PowerPoint File available:

http://bl831.als.lbl.gov/~jamesh/powerpoint/BNL_2009.ppt

ALS 8.3.1 Team

Acknowledgements

Ken Frankel Chris Neilson Michael Blum

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Ken Frankel Chris Neilson Michael Blum

8.3.1 PRT: Tom Alber

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Elven Automation

```
unix% Elves process the data in /data/semet/ using ~/orf.seq
```

Elves examine images and set-up data processing

Elves run…

mosflm
scala
solve
mlphare
dm
arp/warp

Holton and Alber *PNAS USA* **101** 1537-42 (2004)

Elven Automation

How often does it <u>really</u> work?

Turning Data into Models

35 operating US beamlines in 2003

Turning Data into Models

35 operating US beamlines

$2x10^{13}$ ph/s

http://biosync.sdsc.edu/

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

2×10^{13} ph/s

Henderson et al (1990)

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

2×10^9 ph/μm^2/s

http://biosync.sdsc.edu/

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

2×10^9 ph/μm^2/s

= 400,000 datasets/year

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

2×10^9 ph/μm^2/s

~ 200,000 datasets/year

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

2×10^9 ph/μm^2/s

~ 100,000 datasets/year

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

$2x10^9$ ph/μm^2/s

~ 100,000 datasets/year

1324 str in 2003

Jiang & R.M. Sweet (2004)

Turning Data into Models

35 operating US beamlines

~10^{11} ph/μm^2 exposure limit

$2x10^9$ ph/μm^2/s

~ 100,000 datasets/year

1324 str in 2003

~ 2% efficient

DVD data archive

Why do structures fail?

Overlaps

Radiation Damage

Signal to noise

Why do structures fail?

Overlaps

Radiation Damage

Signal to noise

Why do structures fail?

Overlaps

Radiation Damage

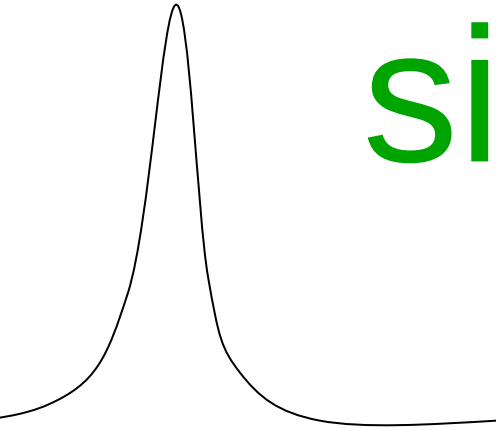
Signal to noise

Why do structures fail?

Overlaps

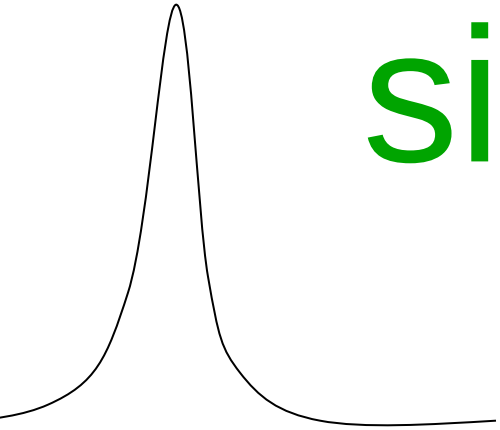
Radiation Damage

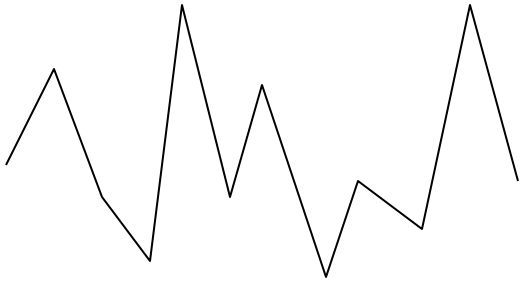
Signal to noise



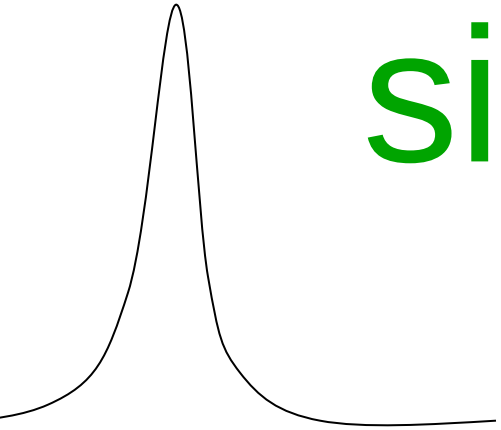
signal

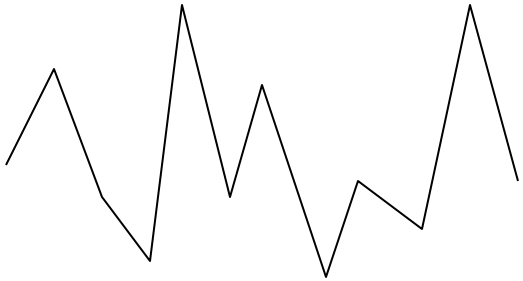
signal *vs* noise





signal *vs* noise

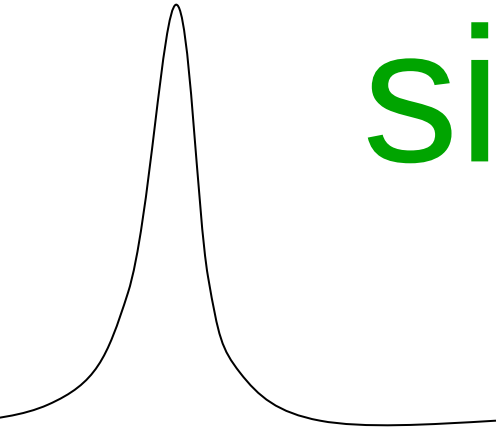




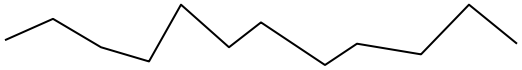
"If you don't have
good data,
then you have
no data at all."

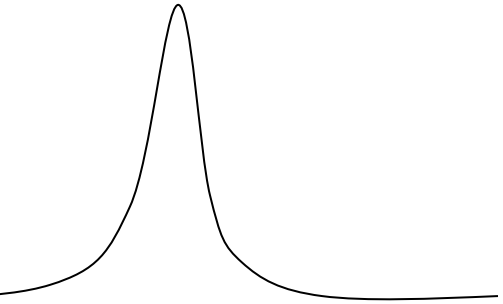
-Sung-Hou Kim

signal *vs* noise

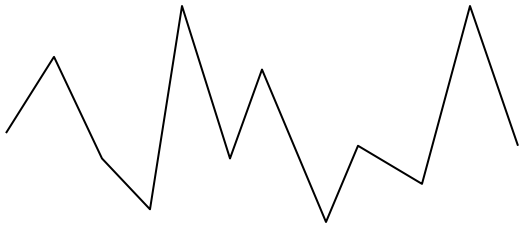


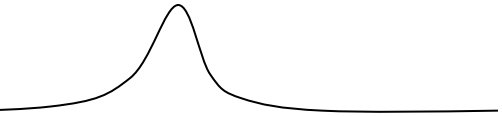
easy



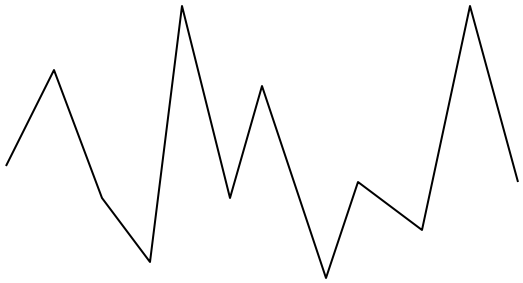


hard

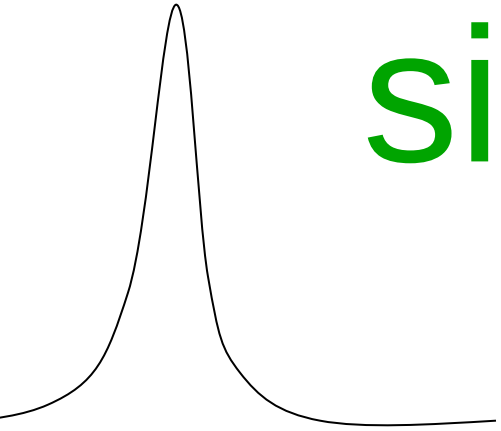




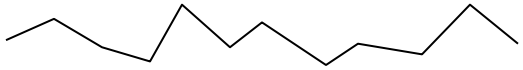
impossible

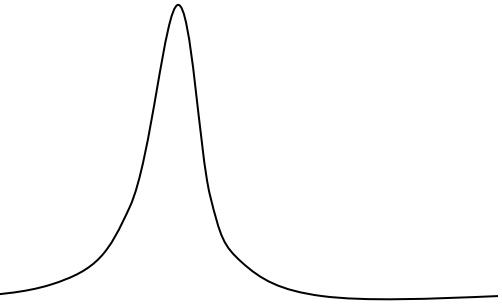


signal *vs* noise

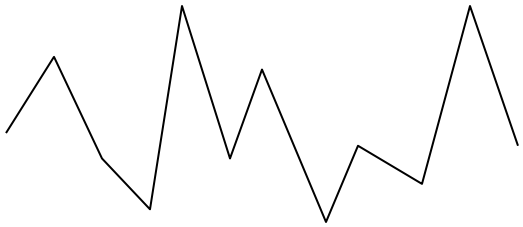


easy

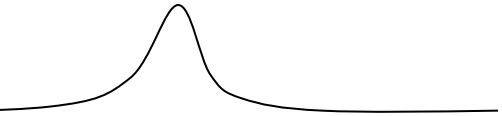




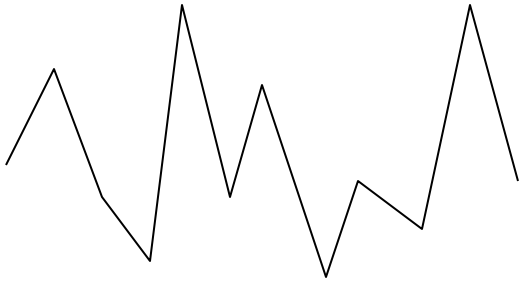
hard



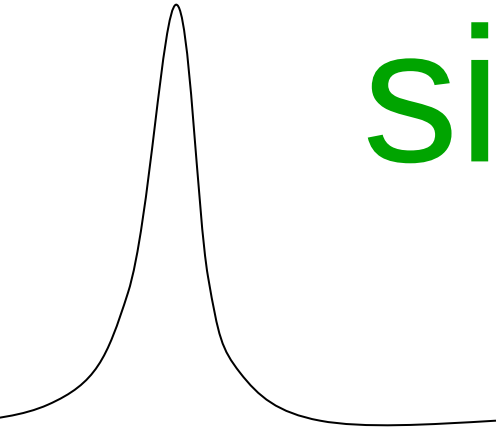
threshold of “solvability”

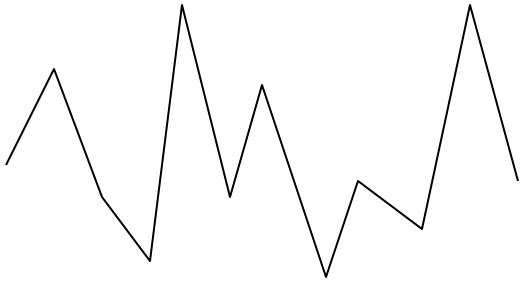


impossible



signal *vs* noise





"If you don't have
good data,
then you must
learn statistics."

-James Holton

Adding noise

Adding noise

$$1 + 1 = 1.4$$

Adding noise

$$1 + 1 = 1.4$$

$$\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2$$

Adding noise

$$1^2 + 1^2 = 1.4^2$$

$$\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2$$

Adding noise

$$1^2 + 1^2 = 1.4^2$$

$$3^2 + 1^2 = 3.2^2$$

$$\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2$$

Adding noise

$$1^2 + 1^2 = 1.4^2$$

$$3^2 + 1^2 = 3.2^2$$

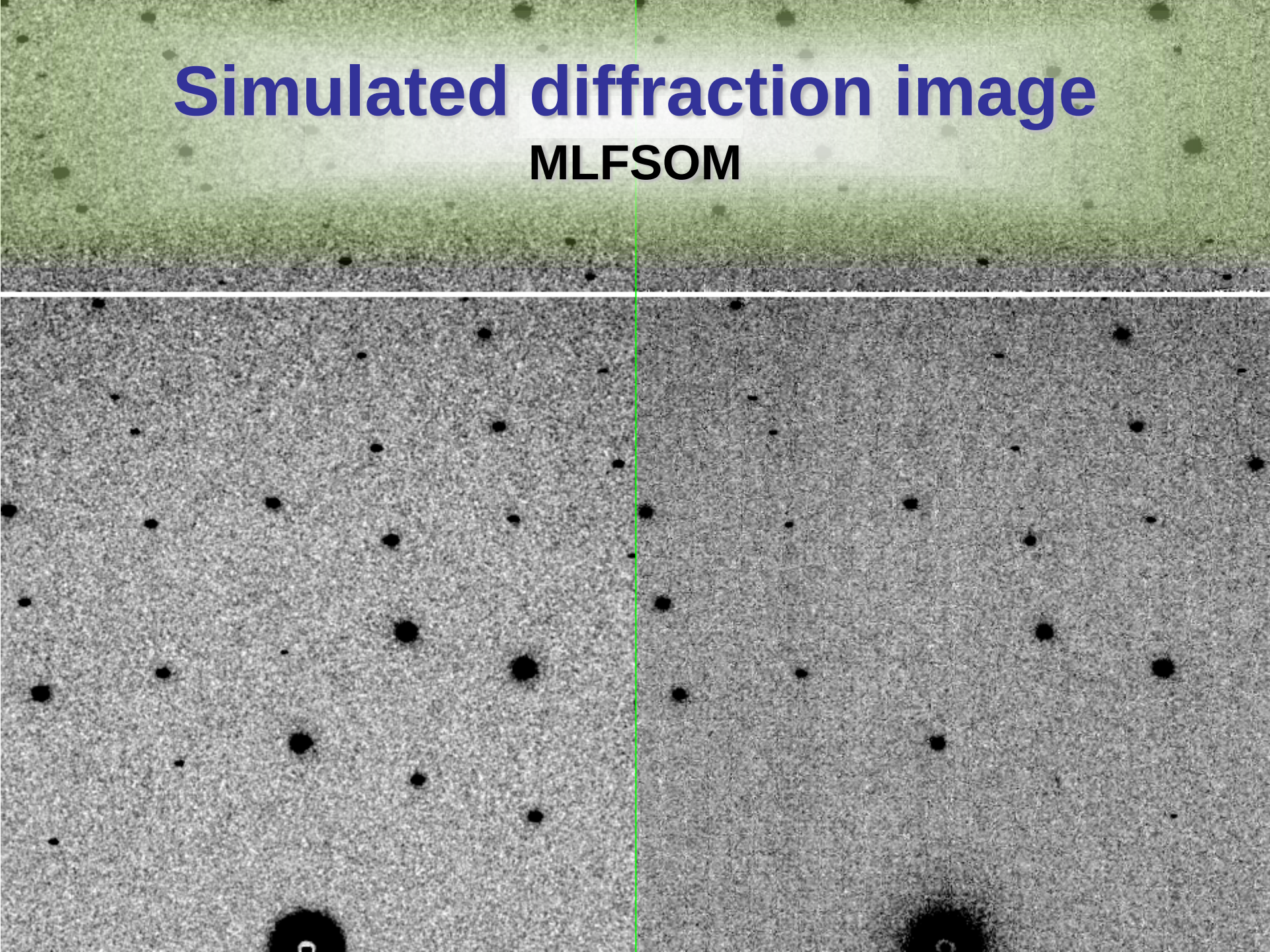
$$10^2 + 1^2 = 10.05^2$$

Sources of noise

“photon counting”	$\sigma(N) = \mathrm{sqrt}(N)$
Read-out noise	rms 11.5 e-/pixel
Shutter jitter	rms 0.57 ms
Beam flicker	0.15 %/$\sqrt{\mathrm{Hz}}$
spot shape	pixels? mosaicity?
radiation damage	B/Gray?

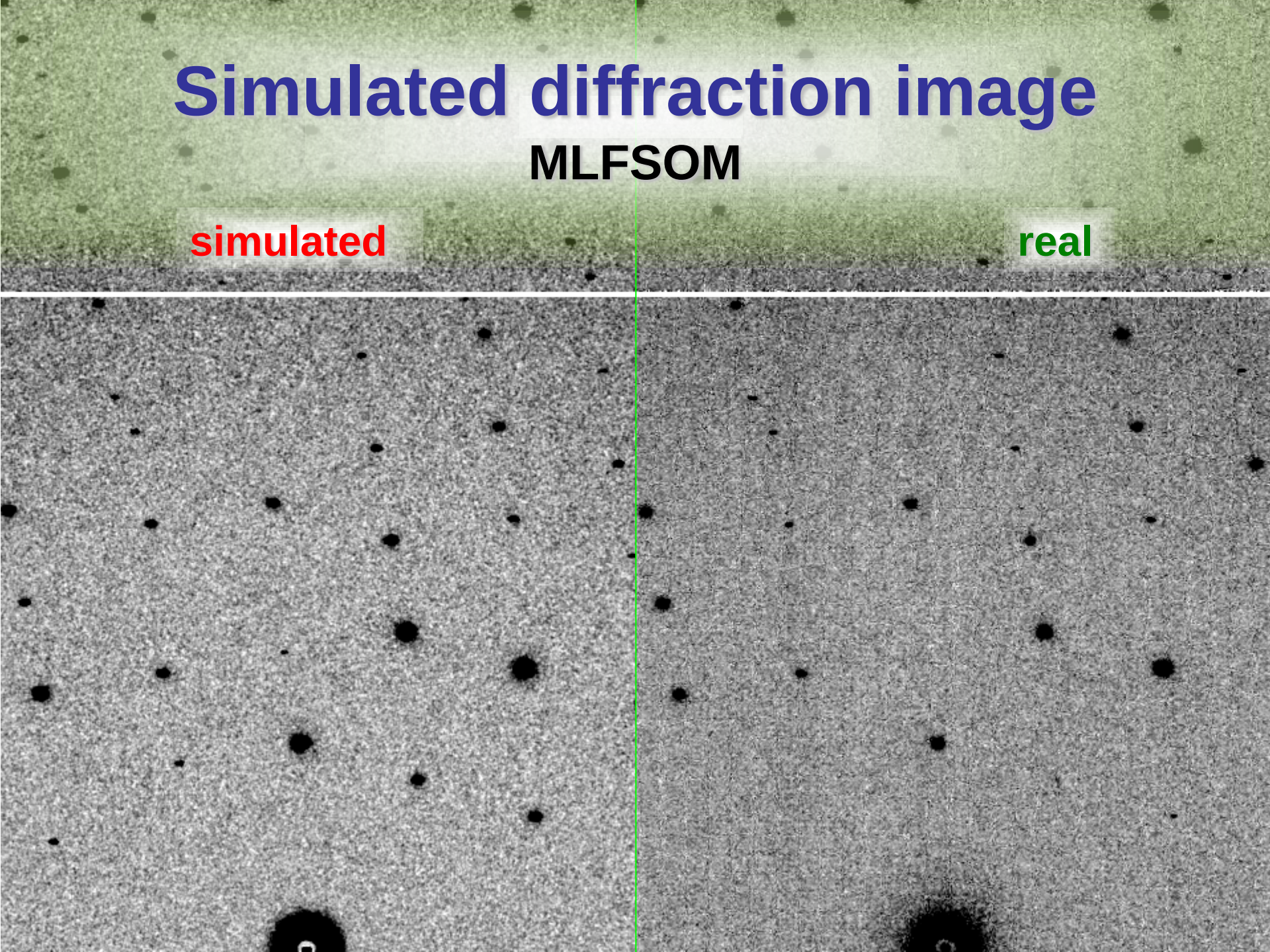
Simulated diffraction image

MLFSOM



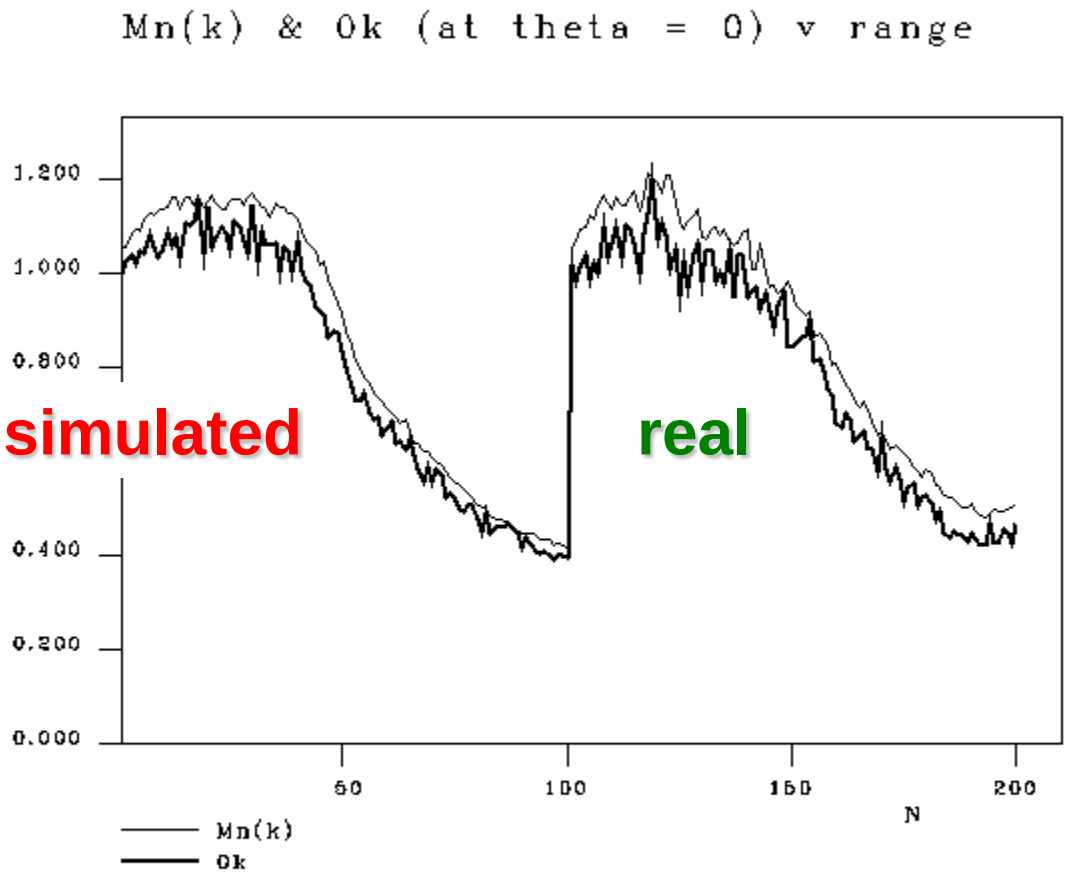
Simulated diffraction image

MLFSOM



Mn(k) & Ok (at theta = 0) v range

Quit Plot



Simulated	statistic	Real
5.4%	R_{merge}	6.2%
18.9	I/sd	16.2
1.9	I/sd (1.4 Å)	1.6
1.7 4.0 0.020	SDCORR	1.0 2.2 0.065
36.8	PADFPH	31.46
3.871	mlphare f”	3.476
0.178	FOM	0.192
0.545	FOMDM	0.664
0.6270	CC(1H87)	0.6090
0.170	R_{cryst}	0.184
0.205	R_{free}	0.231

Reference experiment

Beamline:

ALS 8.3.1

0.1 s exposures

total dose = 0.47 MGy

Detector:

ADSC Quantum 315r

Crystal:

PDB id 1H87

tetragonal HEWL soaked with

Gd complex (2 sites)

Gd f” at 12660 eV ~ Se

Bijvoet ratio: 3.8%

What goes into the simulation?

