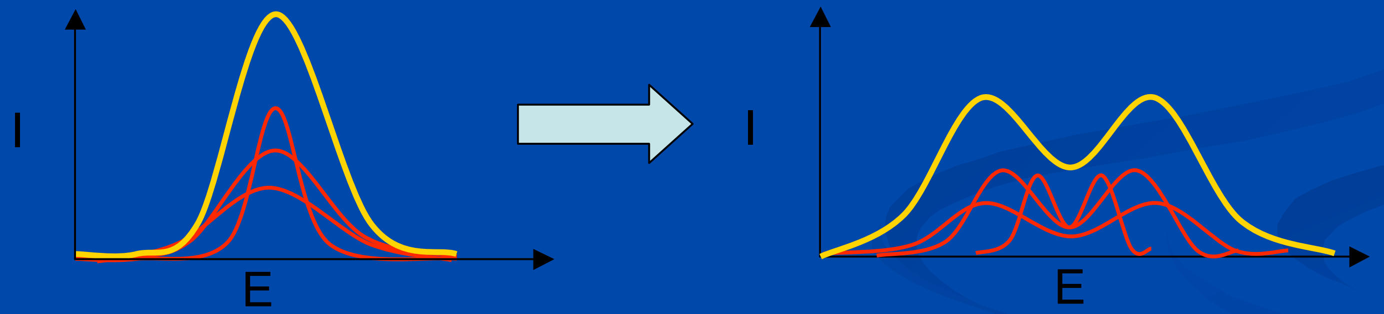
(ex. 1'@100 m ⇒ 3cm)