What goes into the simulation?

Crystal:
- “pristine” PDB
- “decayed” PDB
- Crystal size (μm)
- orientation matrix/angles
- mosaic spread (deg)
- absorption envelope (facet planes)

Non-crystal:
- “air” path (mm)
- cryo types & thicknesses (μm)
- ice rings

Beam:
- Flux (photons/s)
- beam size (μm)
- Wavelength (Å)
- dispersion ($\Delta\lambda/\lambda$)
- divergence (deg)
- flicker noise (%/$\sqrt{\text{Hz}}$)
- shutter jitter (ms)

Detector:
- Distance, beam center
- tilt, twist, omega (deg)
- pixels x pixels, pixel size
- E-O gain, amplifier gain
- DQE, vignette
- read noise (rms e^-/pixel)
- “ripple” noise (%)
- point-spread function
- PSF variation

What goes into the simulation?

Crystal:

- "pristine" PDB
- "decayed" PDB
- Crystal size (μm)
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Beam:

- Flux (photons/s)
- beam size (μm)
- Wavelength (Å)
- dispersion ($\Delta\lambda/\lambda$)
- divergence (deg)
- flicker noise (%/√Hz)
- shutter jitter (ms)

Detector:

- Distance, beam center
- tilt, twist, omega (deg)
- pixels x pixels, pixel size
- E-O gain, amplifier gain
- DQE, vignette
- read noise (rms e^-/pixel)
- "ripple" noise (%)
- point-spread function
- PSF variation

What does not go into the simulation?

Crystal:

- "one dimensional"
  (but variable)
- uniform damage
- assumed "top hat" mosaic spread
- kinematical diffraction

Non-crystal:

- no polarization correction
- no 2θ support

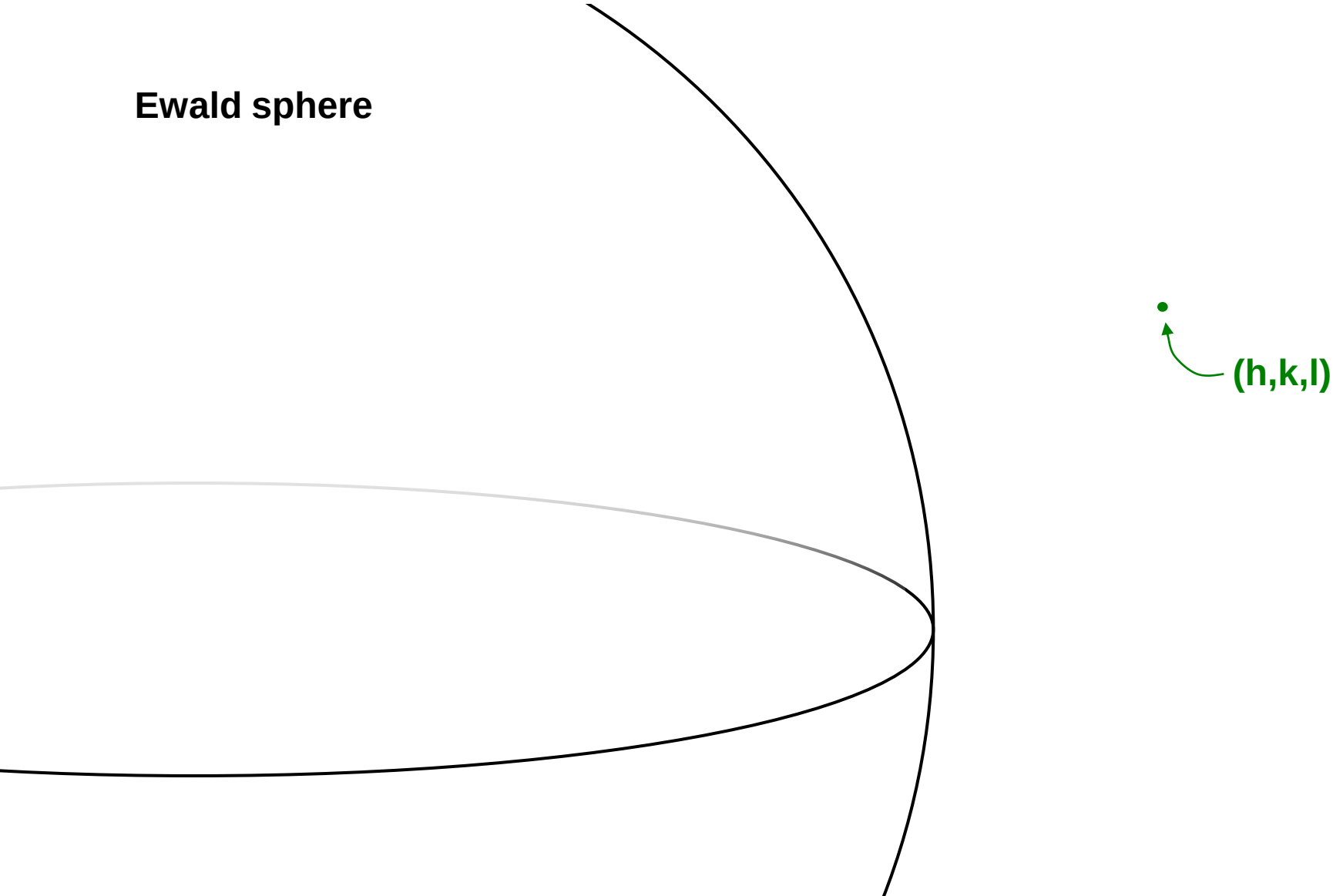
Beam:

- assumed uniform square "top hat" profiles for beam size, divergence dispersion
- flicker and jitter follow normal distribution

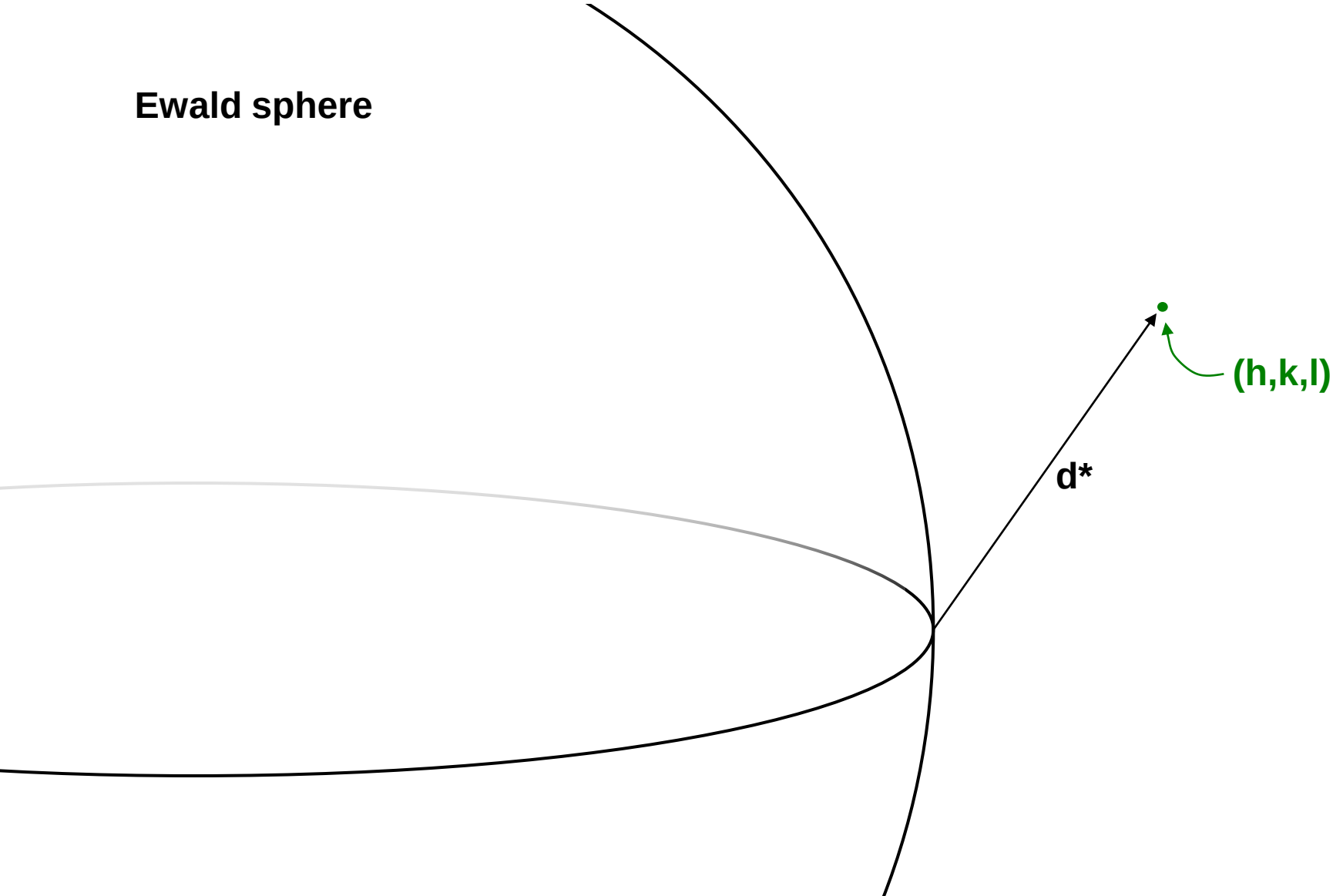
Detector:

- no spatial transformation
- no flood/dark correction
- no read-noise anisotropy
- no electron-counting noise