Cont. sensitivity ~ F_{∞}

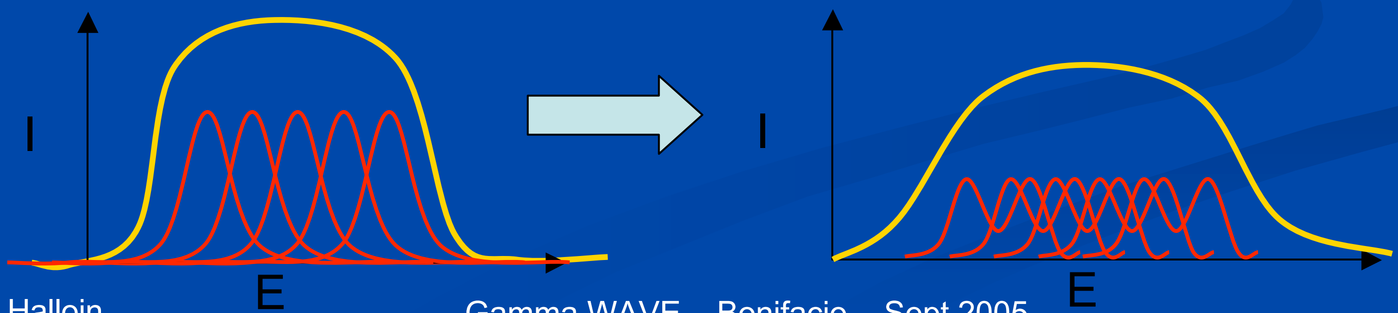
Short vs. long focal length

- Spectral response vs. pointing accuracy

Short focal length :
strong spectral deformation for off-axis source

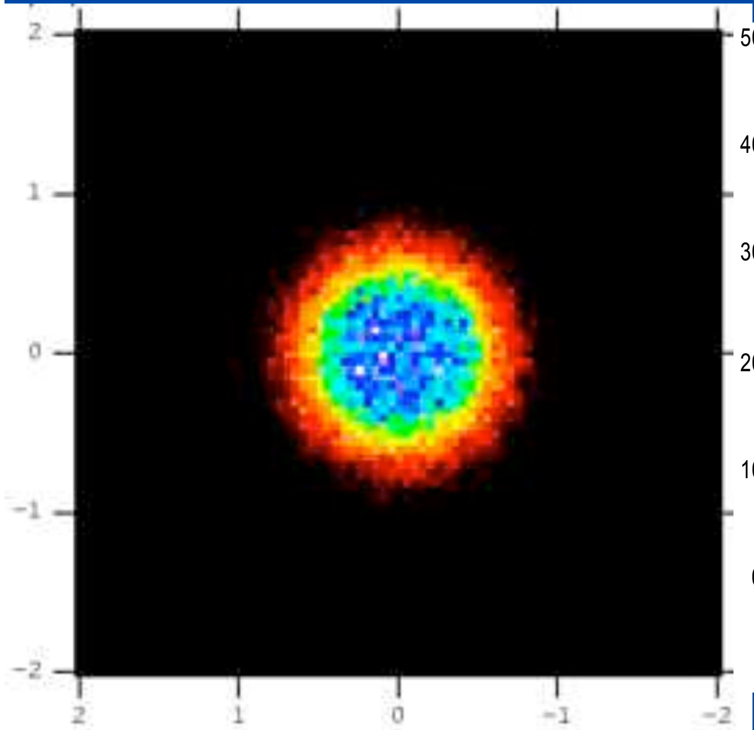


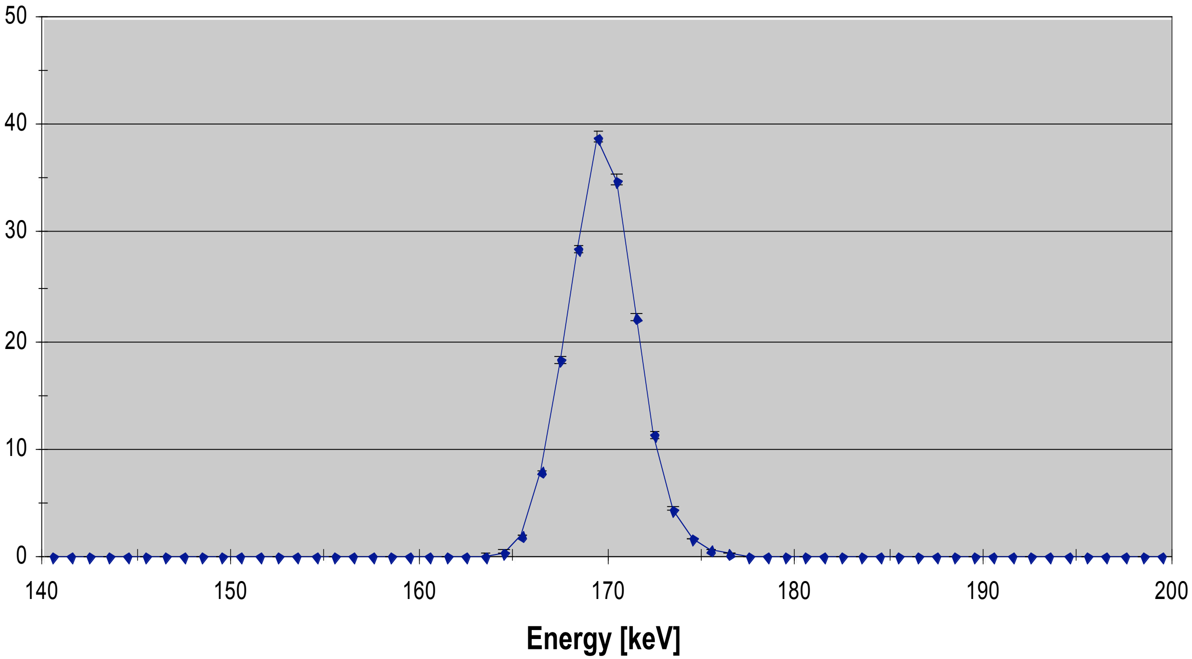
Long focal length :
energy overlap ⇒ small spectral deformation