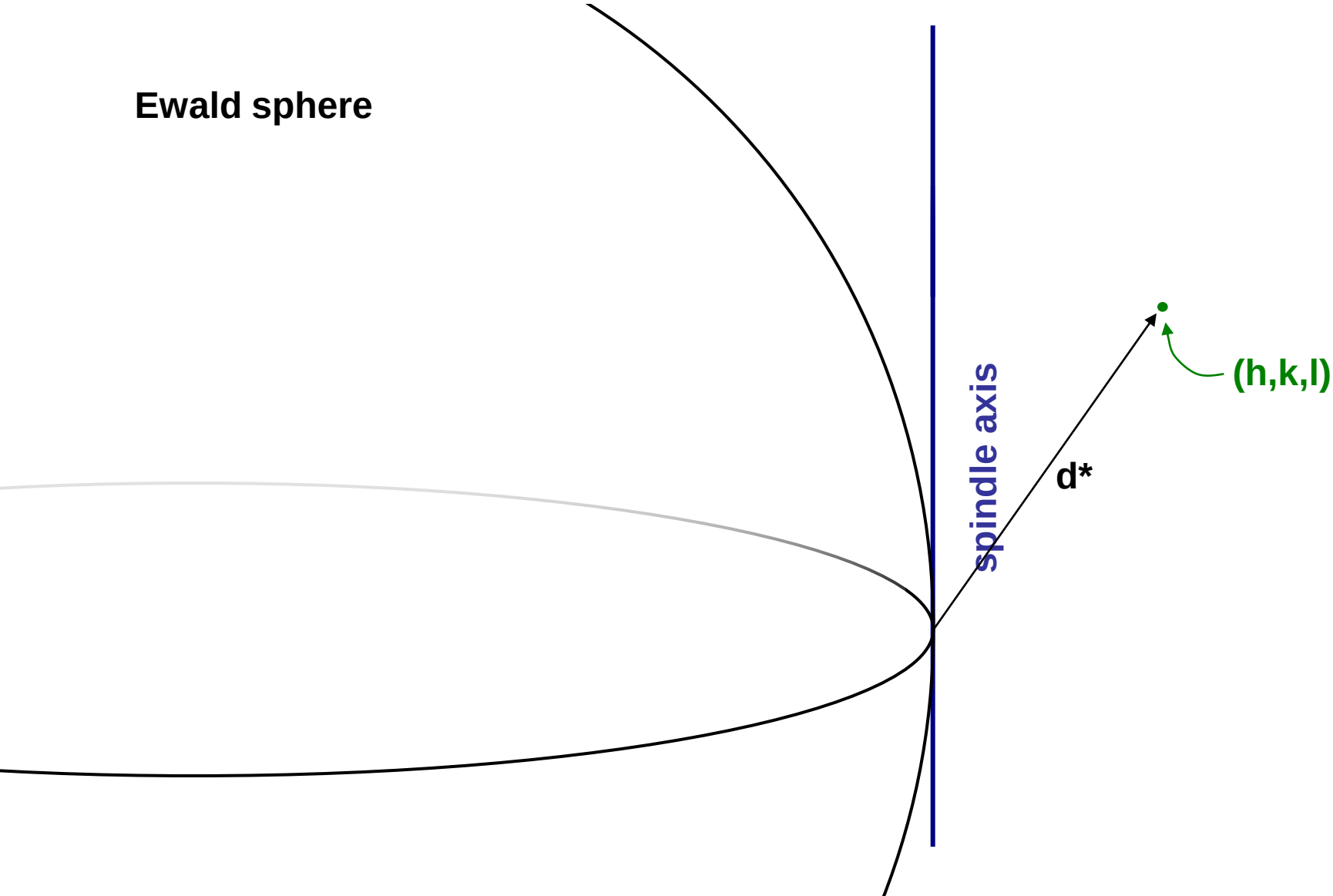
Spot shape



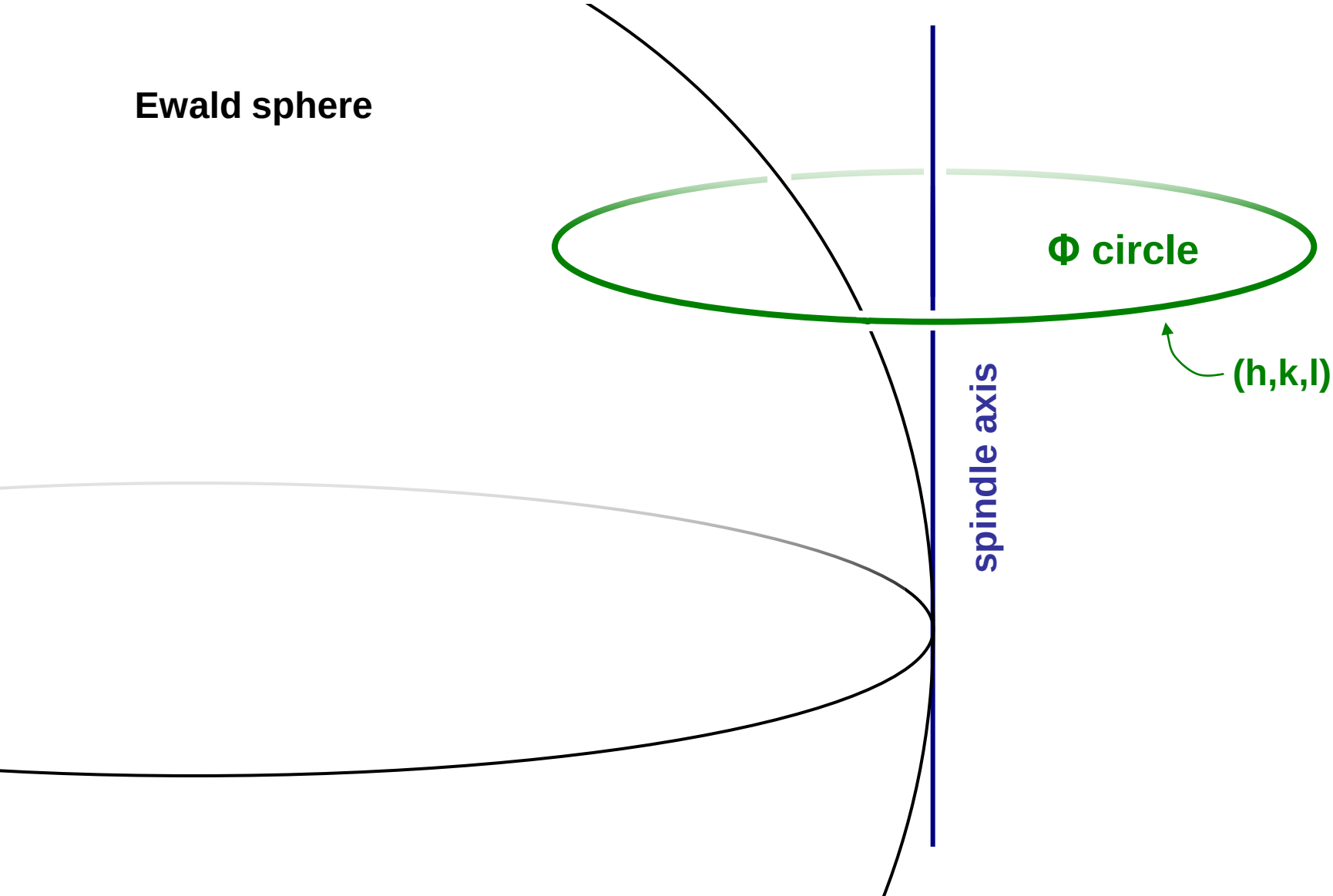
Spot shape



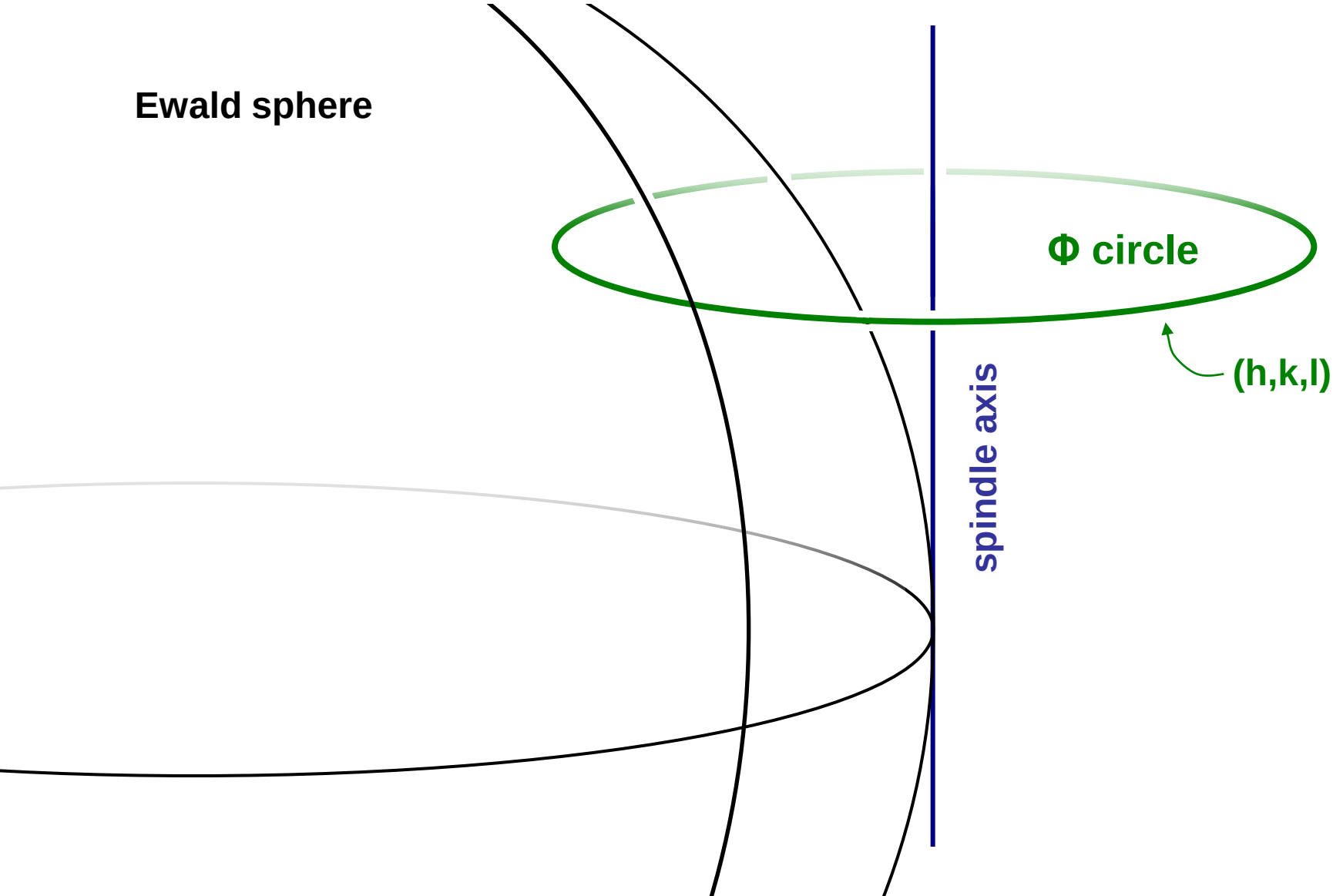
Spot shape



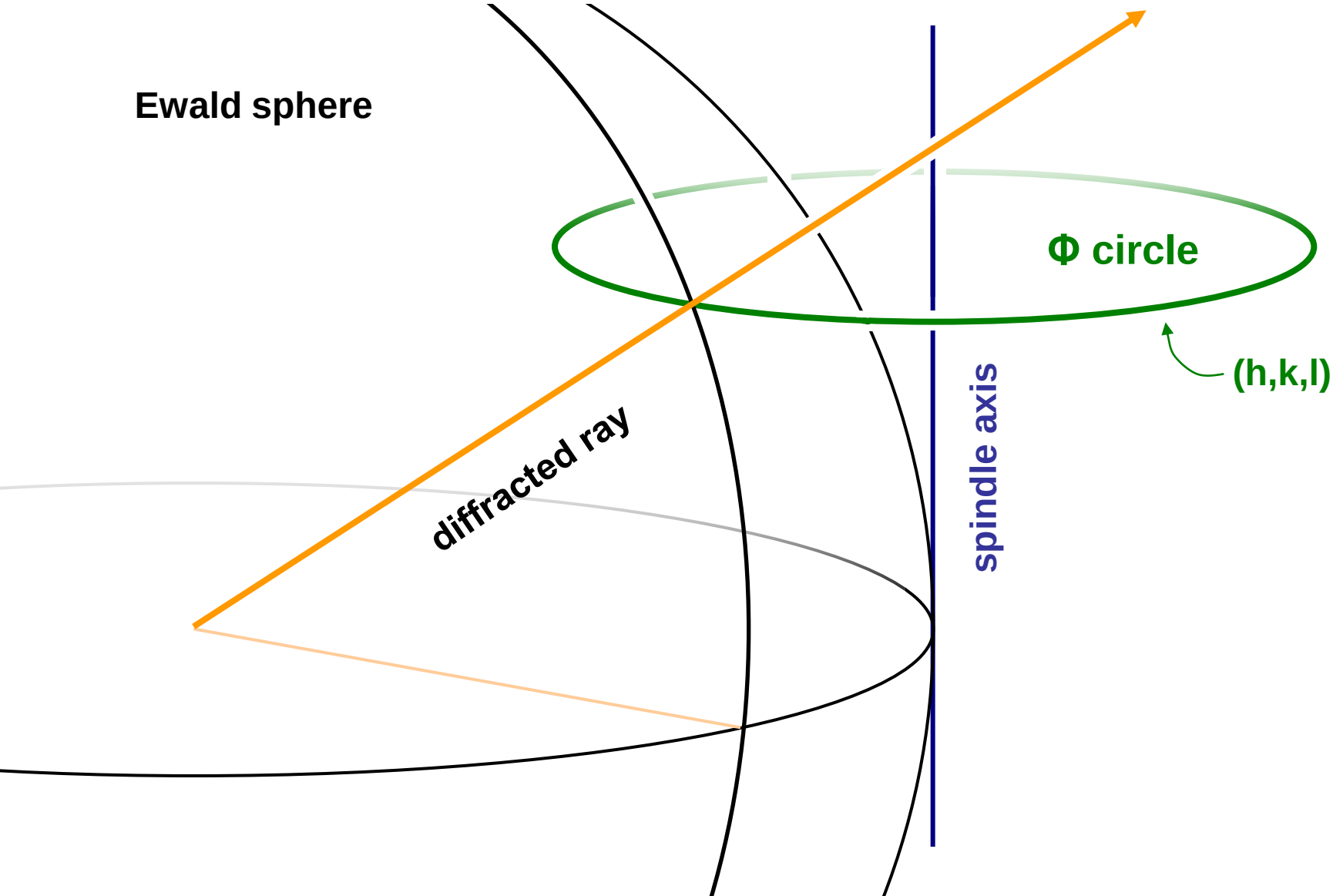
Spot shape



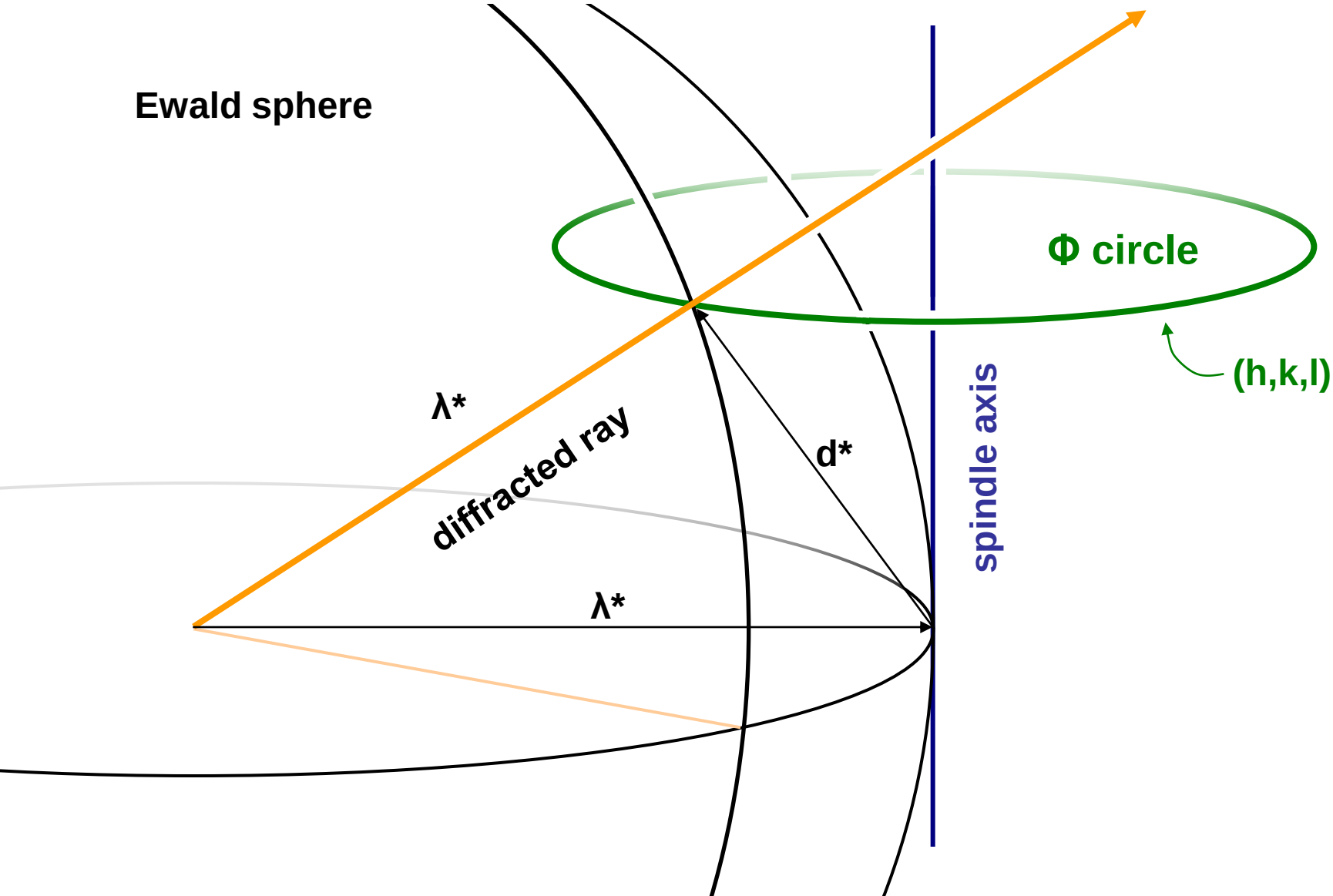
Spot shape



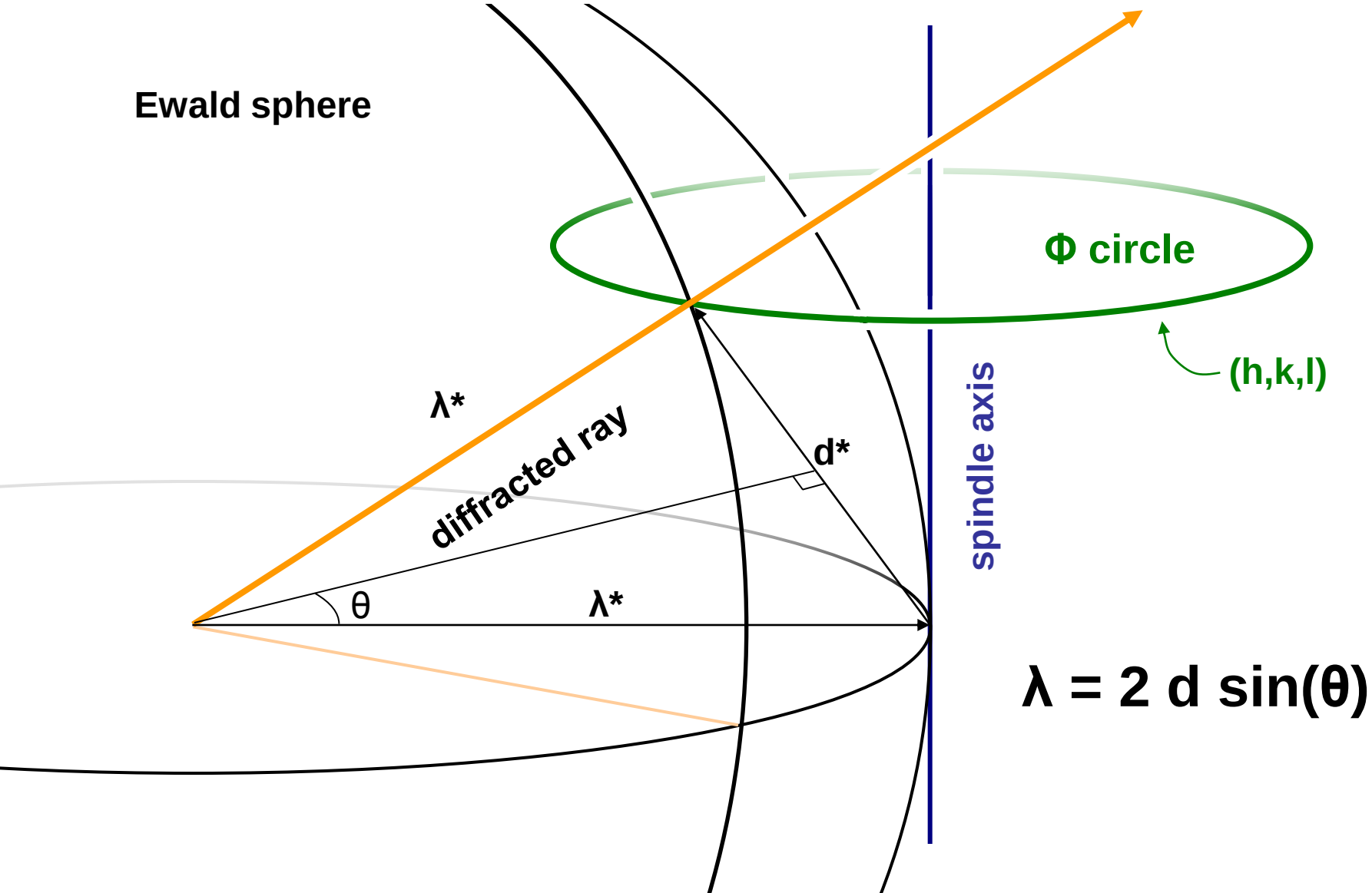
Spot shape



Spot shape

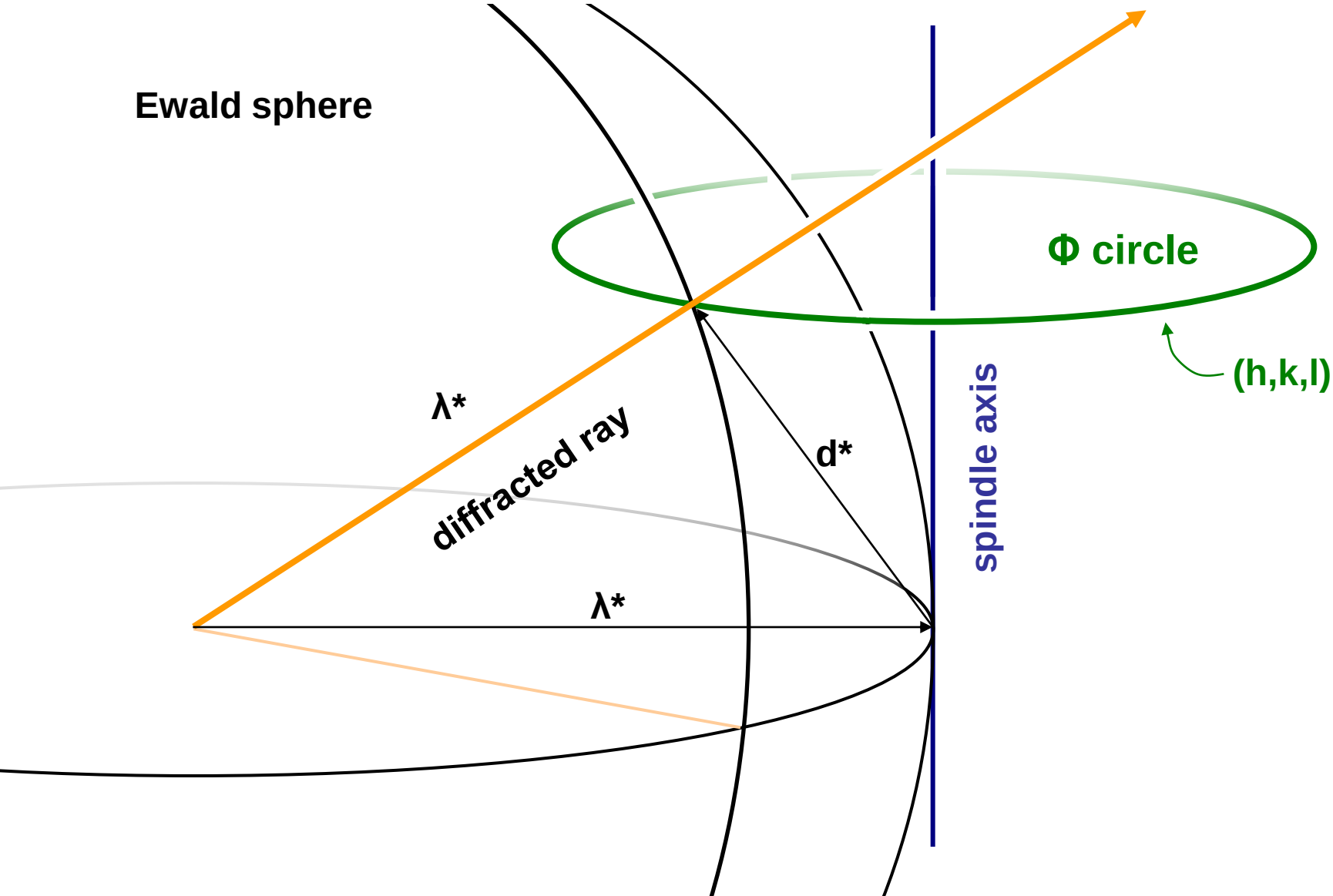


Spot shape

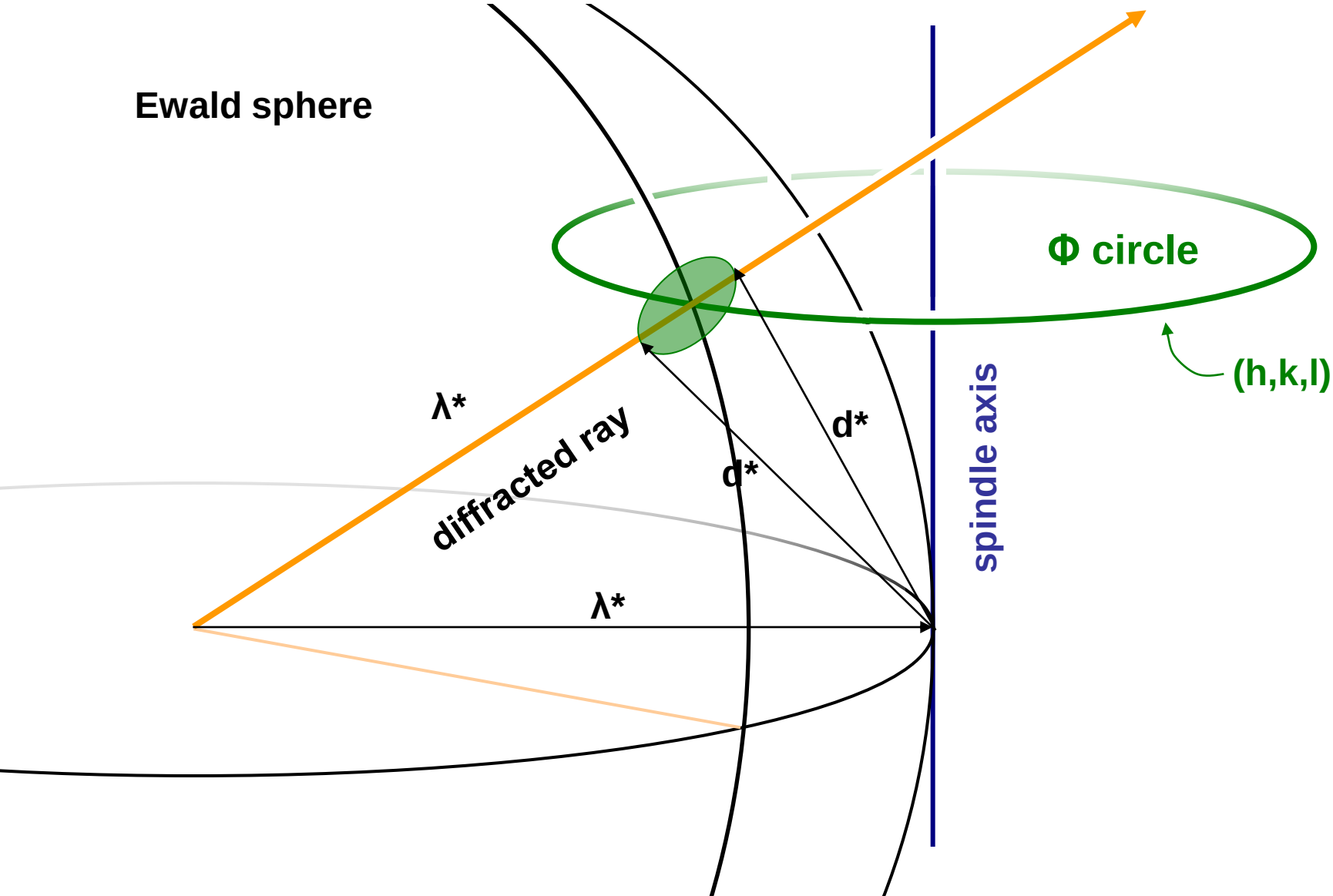


$$\lambda = 2\ d\ \sin(\theta)$$

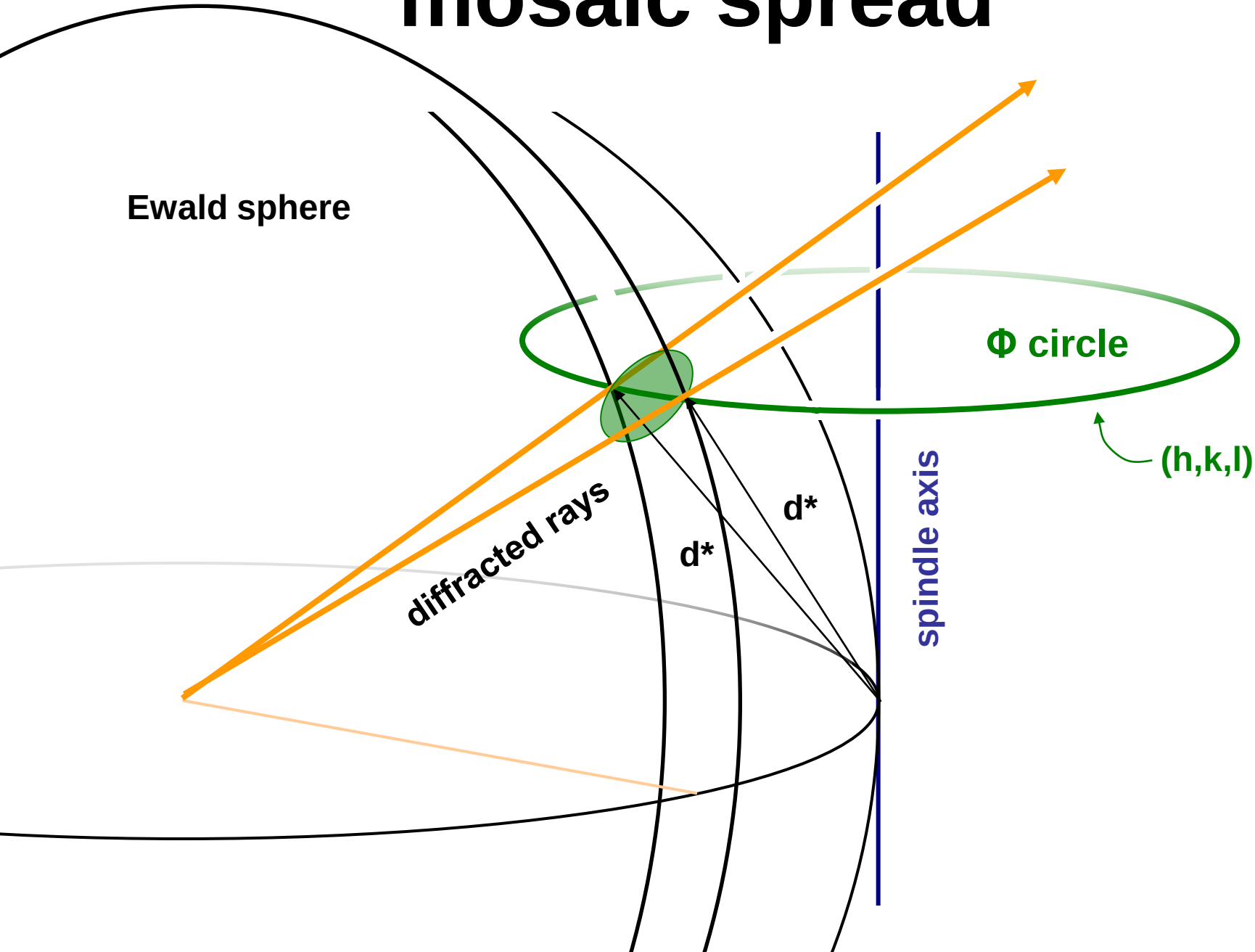
Spot shape

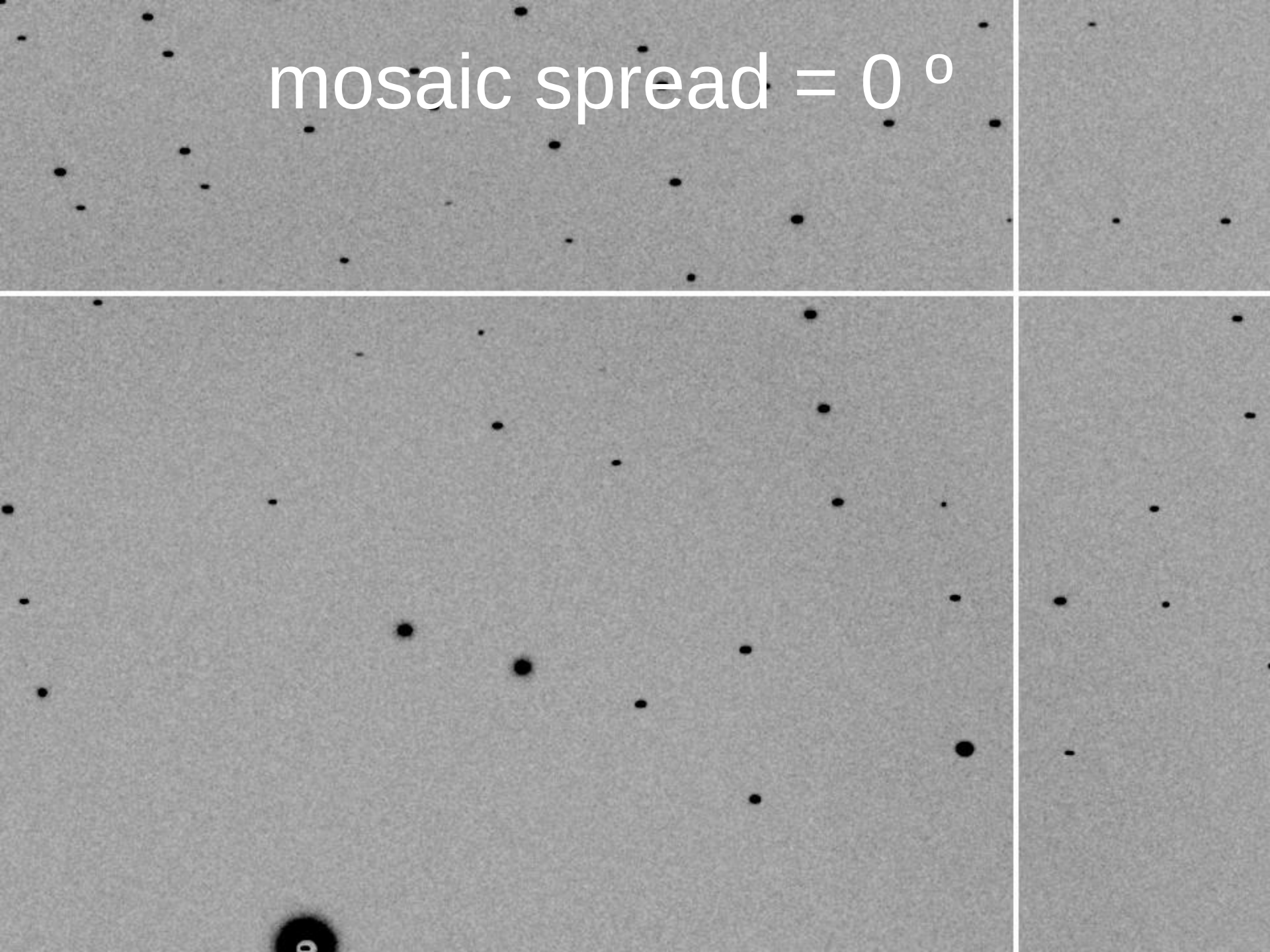


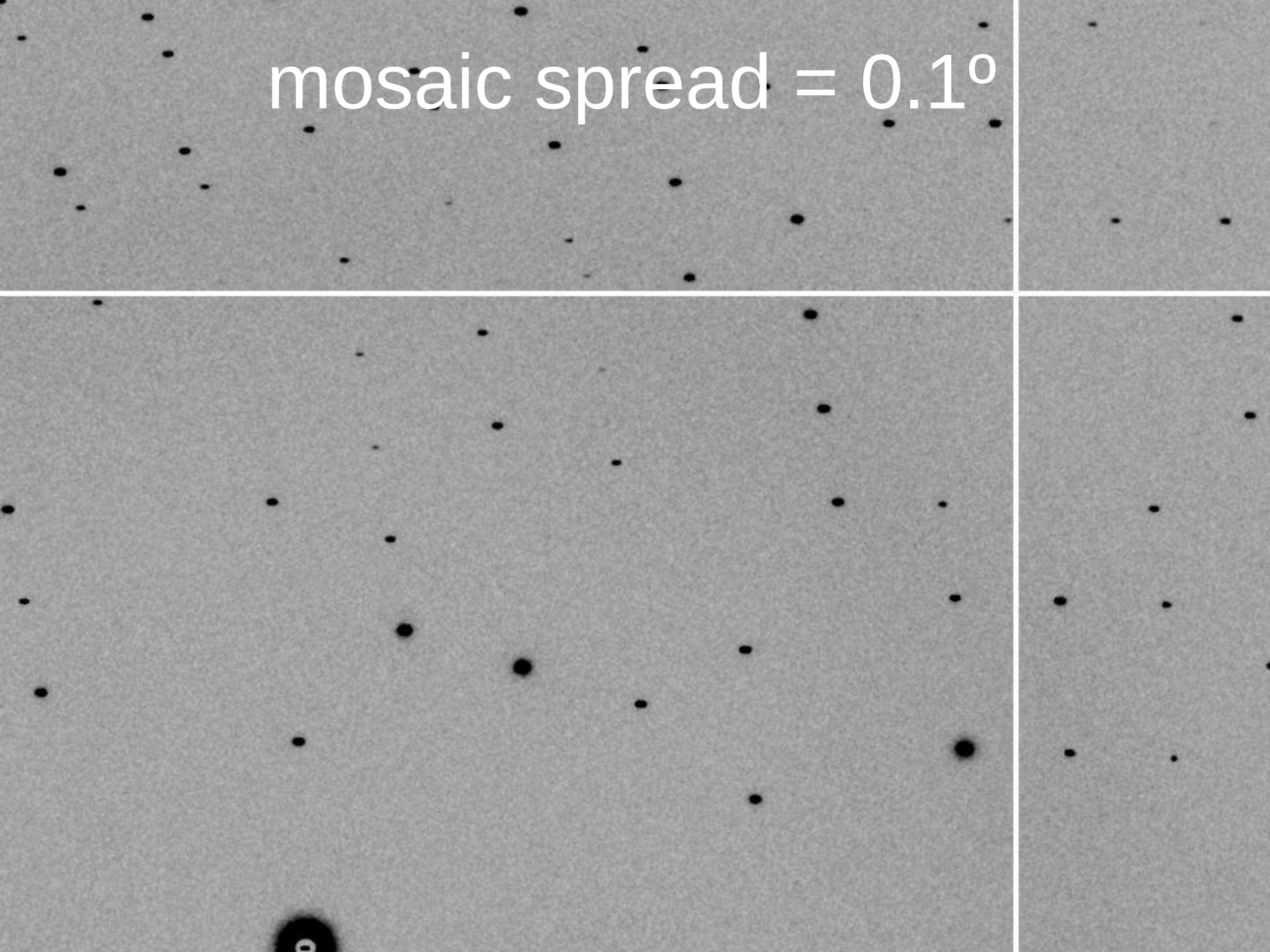
mosaic spread

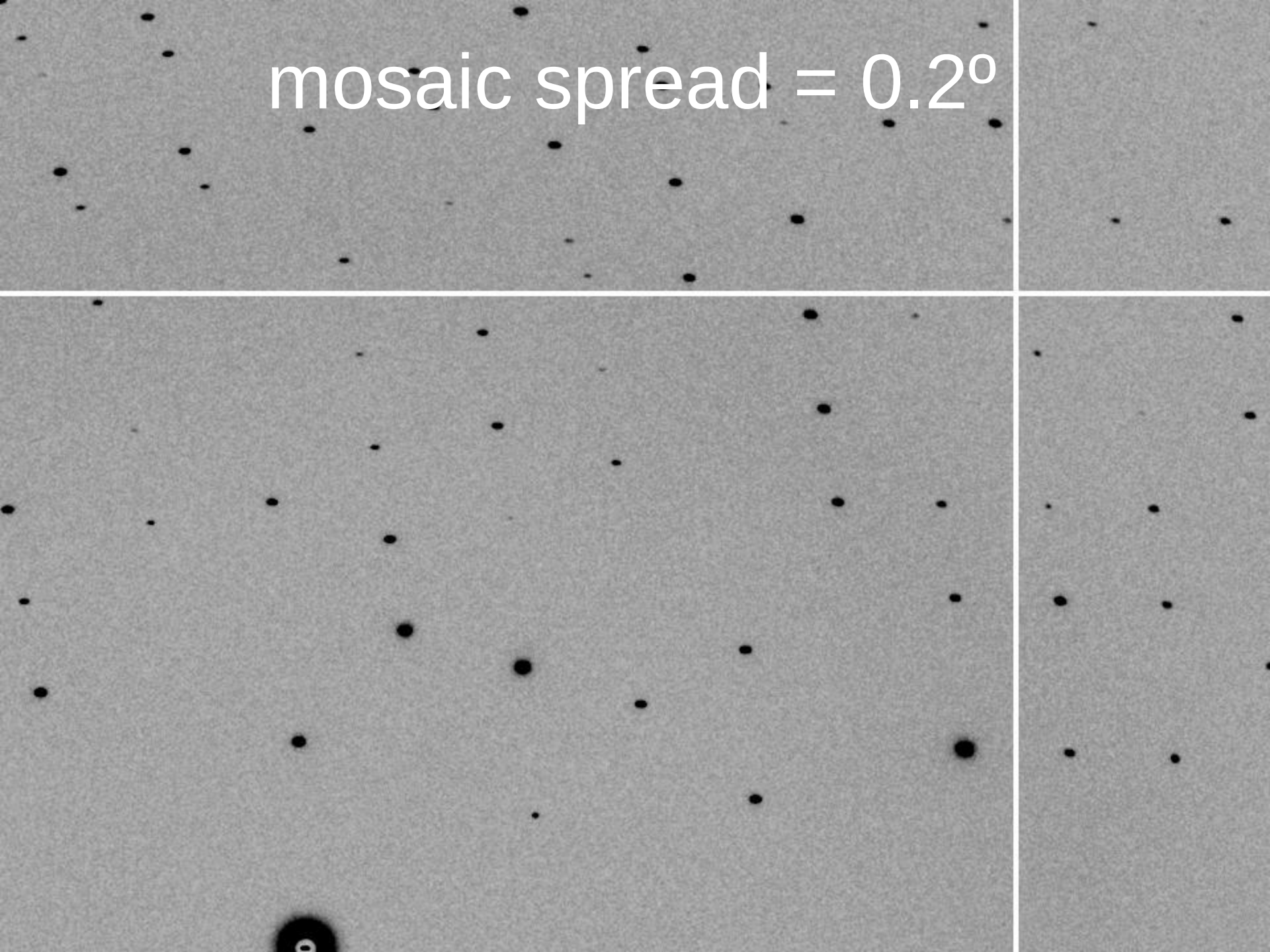


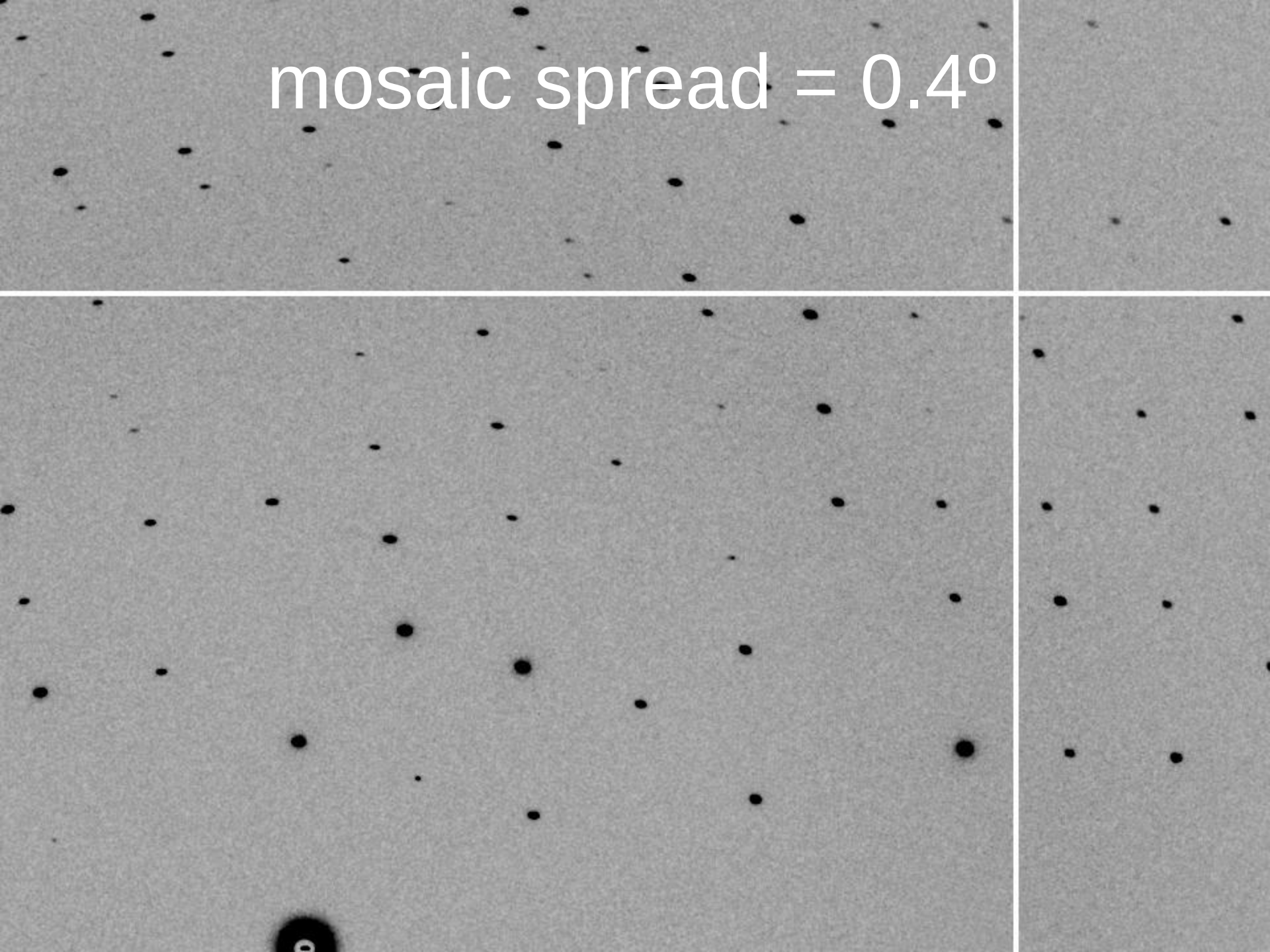
mosaic spread

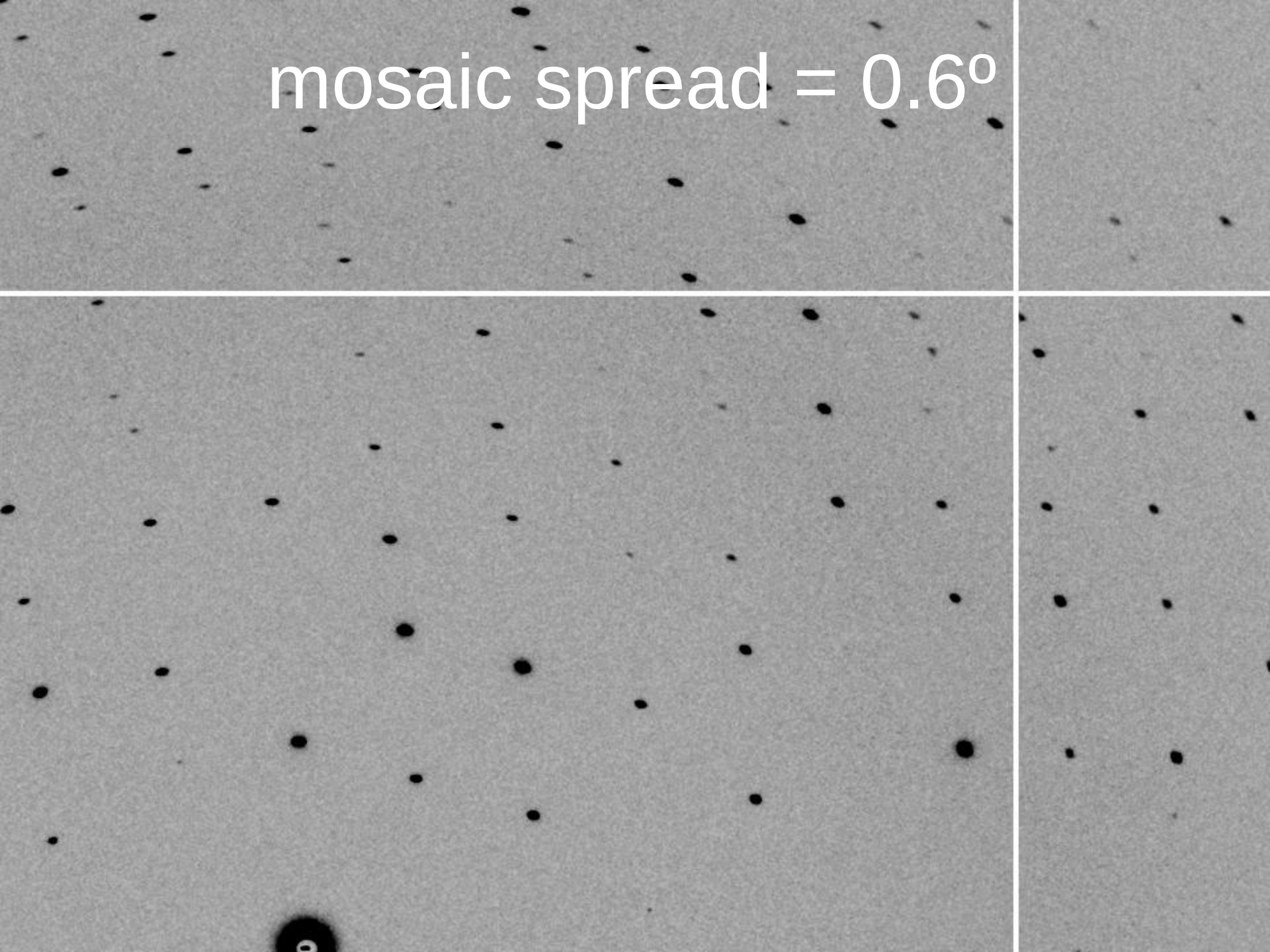


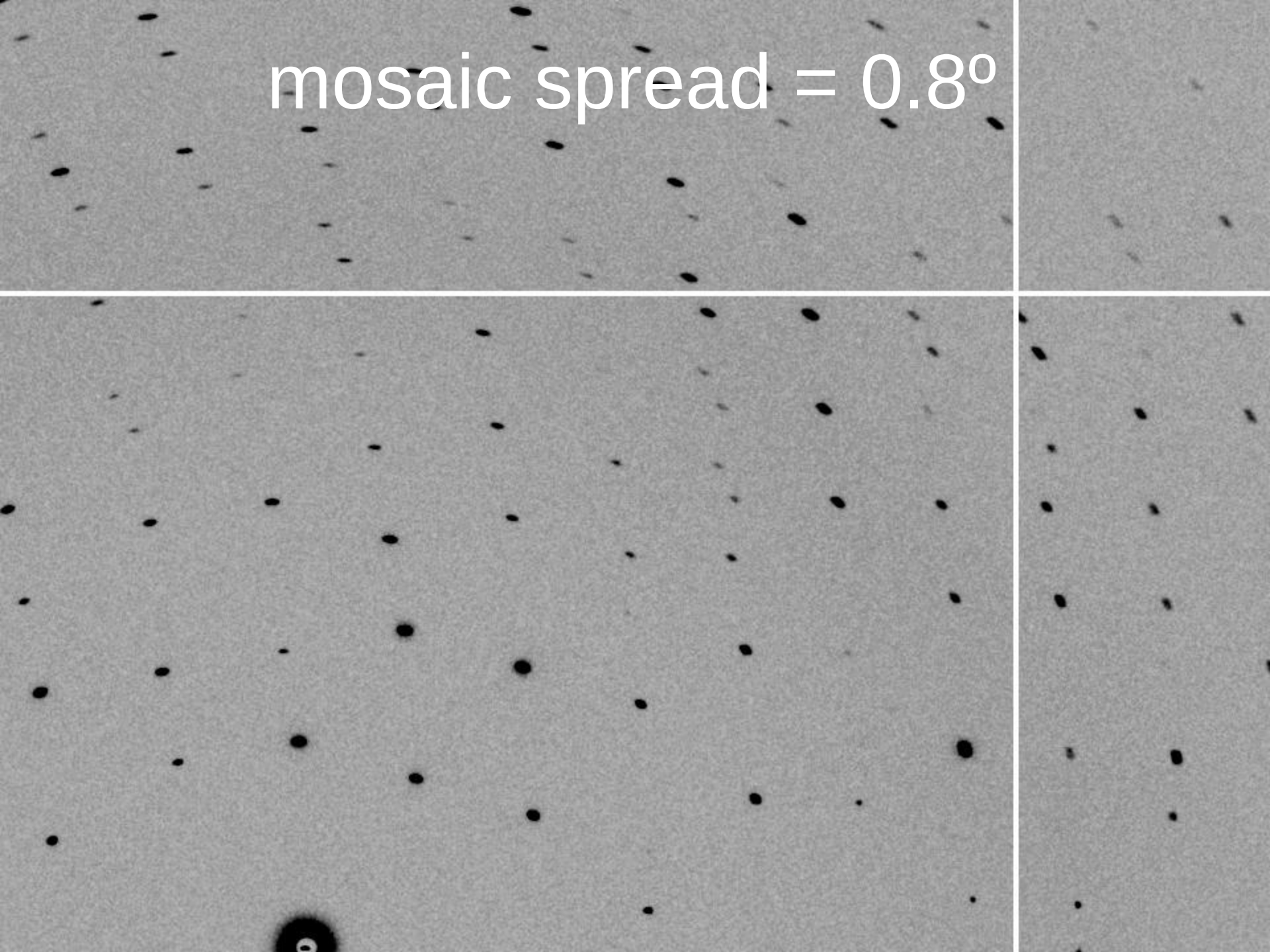

mosaic spread = 0 º

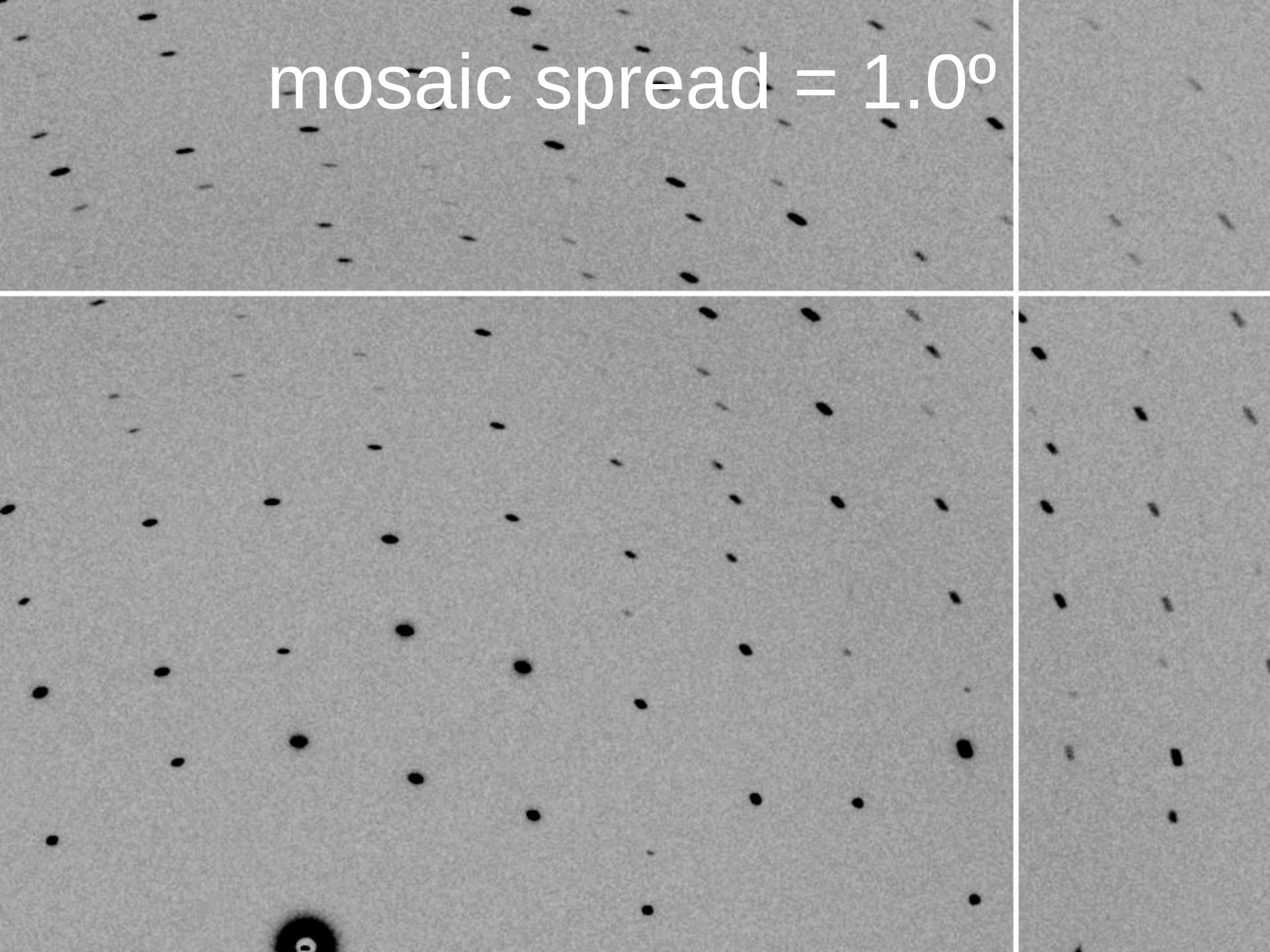