Monte-Carlo simulations

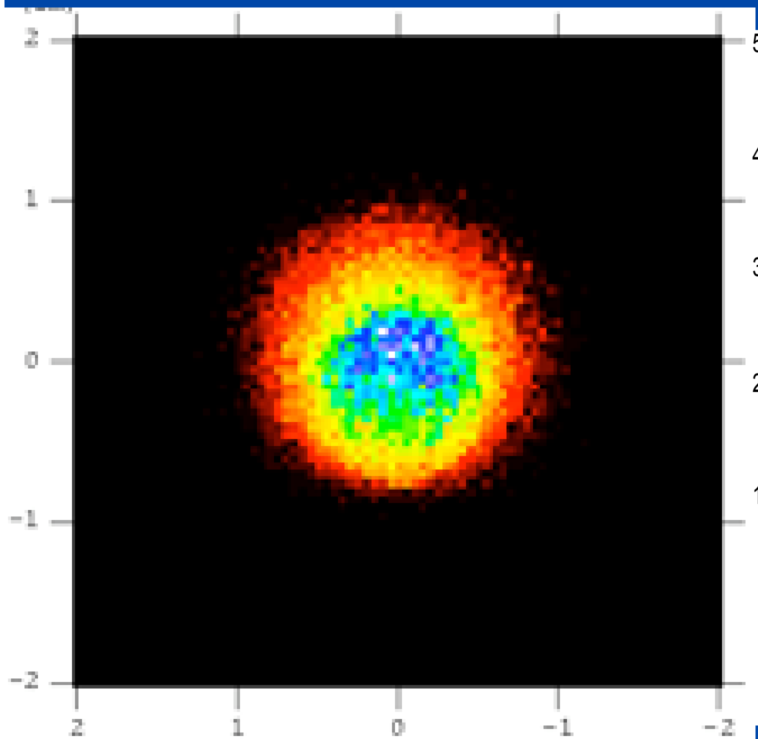
- Short focal length – On axis

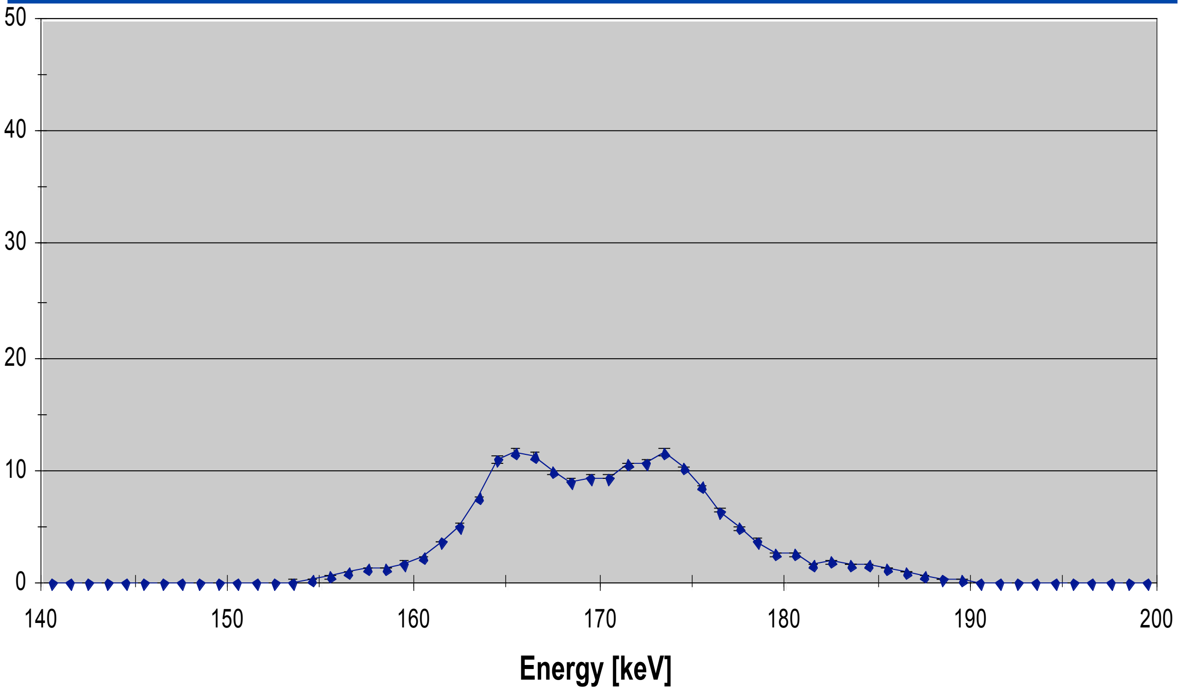