mosaic spread = 0.1º

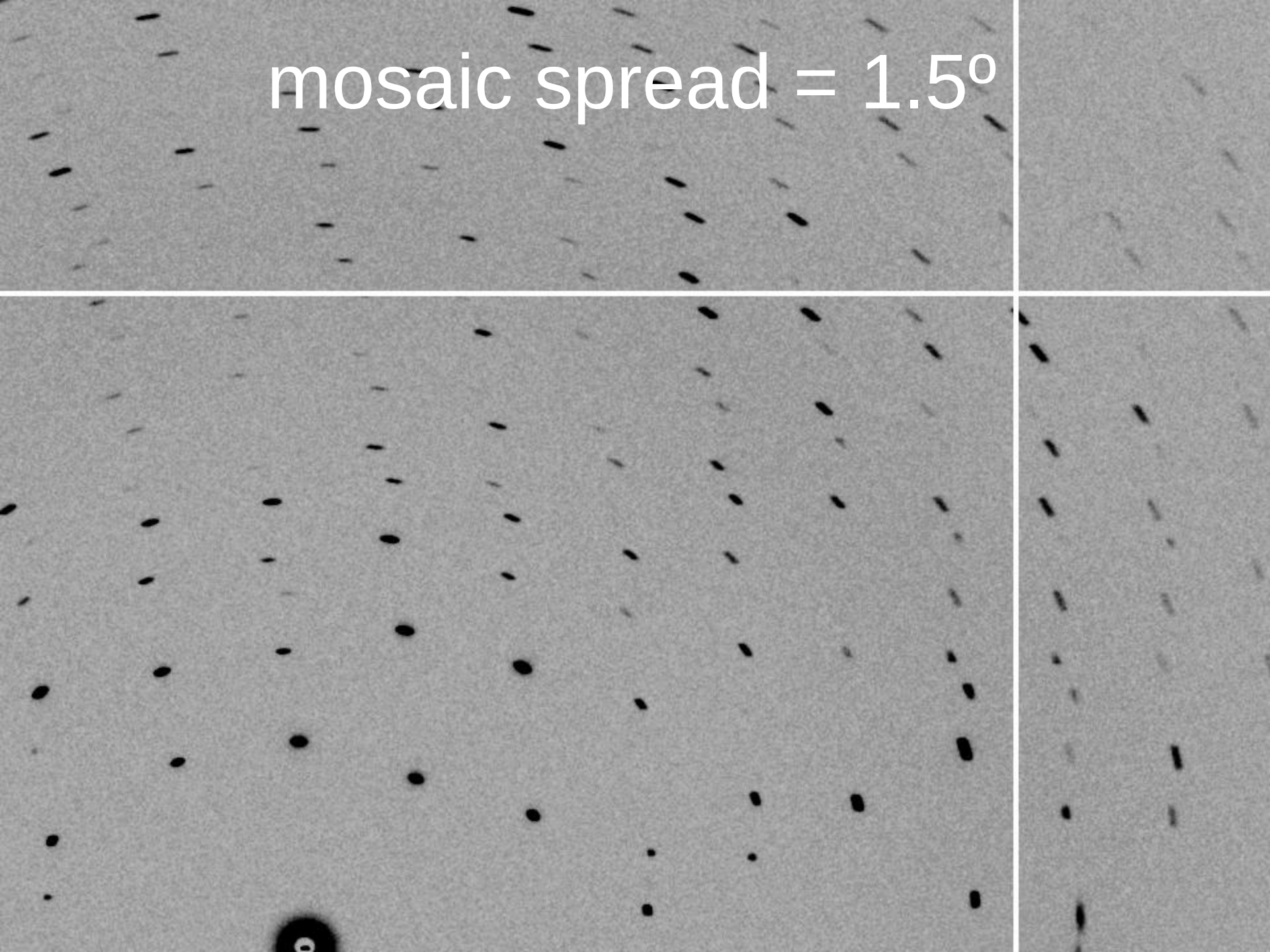

mosaic spread = 0.2º

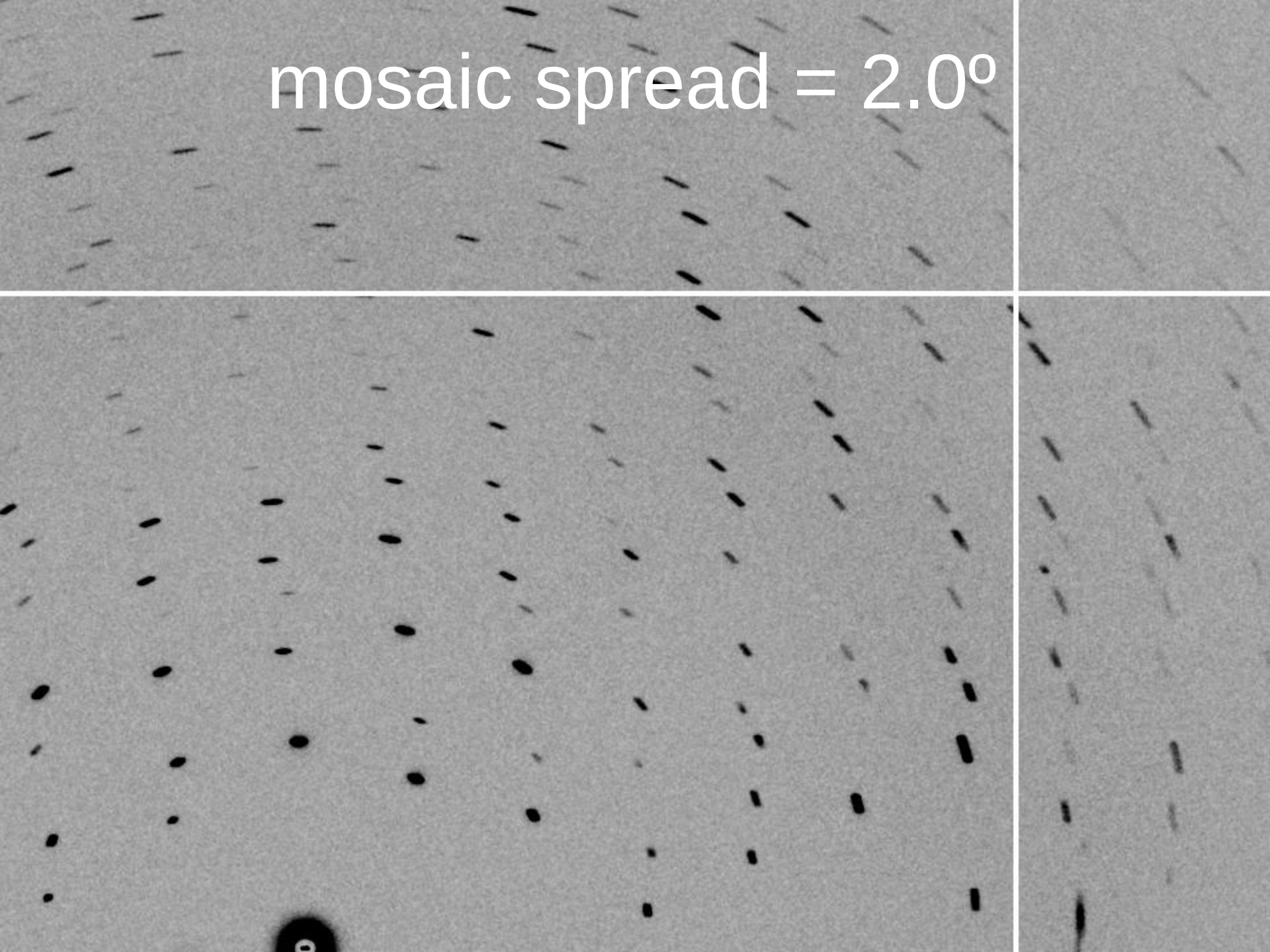

mosaic spread = 0.4º

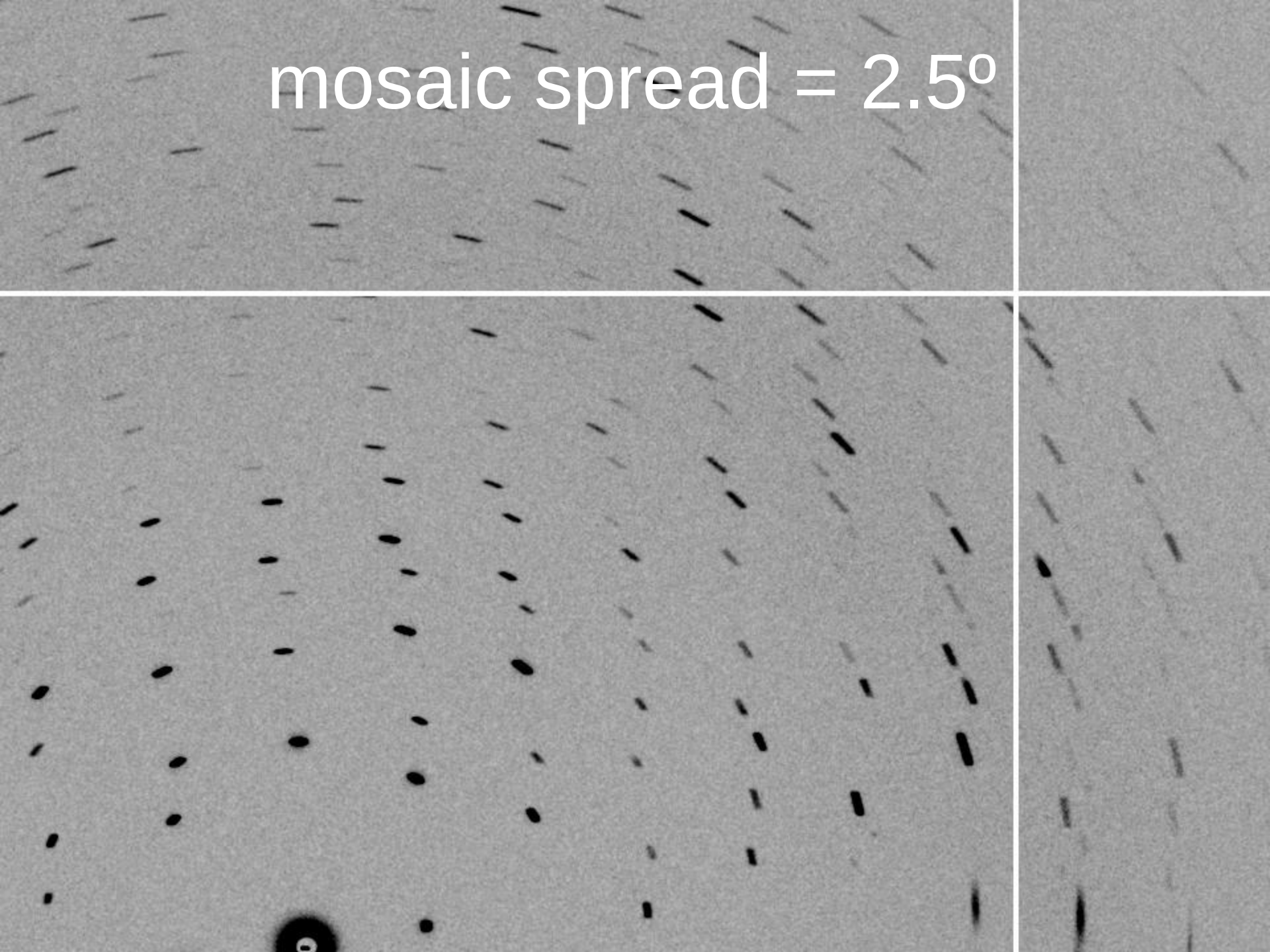

mosaic spread = 0.6º

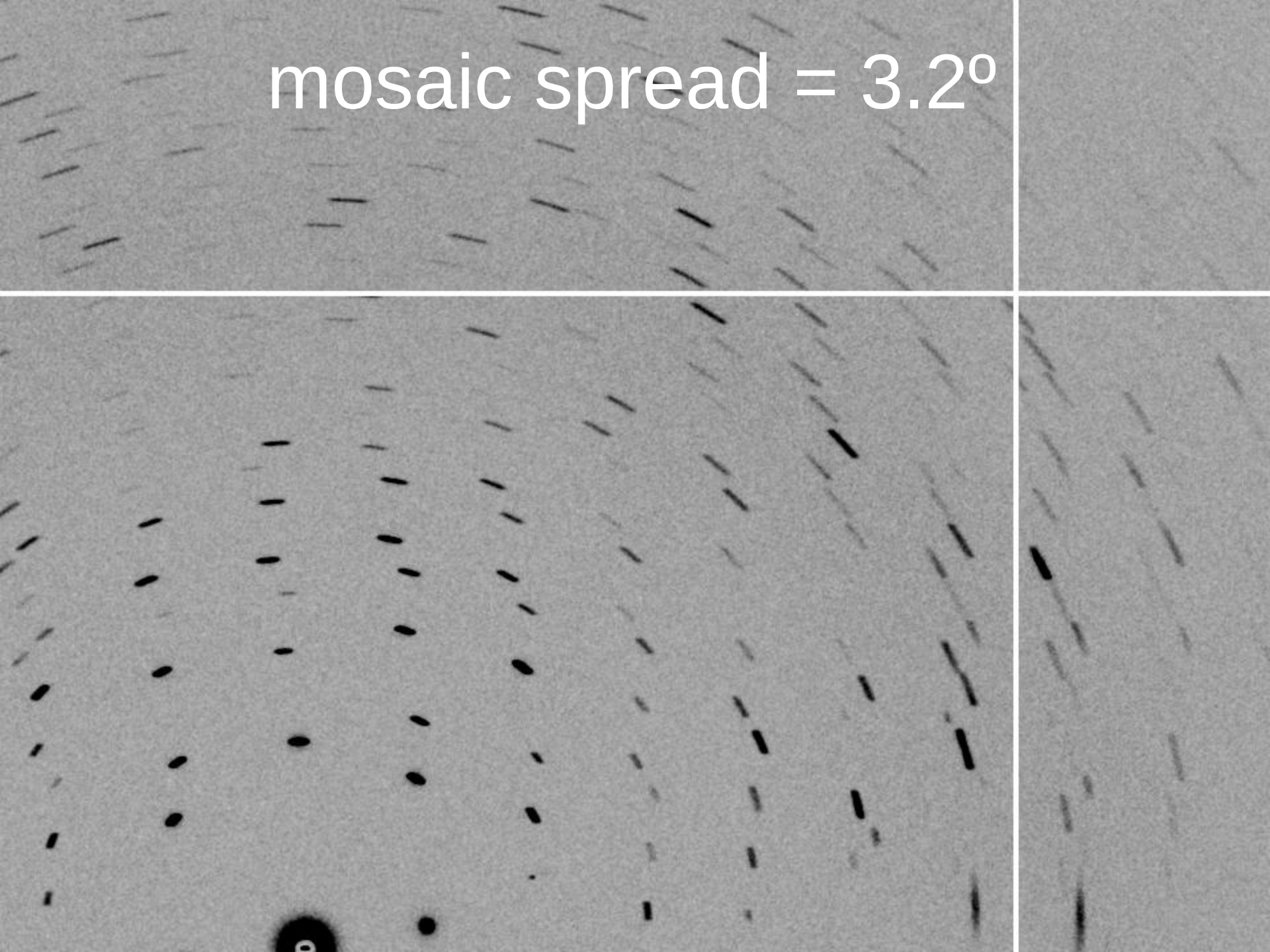

mosaic spread = 0.8º

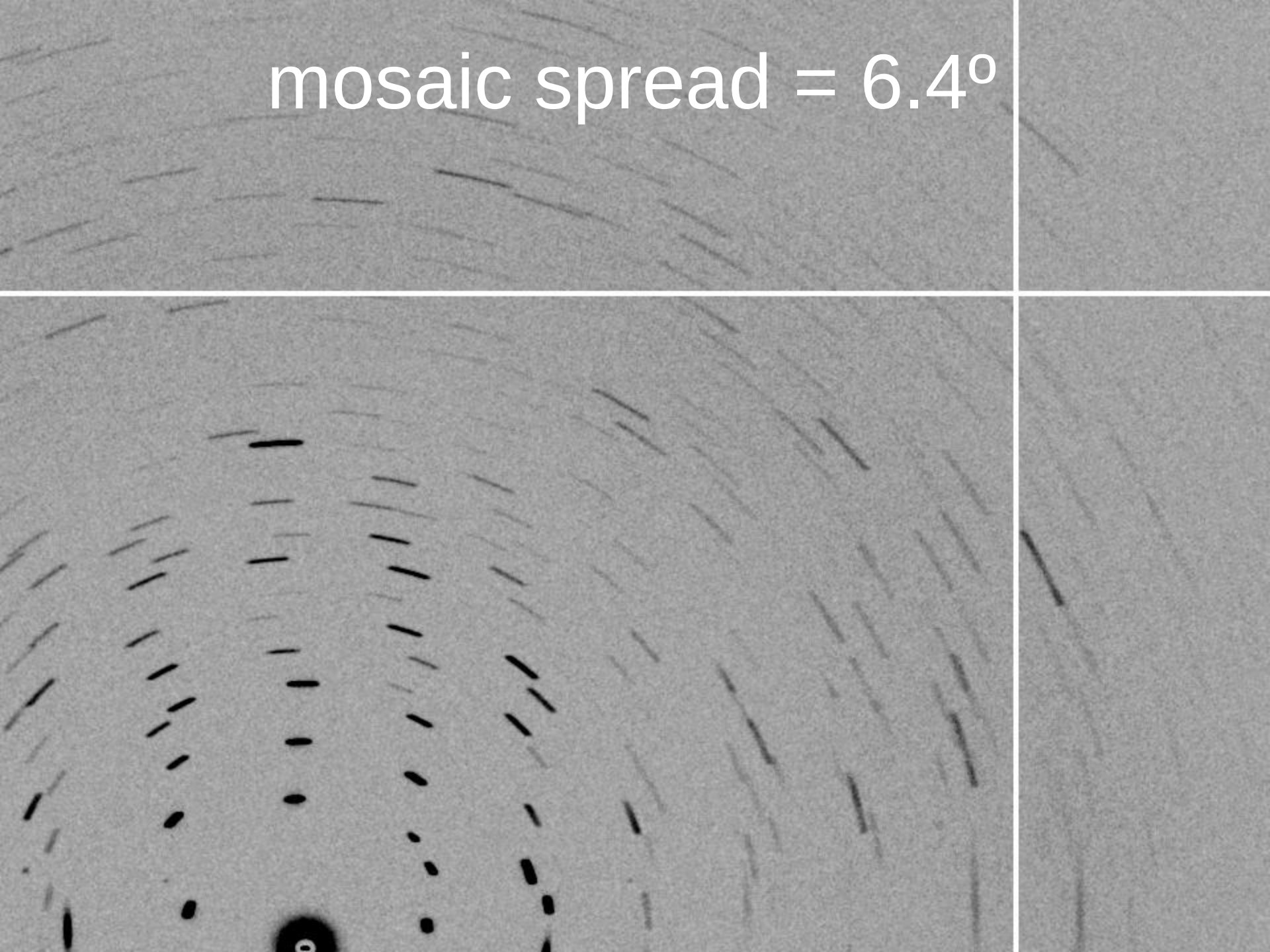

mosaic spread = 1.0º

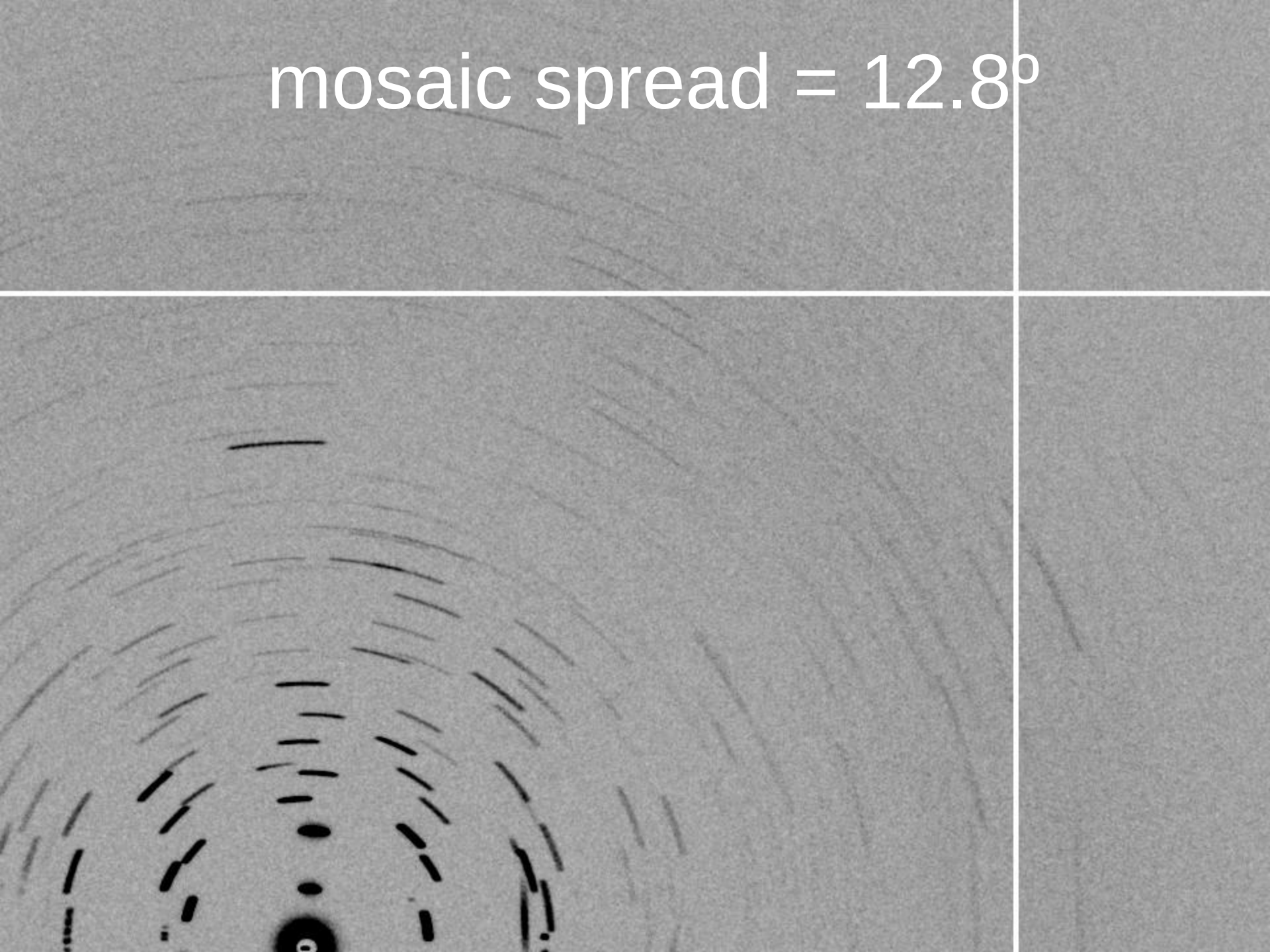

mosaic spread = 1.5º


mosaic spread = 2.0º