Monte-Carlo simulations

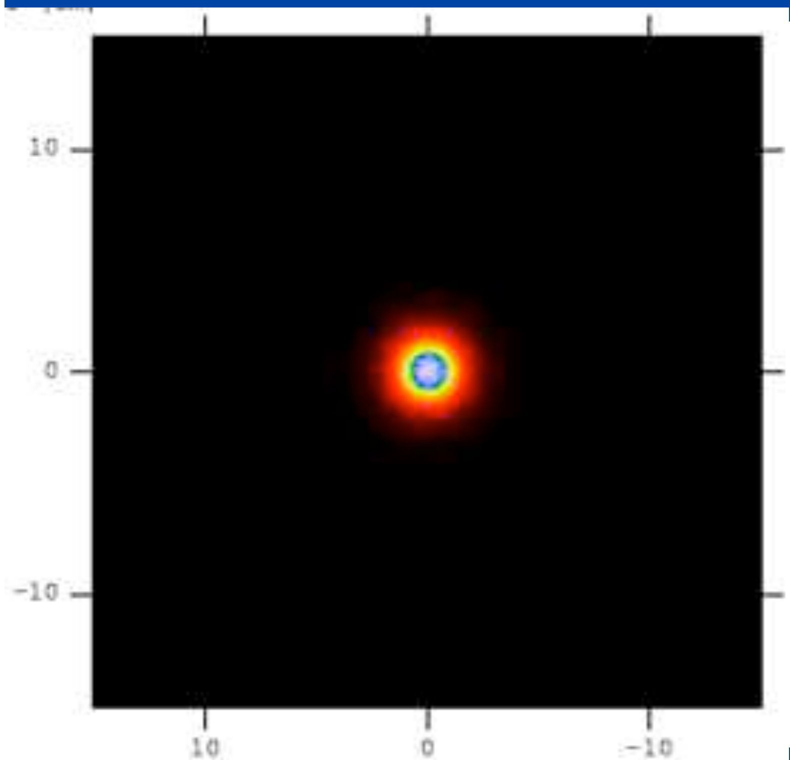
- Short focal length – Off axis (3 arcmin)