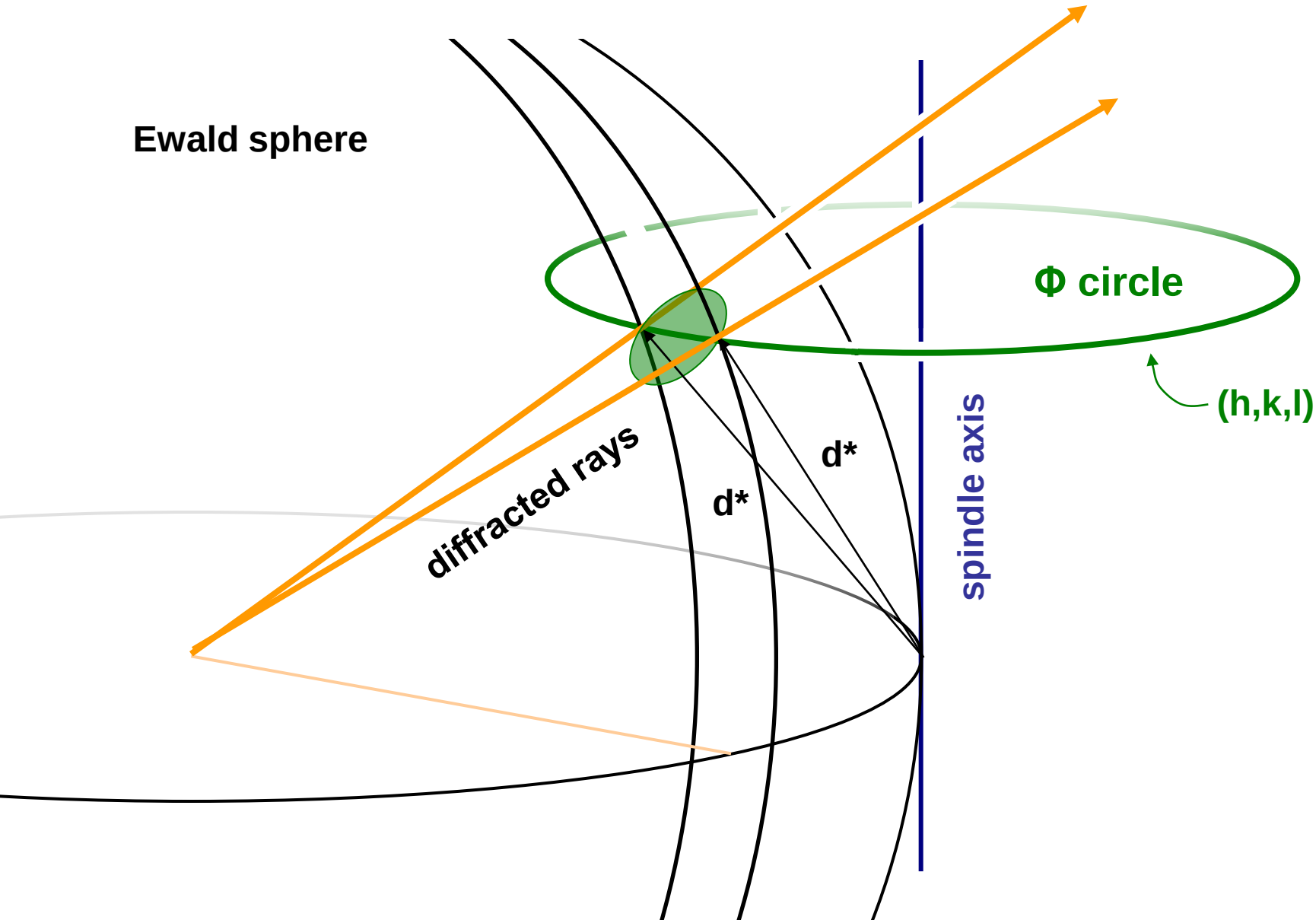

mosaic spread = 2.5º


mosaic spread = 3.2º

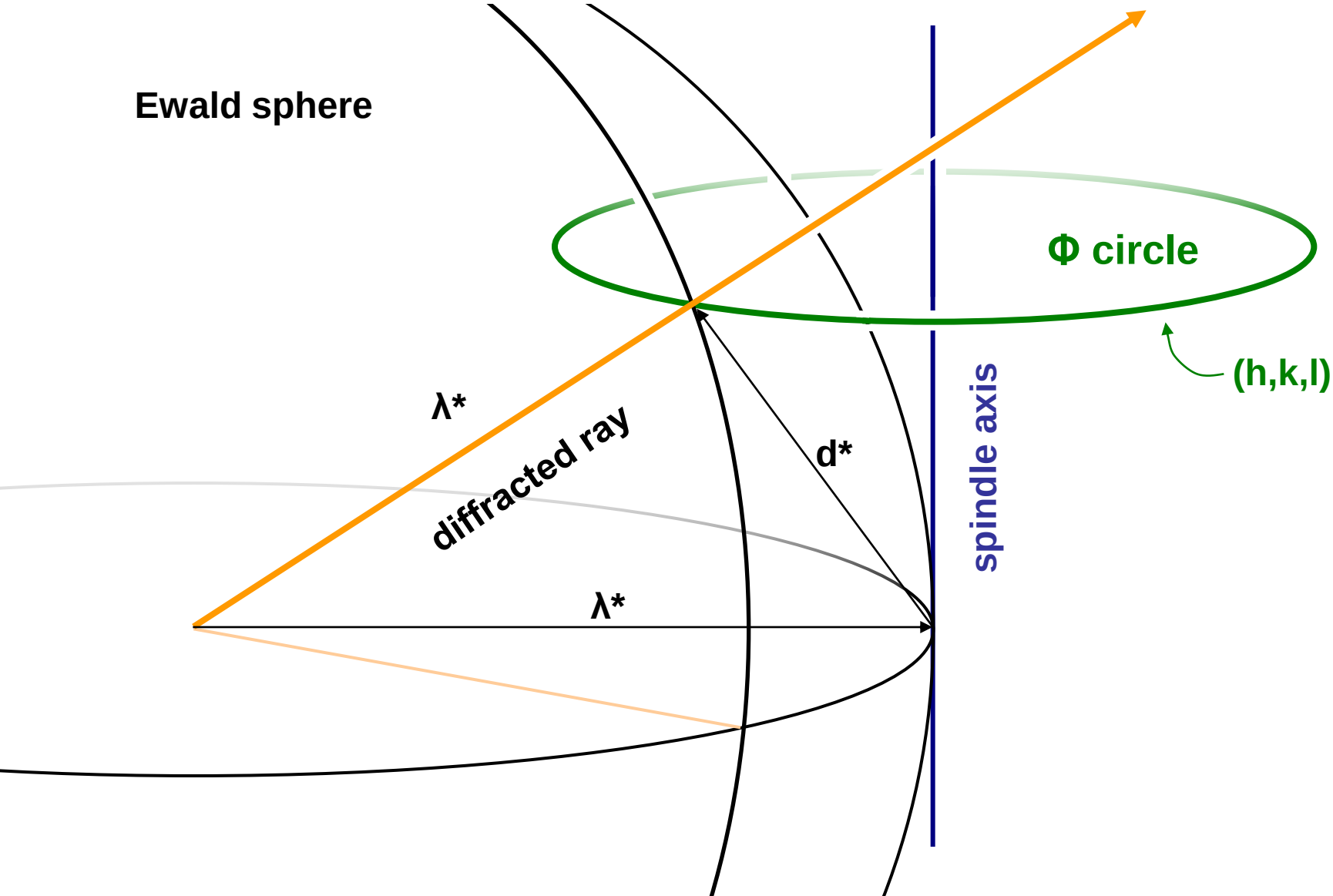

mosaic spread = 6.4º


mosaic spread = 12.8º

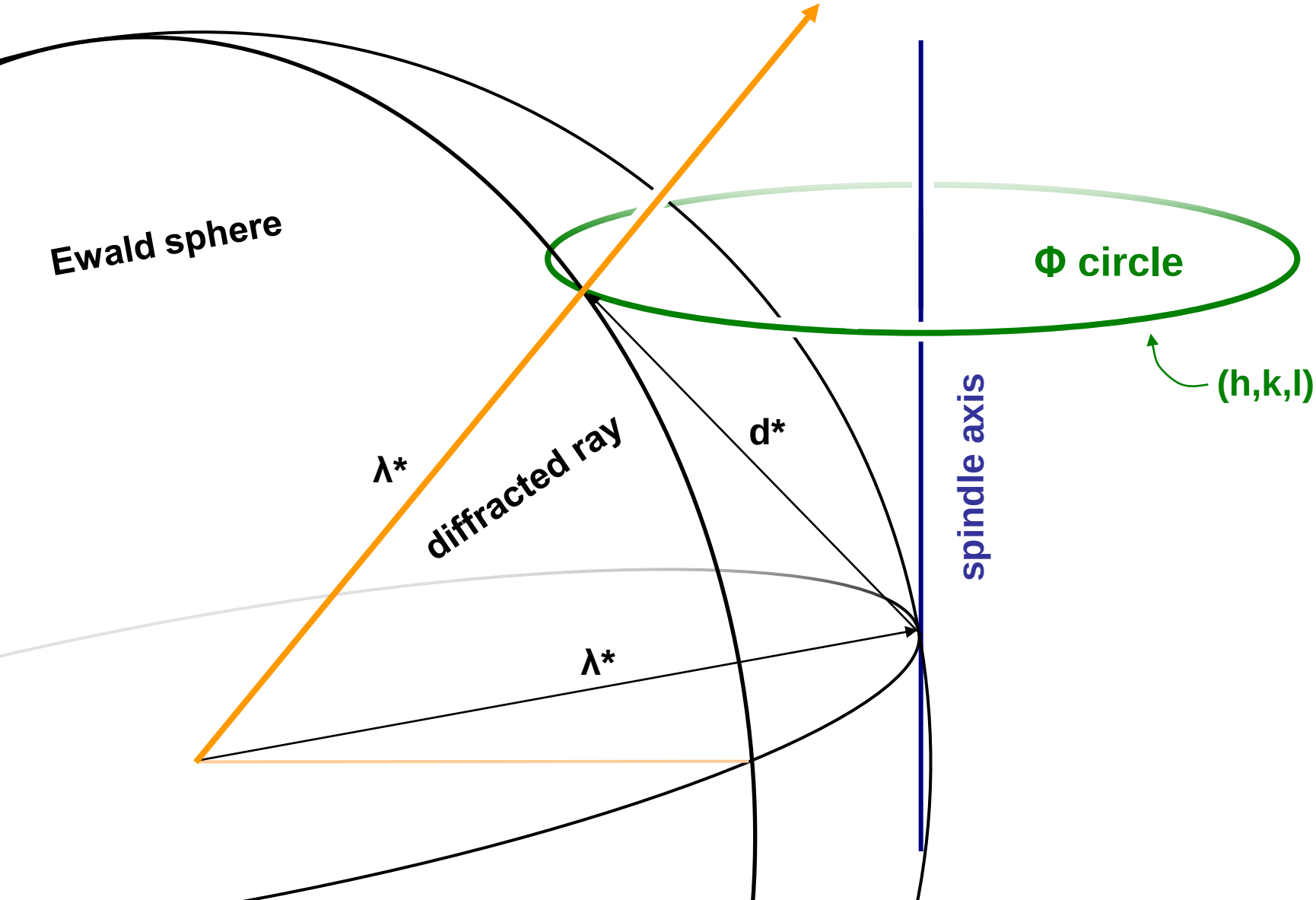
mosaic spread

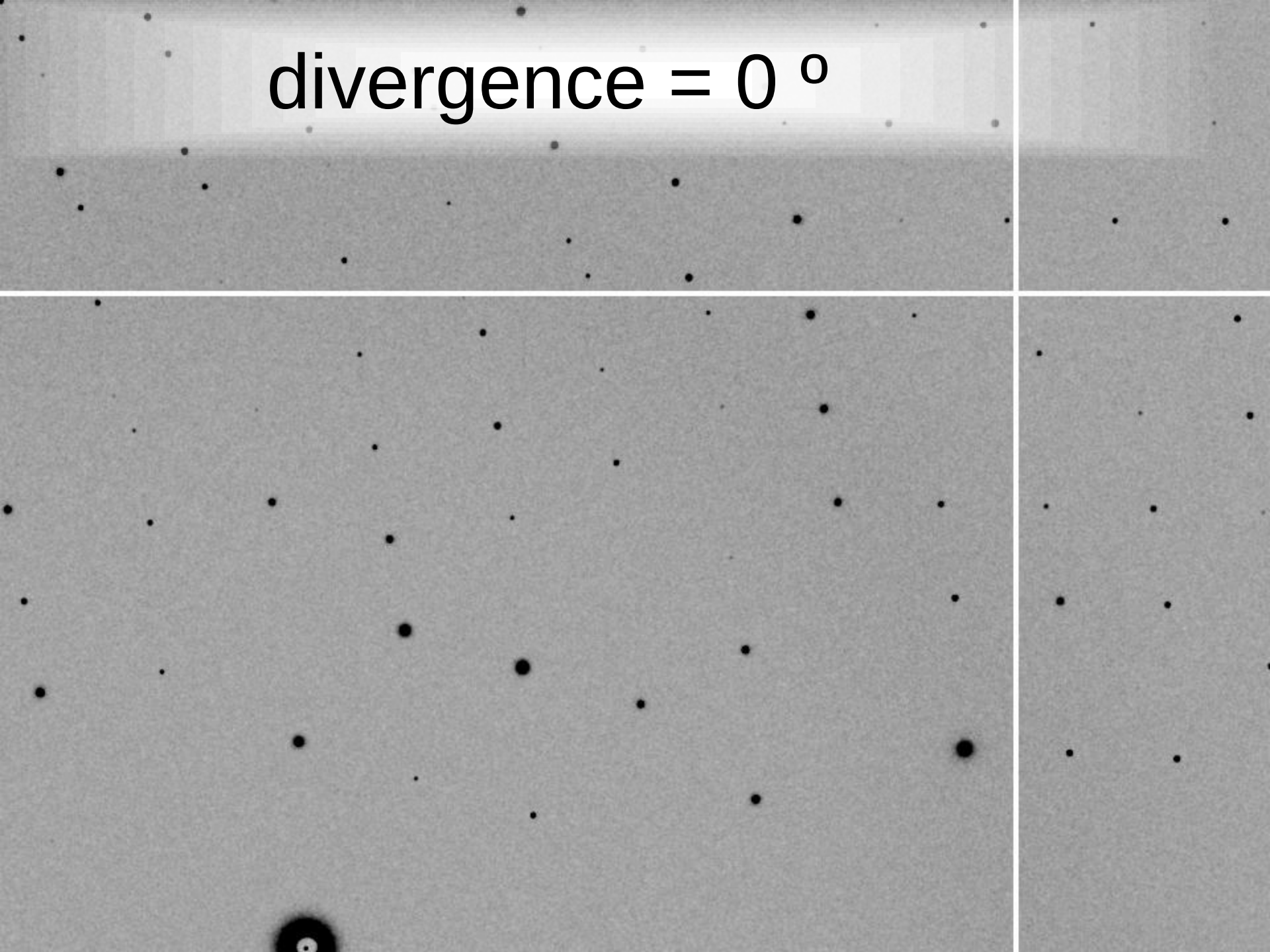


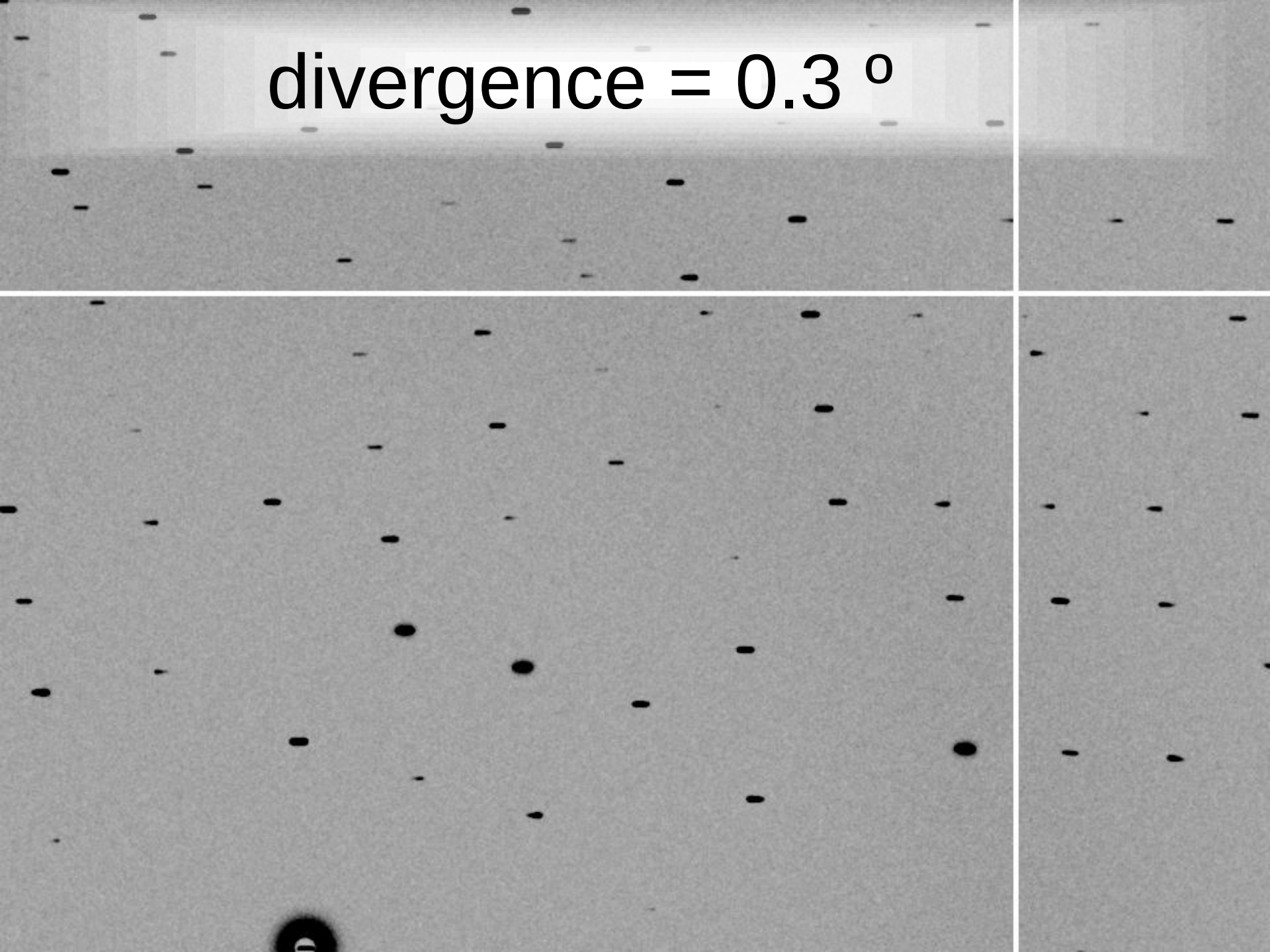
beam divergence



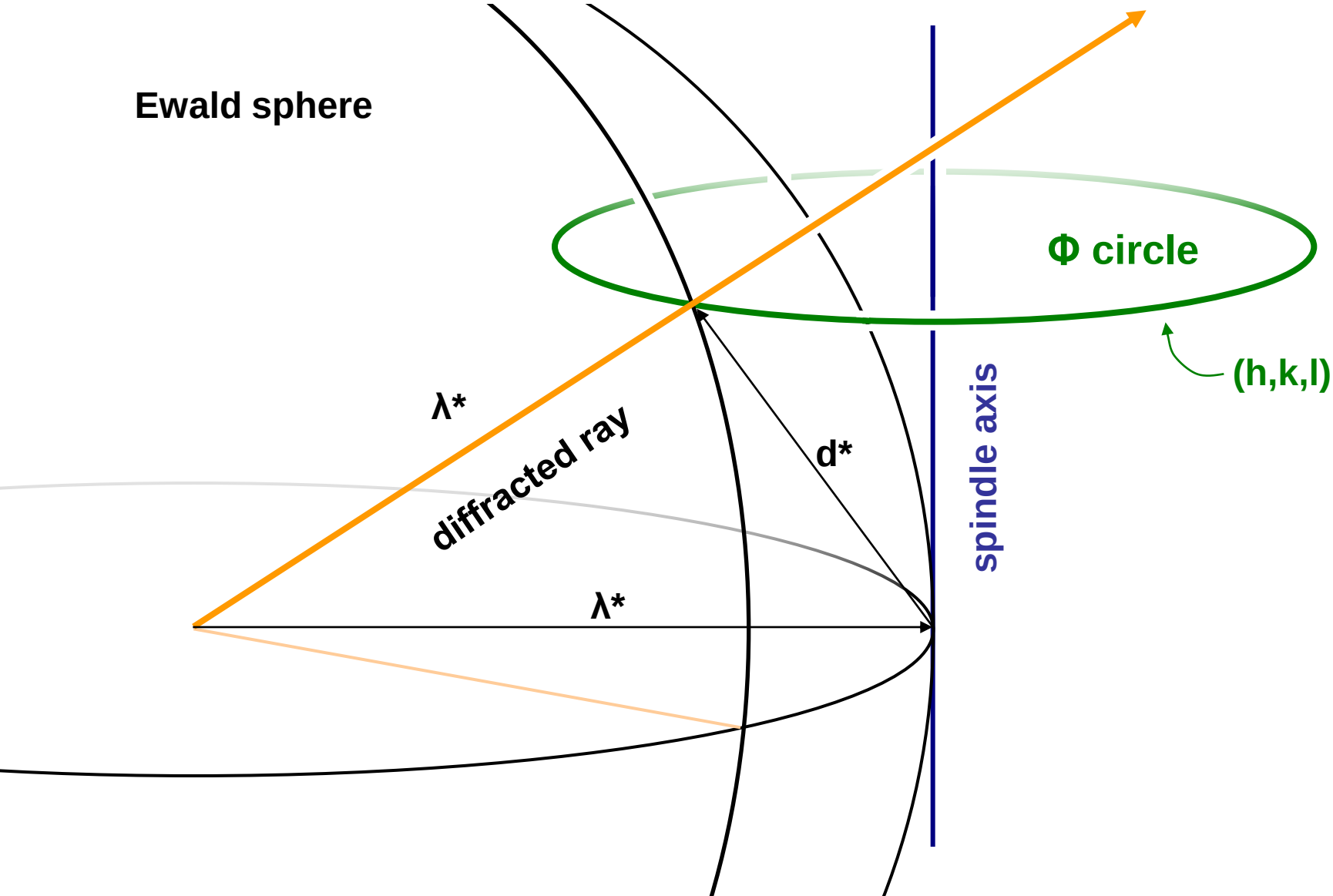
beam divergence



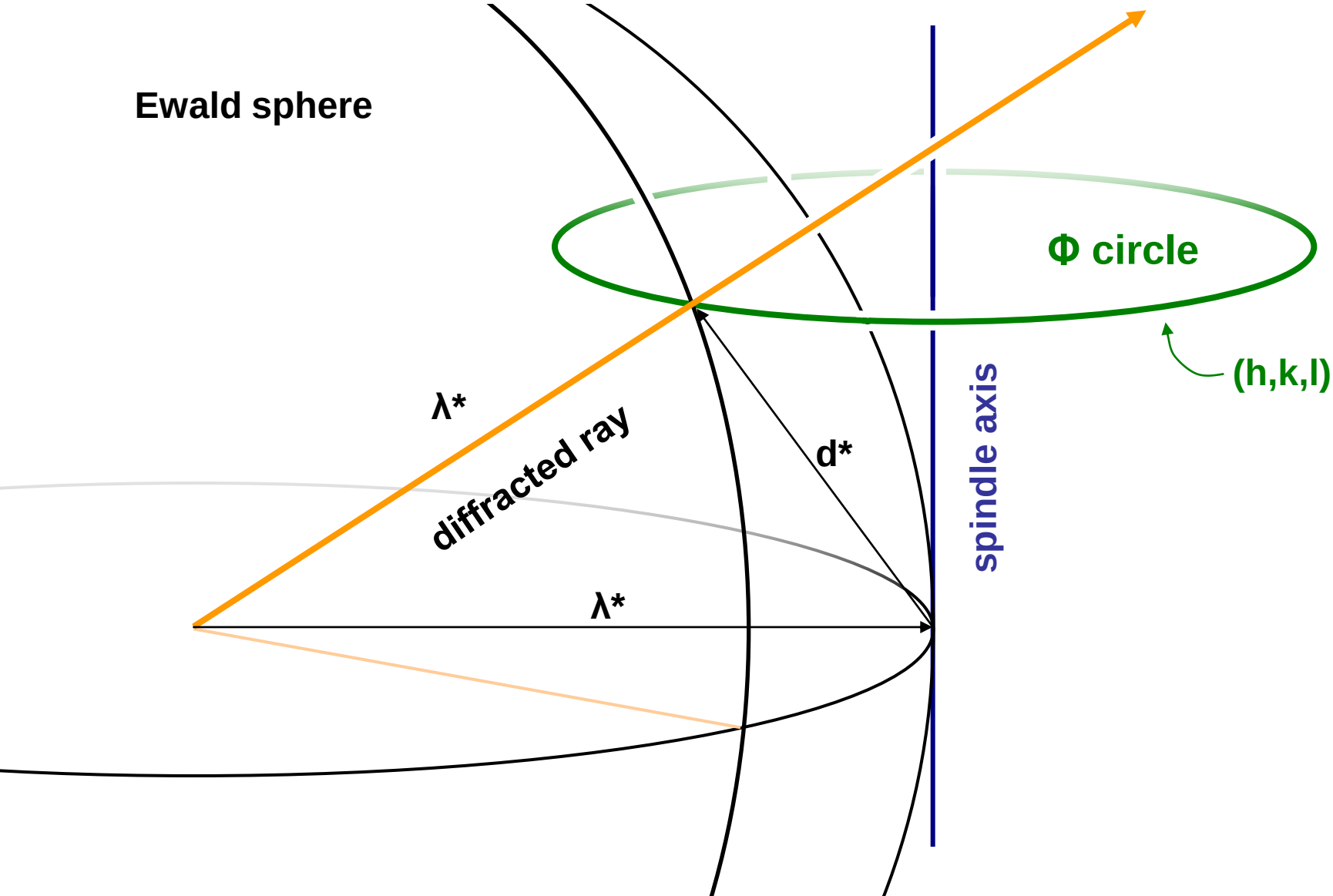

divergence = 0 º