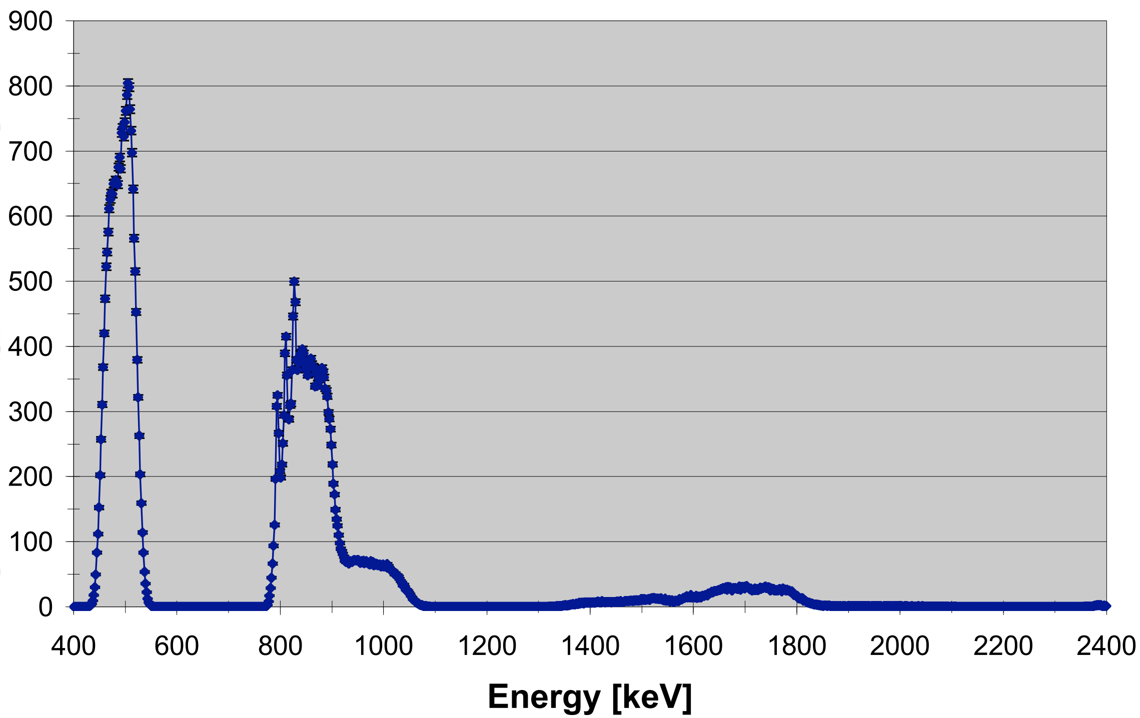




Monte-Carlo simulations

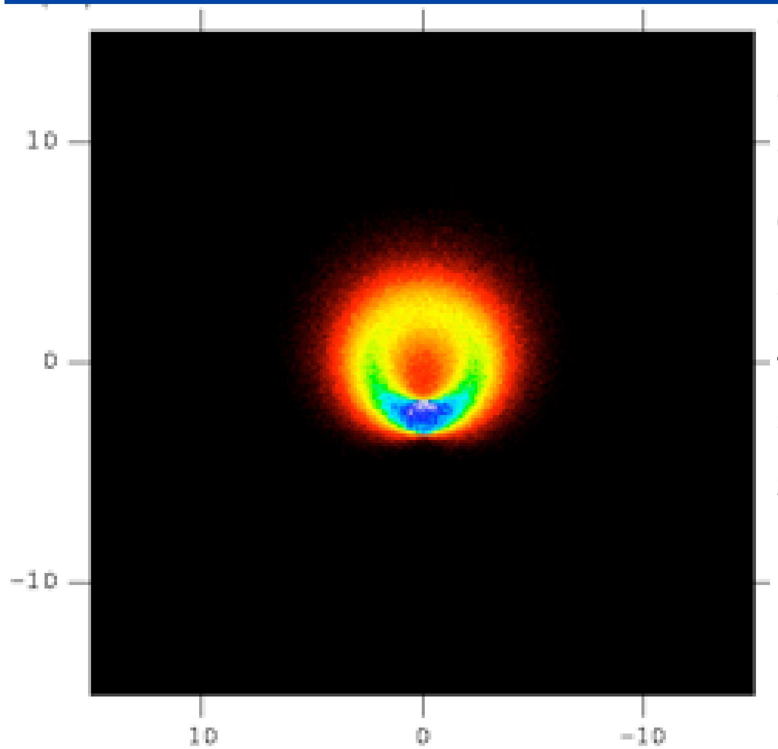
- Long focal length – On axis

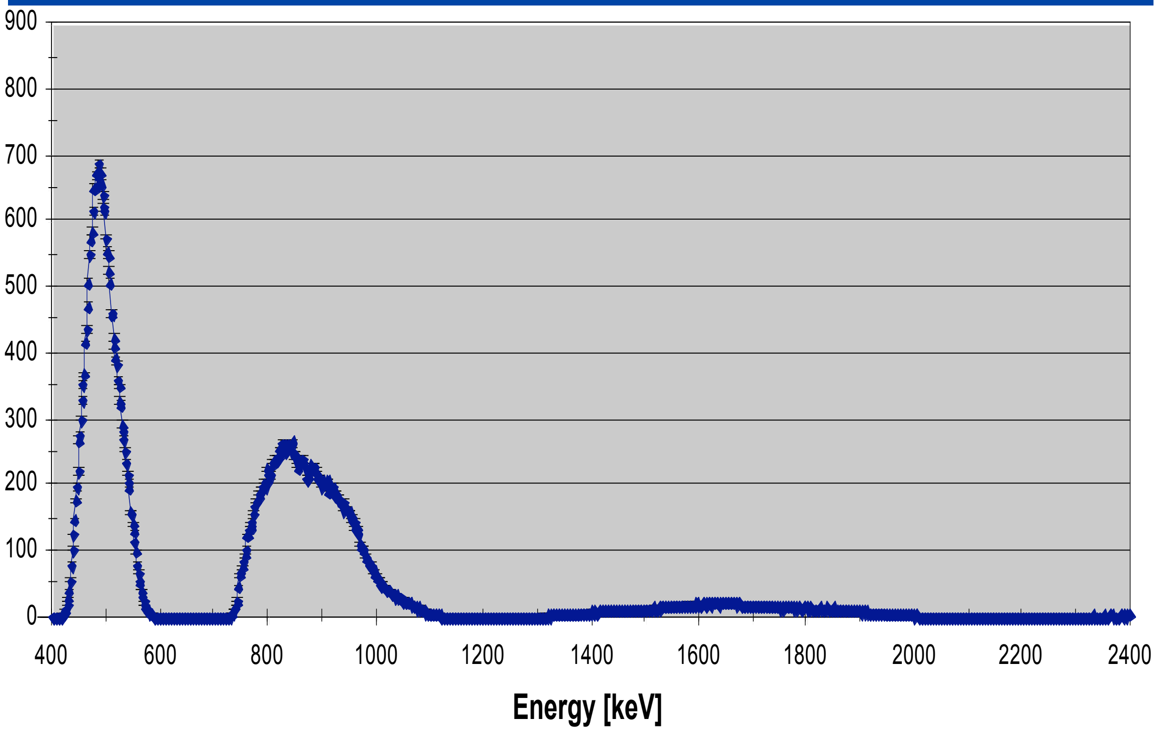




Monte-Carlo simulations

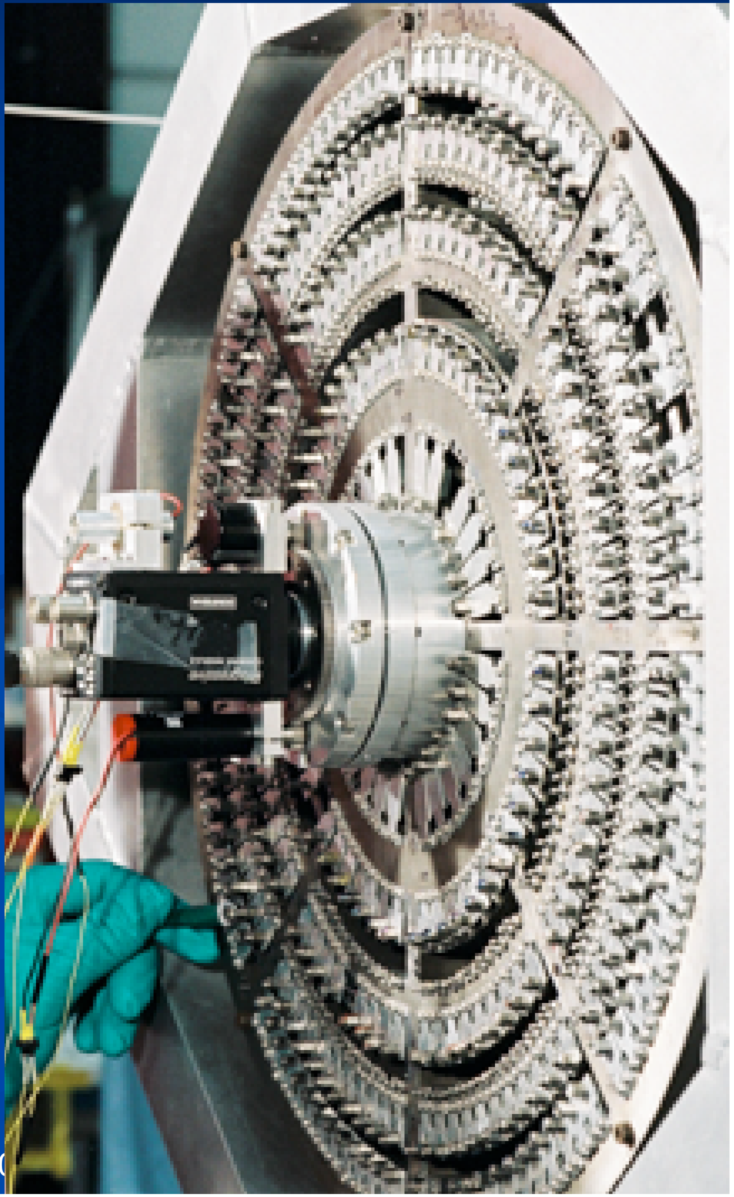
- Long focal length – Off axis (1 arcmin)