divergence = 0.3 º

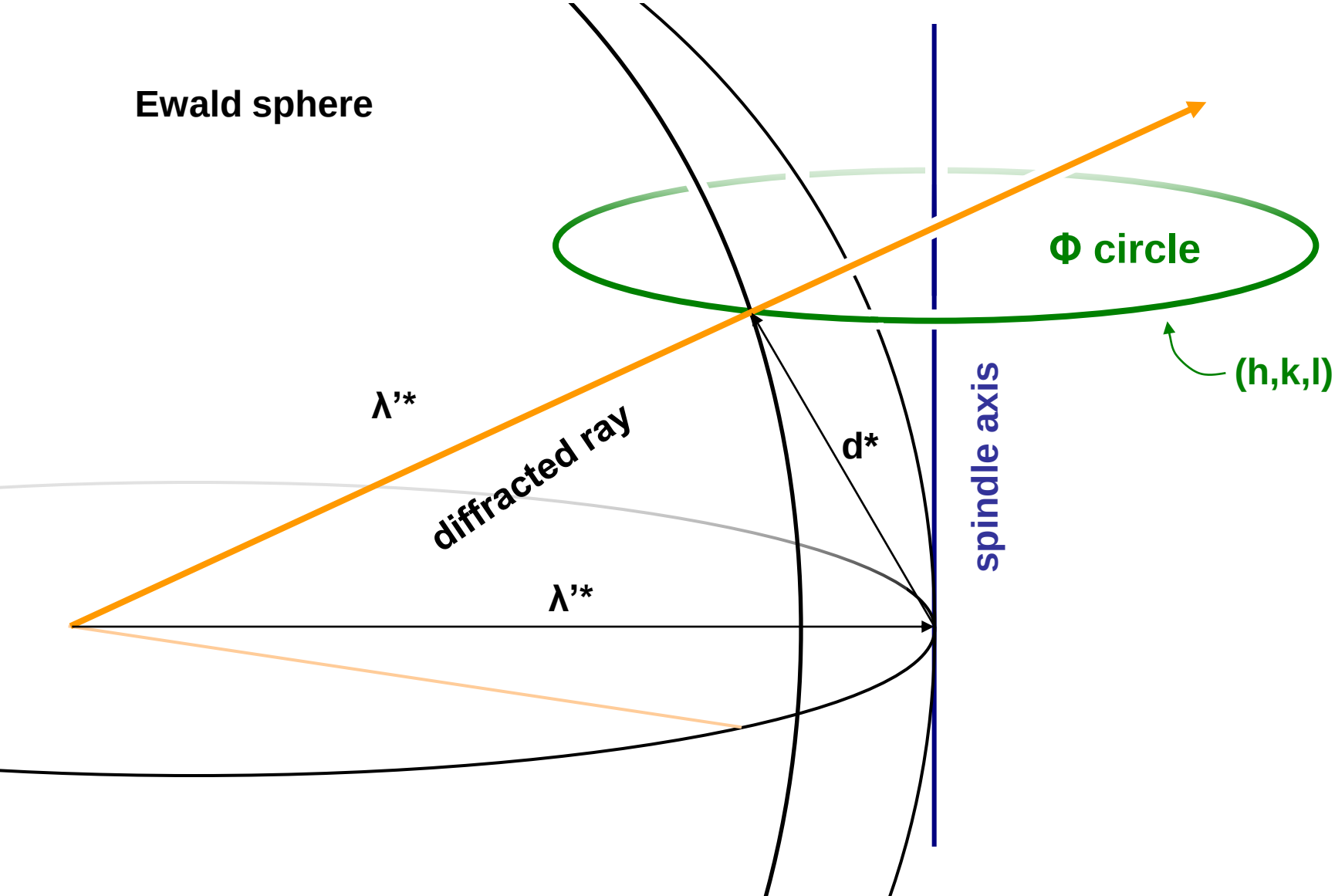
beam divergence

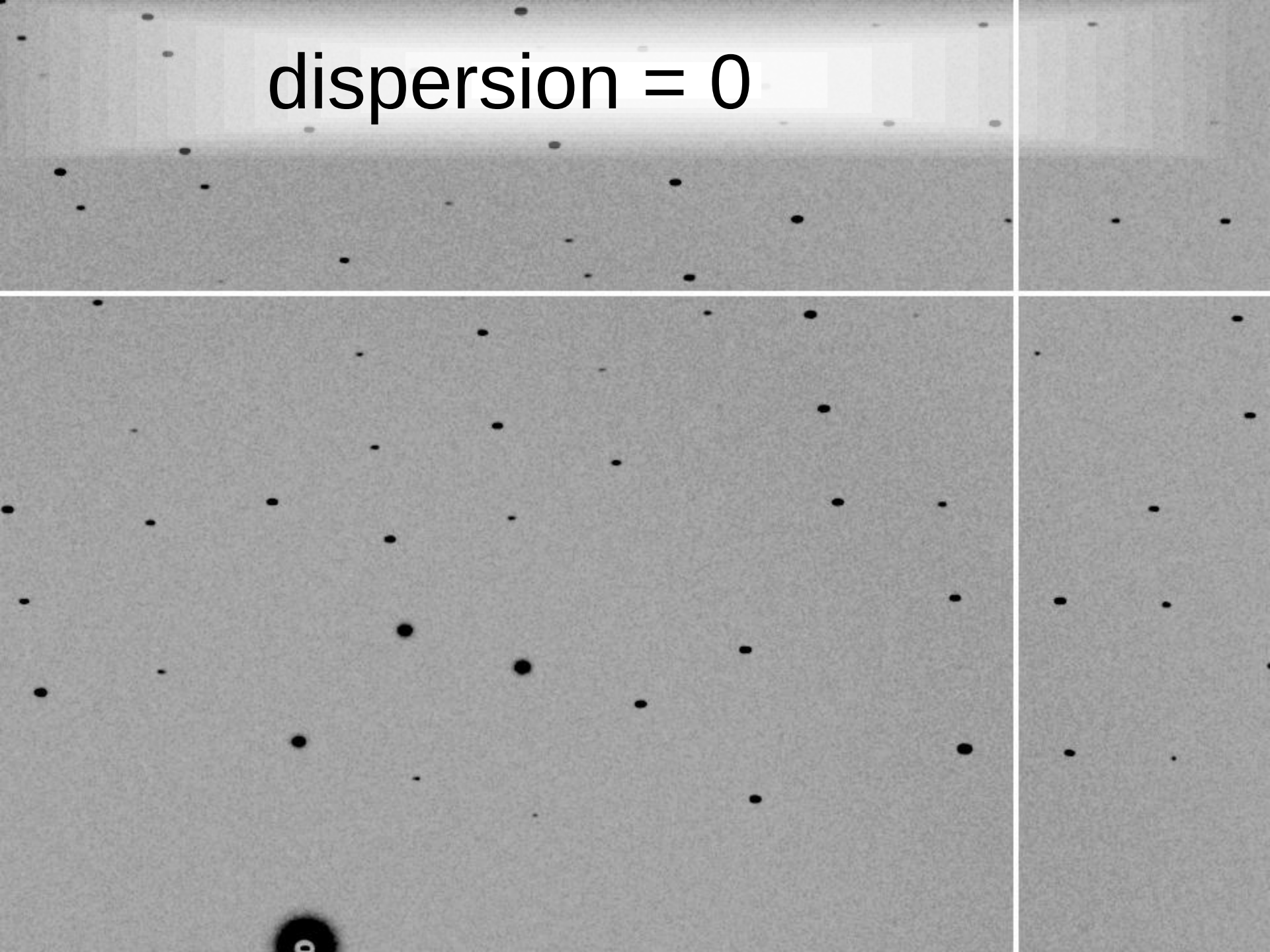


spectral dispersion

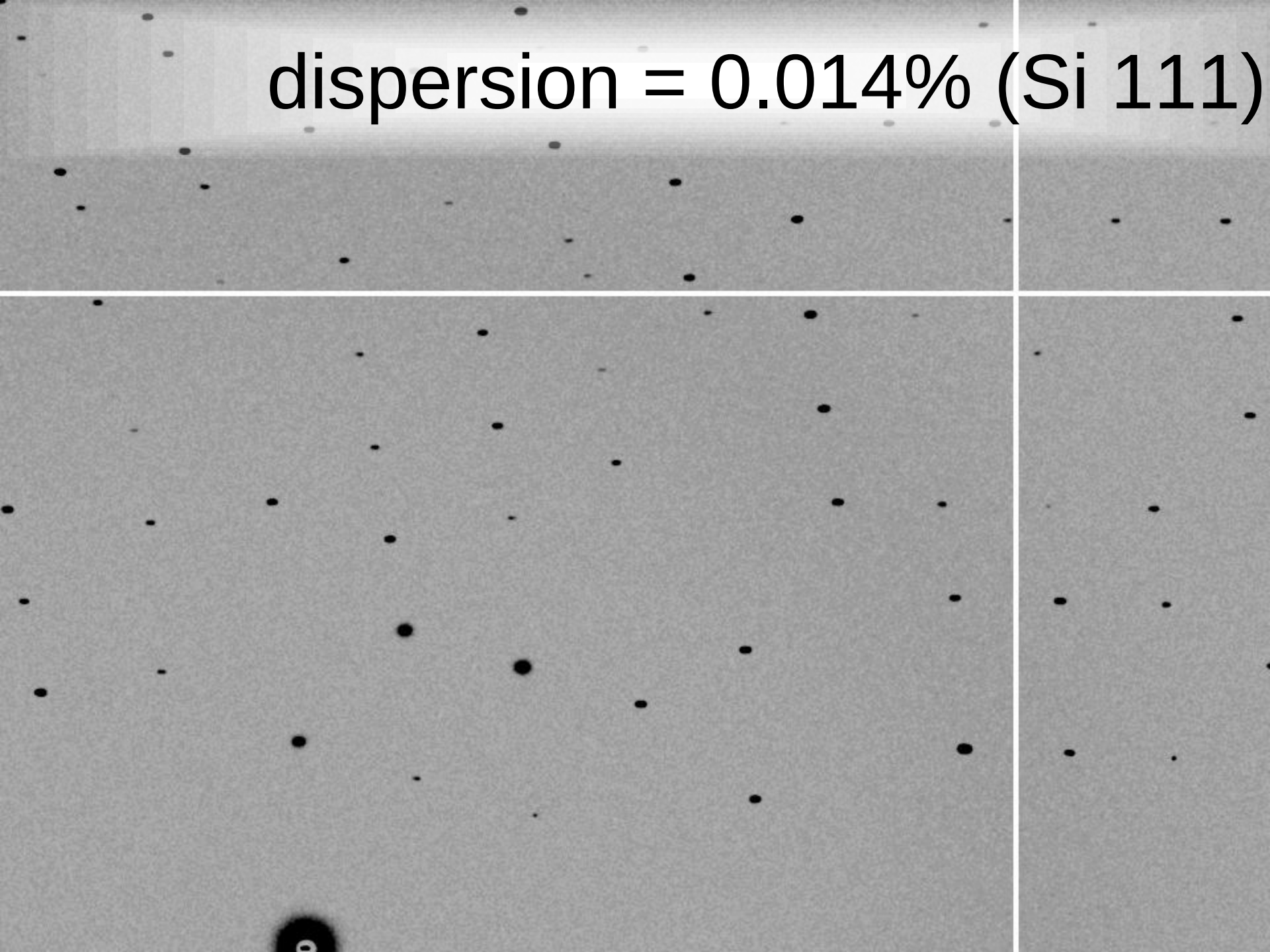


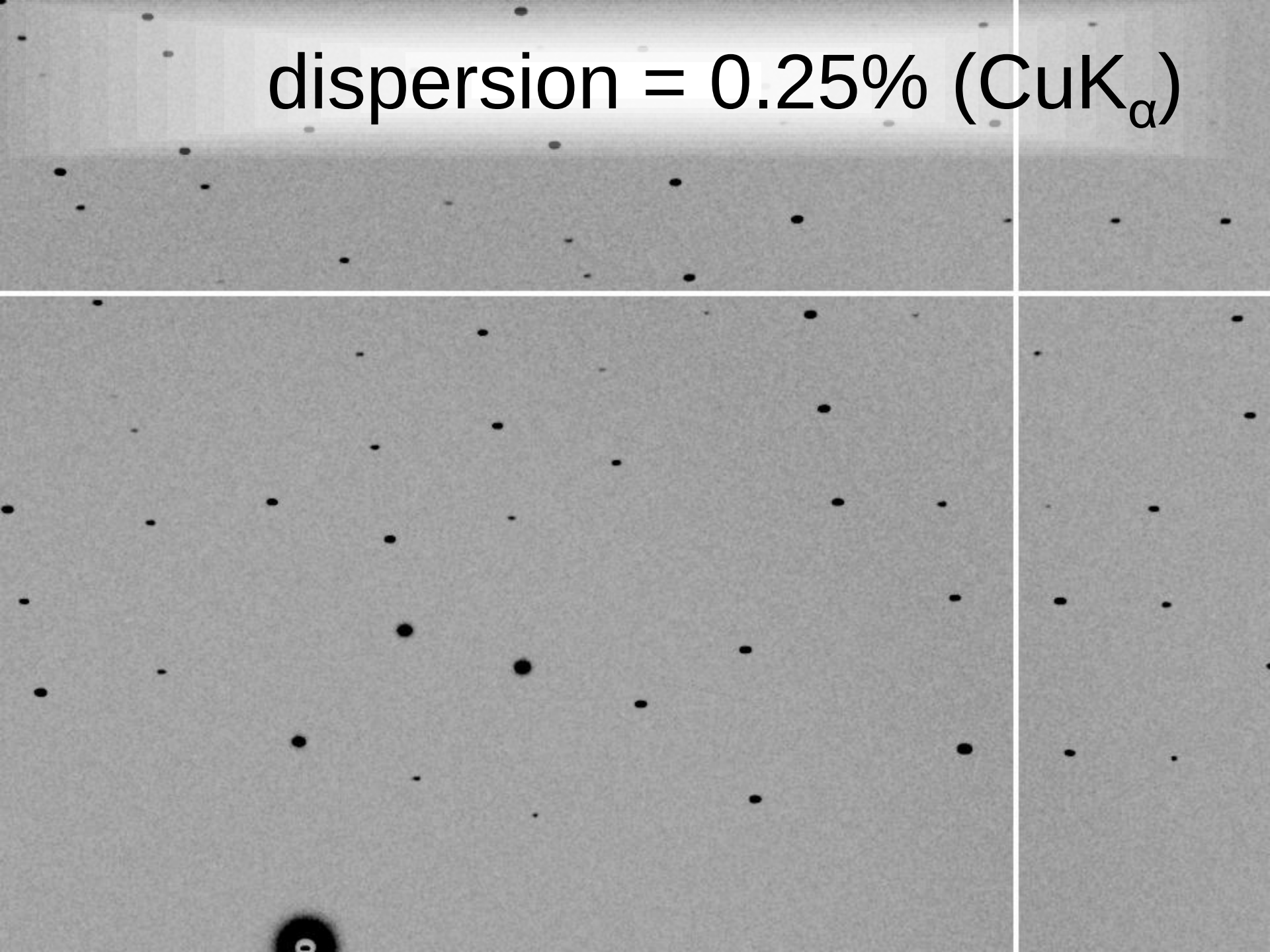
spectral dispersion

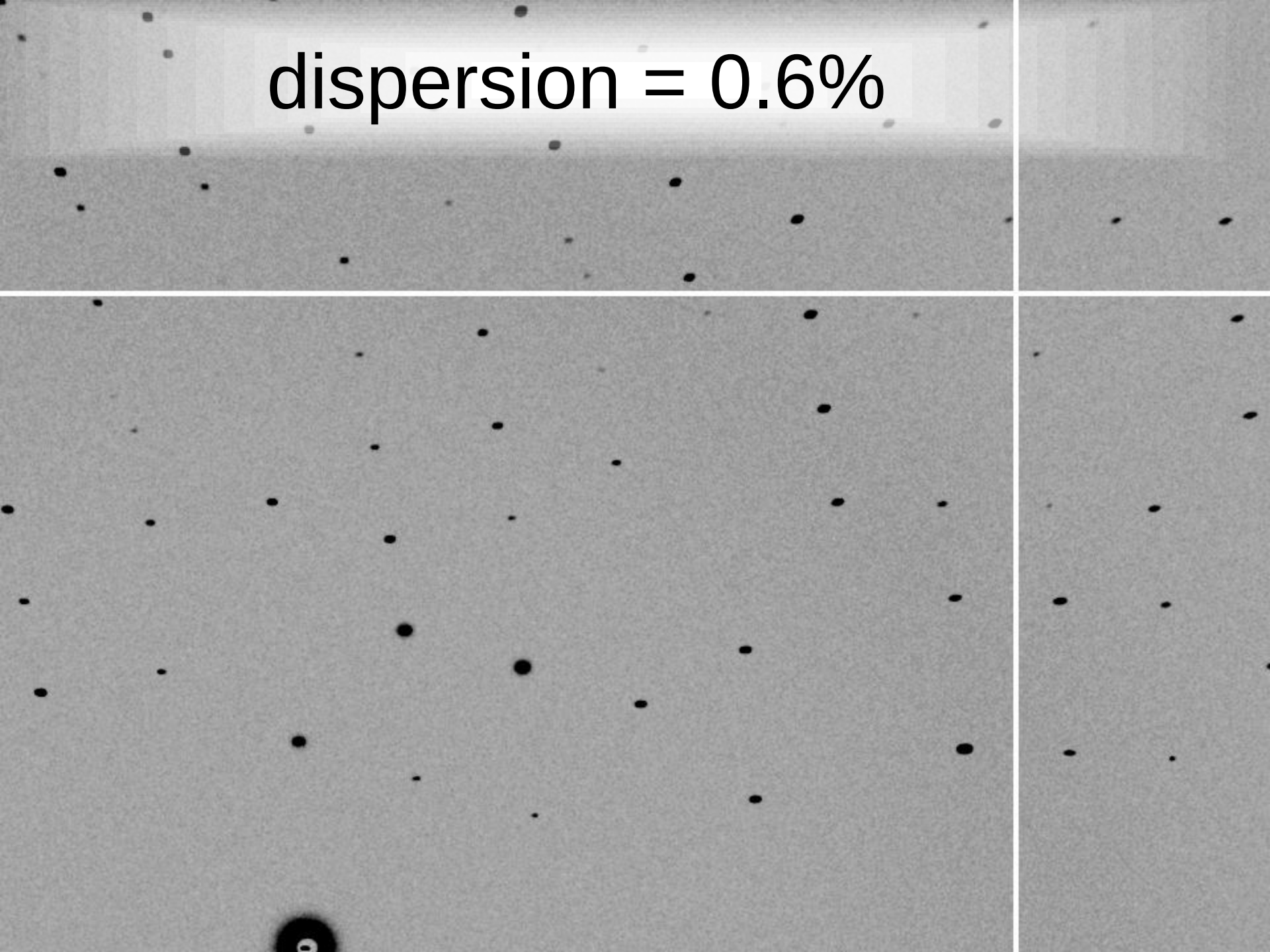


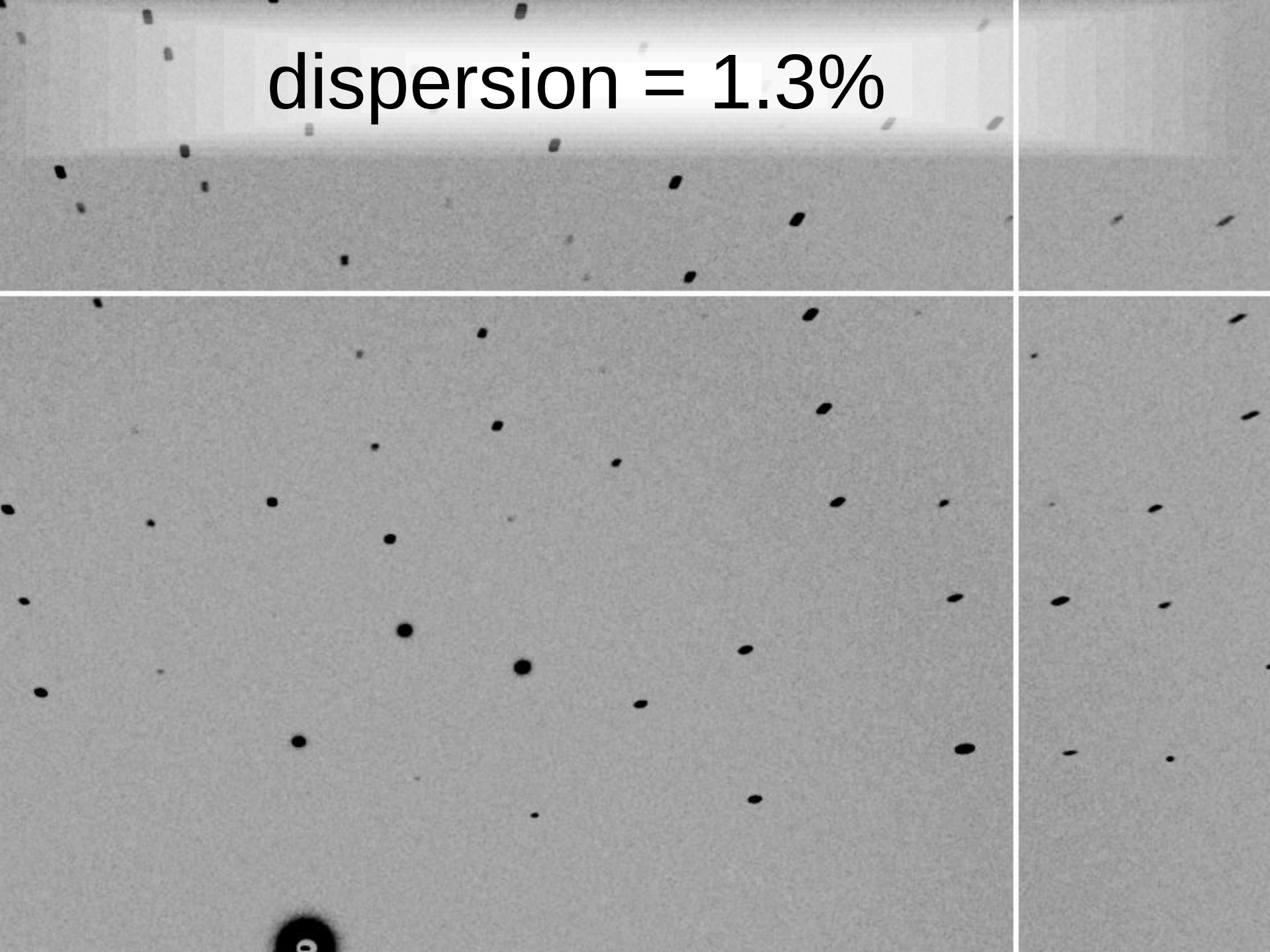

dispersion = 0

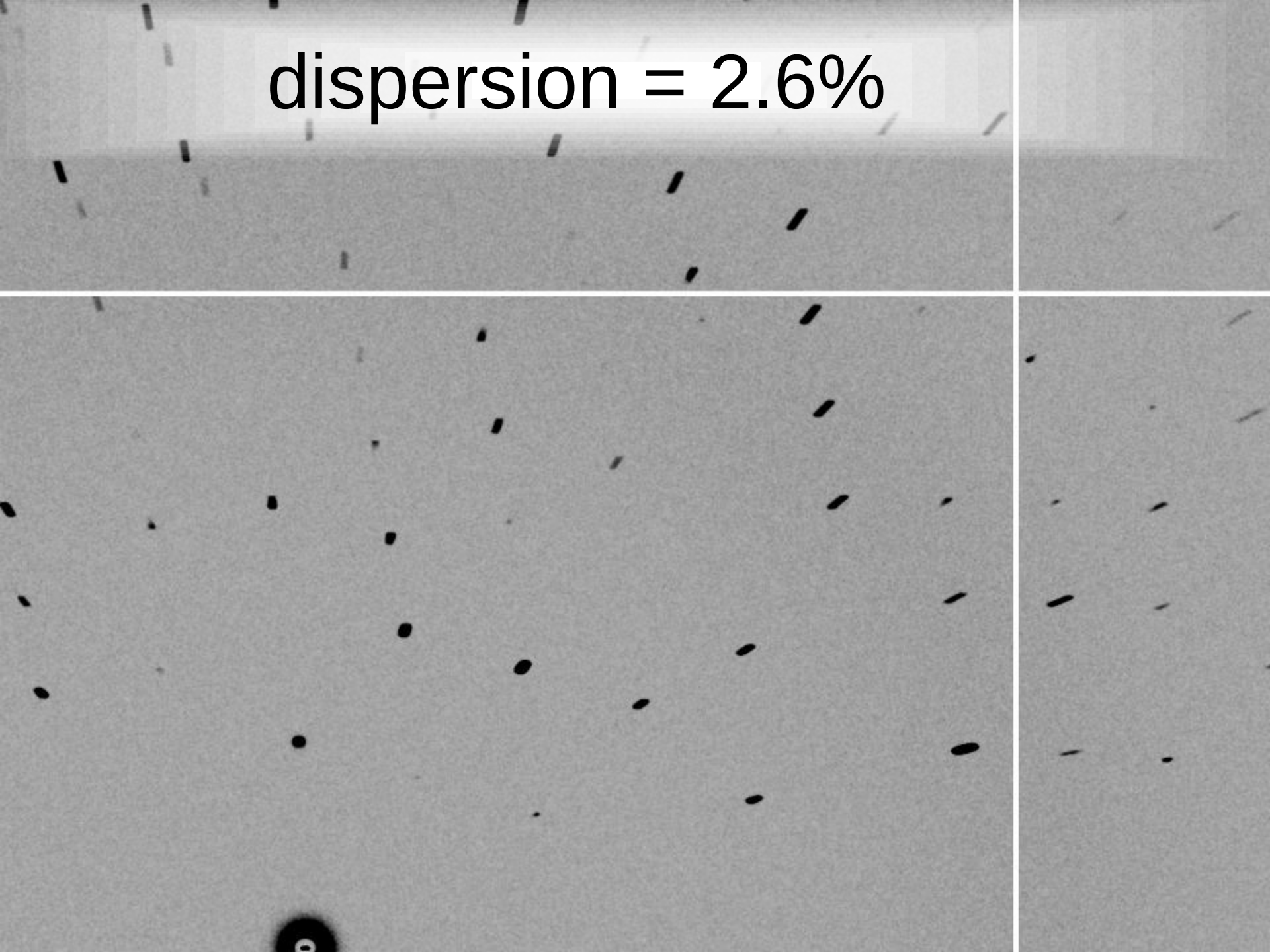
dispersion = 0.014% (Si 111)

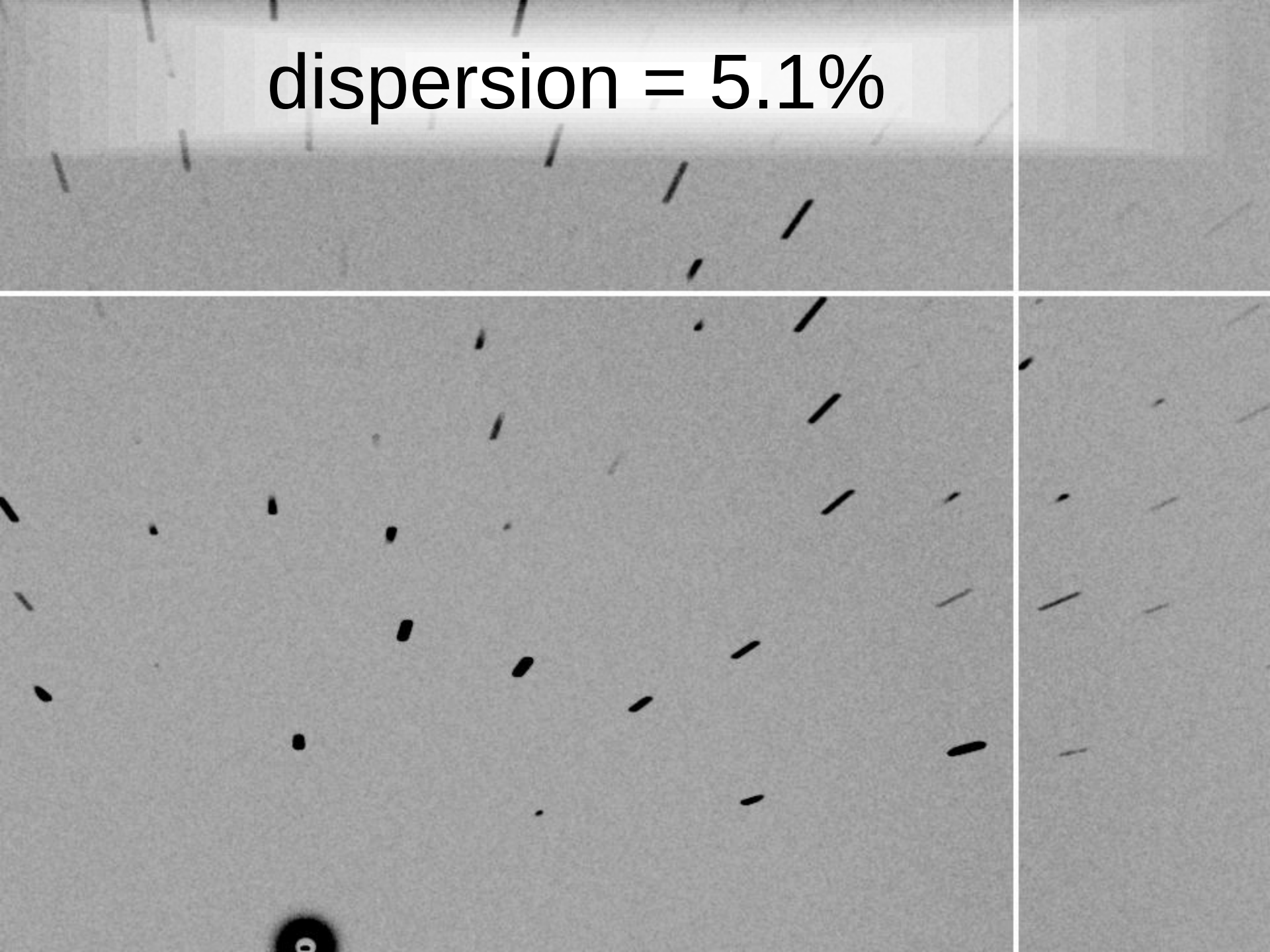