Simulations vs. experiment

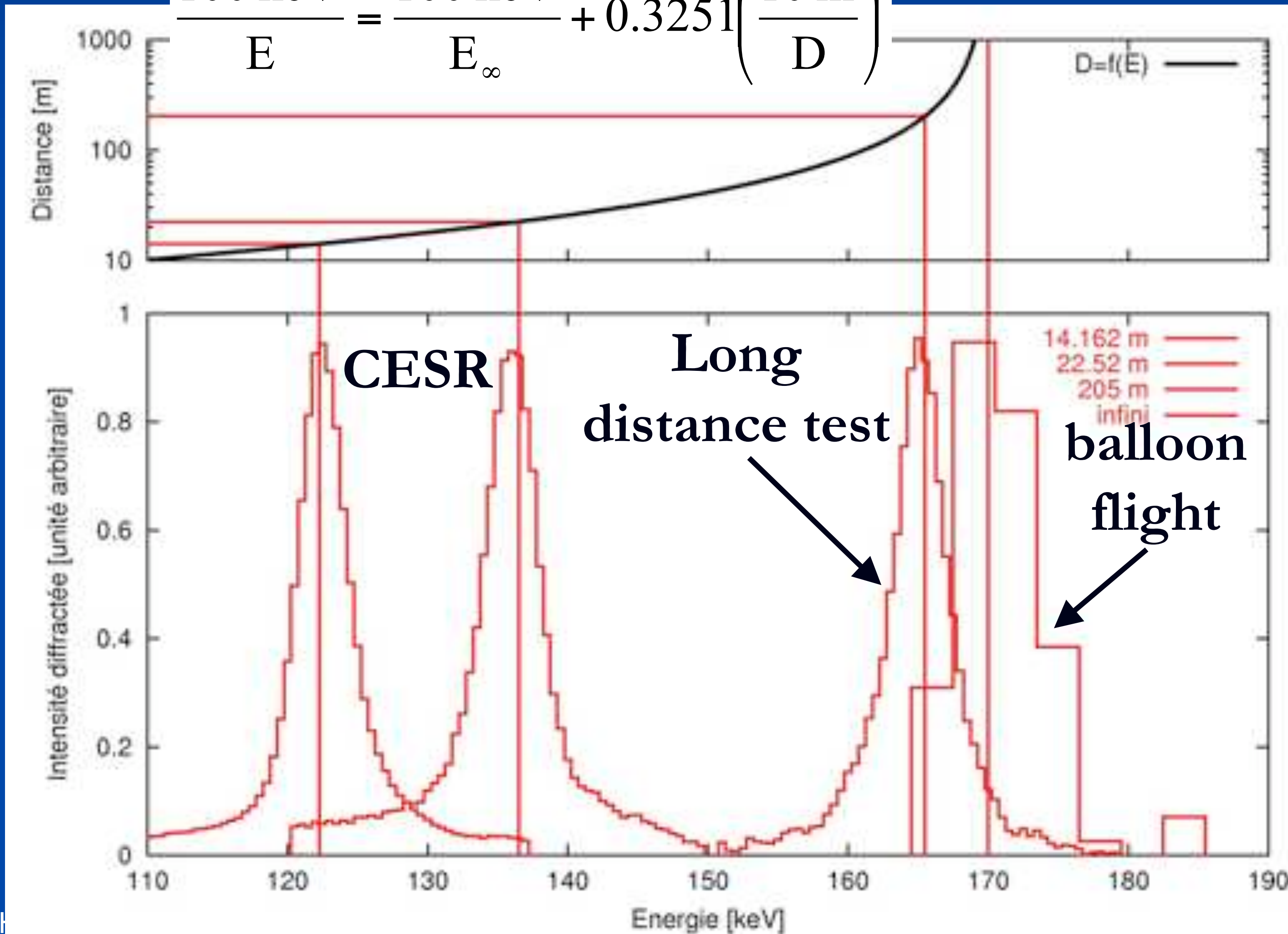
- Results from the CLAIRE project :
  - E_∞ = 170 keV, F = 2.73 m
  - 563 Ge crystals, 511 cm^2
  - 8 rings :
    - R_{111} = 6.2 cm
    - R_{440} = 20.2 cm
  - Crystals individually tuned and compared to the theory (⇒ determination of m and t_0)
  - Crystals parameters used for simulation



Simulations vs. experiment

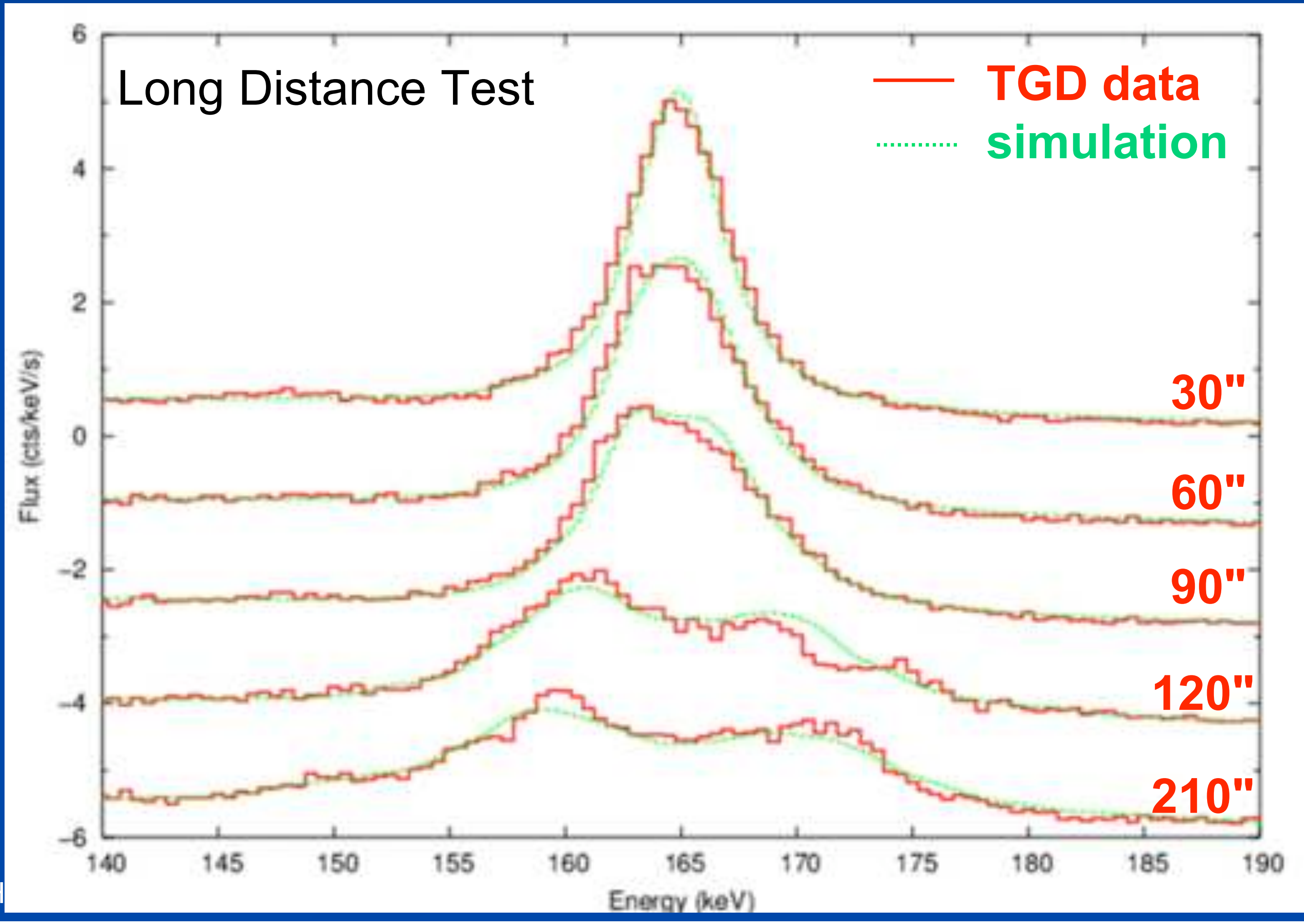
- Diffracted energy dependence on source distance :

$$\frac{100\,\text{keV}}{\text{E}} = \frac{100\,\text{keV}}{\text{E}_\infty} + 0.3251\left(\frac{10\,\text{m}}{\text{D}}\right)$$



Simulations vs. experiment

- Spectral response as a function of pointing



Measurements & Simulations Summary

Simulation / Measurement	Integrated flux [ph/s]	Diffracted FWHM [keV]	Efficiency (FWHM=3keV) [%]	Notes
D=Infinity, continuum@170 keV	312.9E0.6	4.1	19.33E0.04	Ideal case (perfect crystals and pointing)
	143.7E0.3	3.3	8.88E0.02	Perfect pointing Real crystals
	200E65-32	7.6	12.5E4-2	Stratospheric flight
D=205 m, continuum@165 keV	138.0E0.3	3.2	8.53E0.02	Perfect pointing Real crystals
	169.6E14	3.9	8.5E0.7	Long distance test Lorentzian peak
D=14m ^{57}Co@122keV	18.590E0.002	-	3.668E0.004	Perfect pointing Real crystals
	16.1E0.6	-	3.17E0.12	Lab. measurement ⇒ 7.7E1% @infinity