dispersion = 0.25% (CuK$_\alpha$)

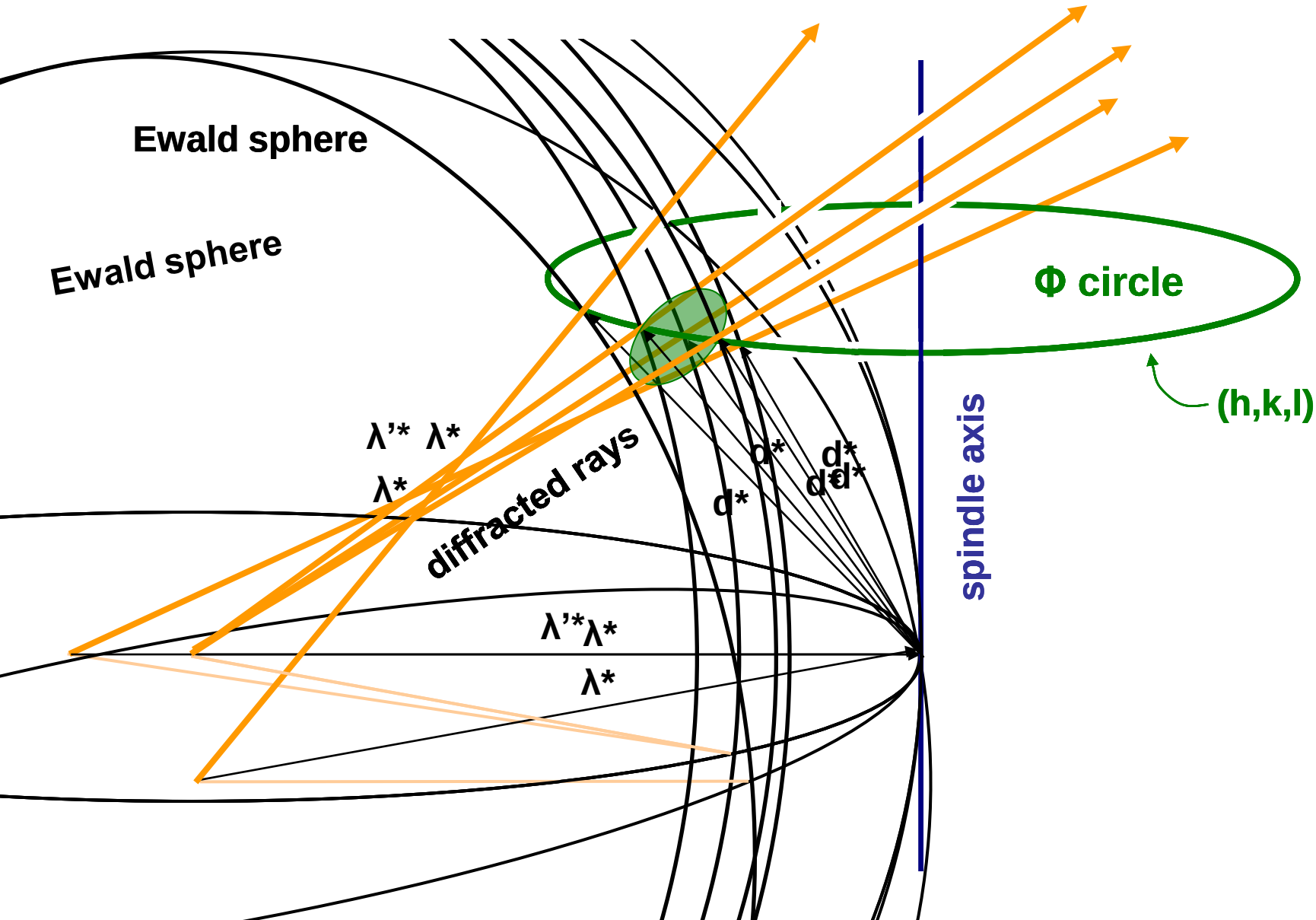

dispersion = 0.6%


dispersion = 1.3%

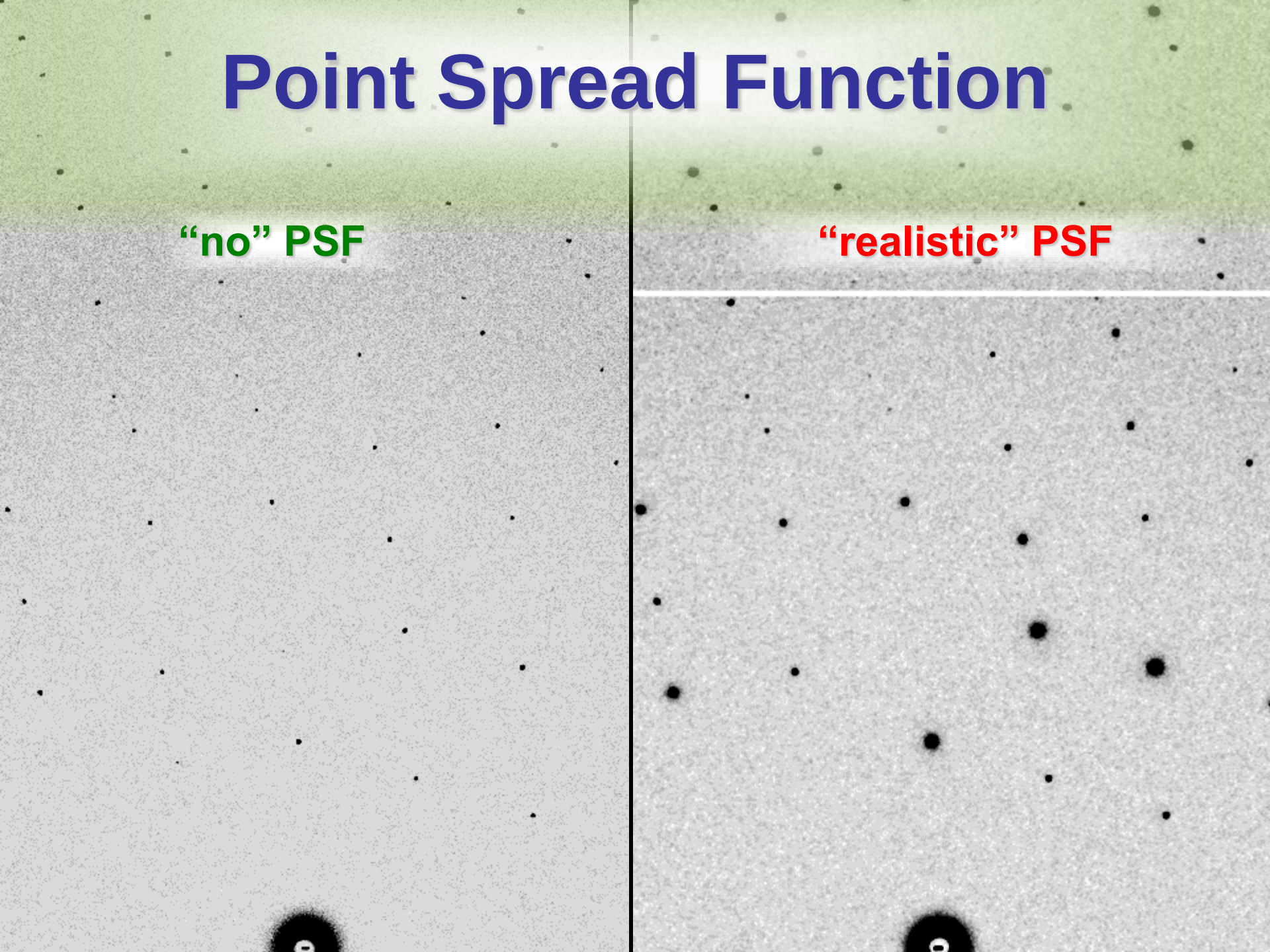

dispersion = 2.6%


dispersion = 5.1%

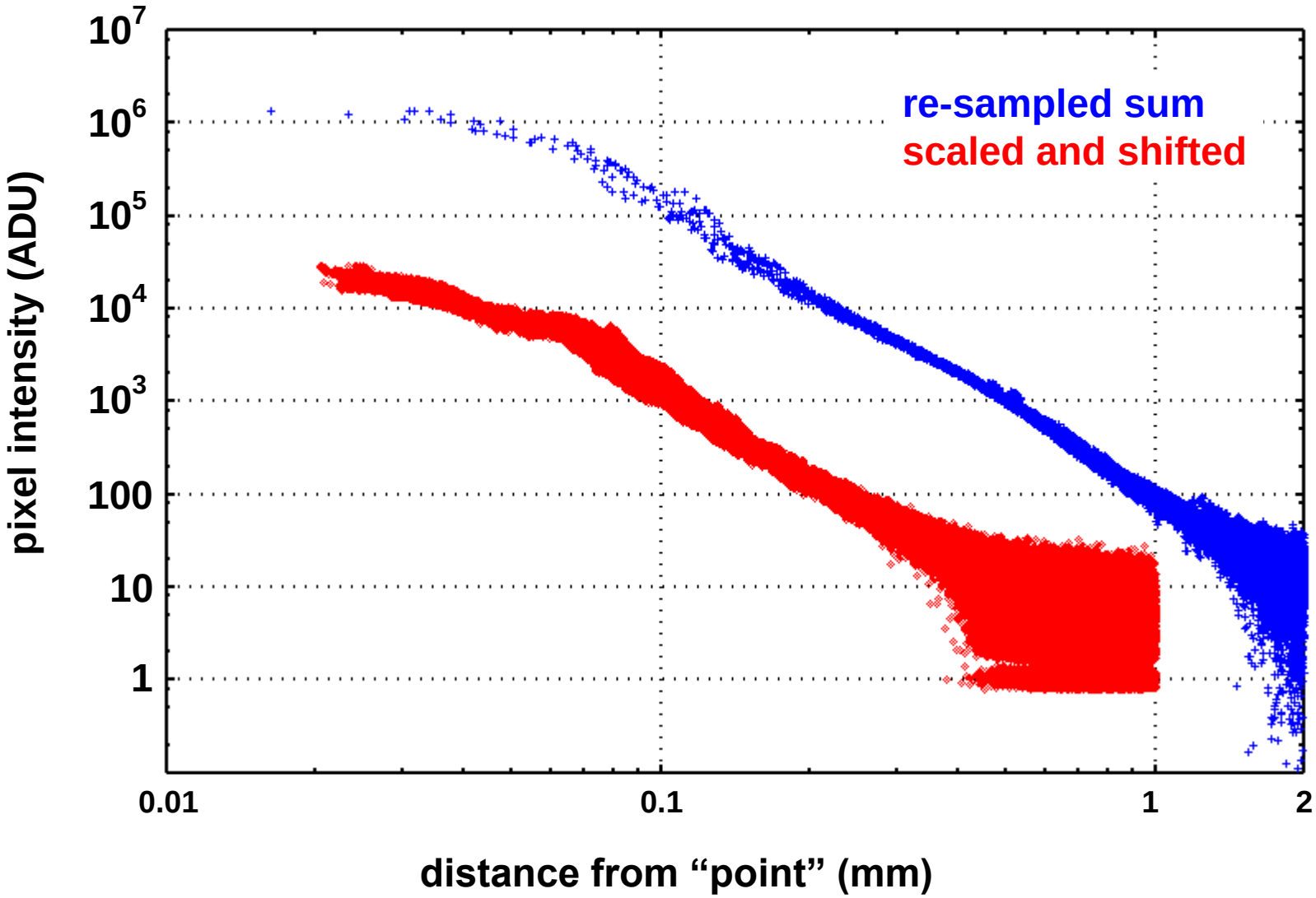
spot shape


Ewald sphere
Ewald sphere
Φ circle
(h,k,l)
spindle axis
λ'* λ*
λ*
diffracted rays
d*
d*
d*
d*
λ'*λ*
λ*

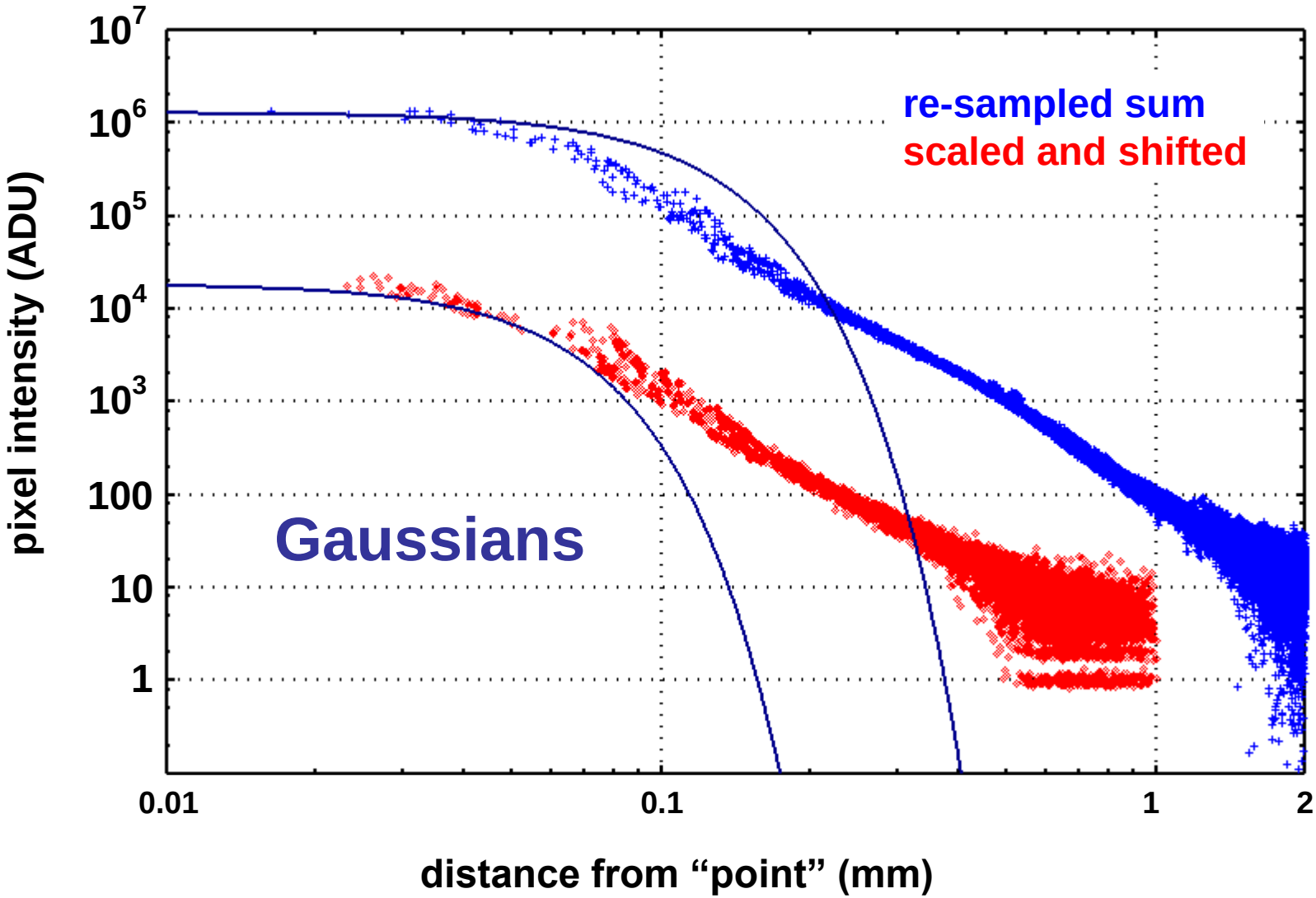
Point Spread Function



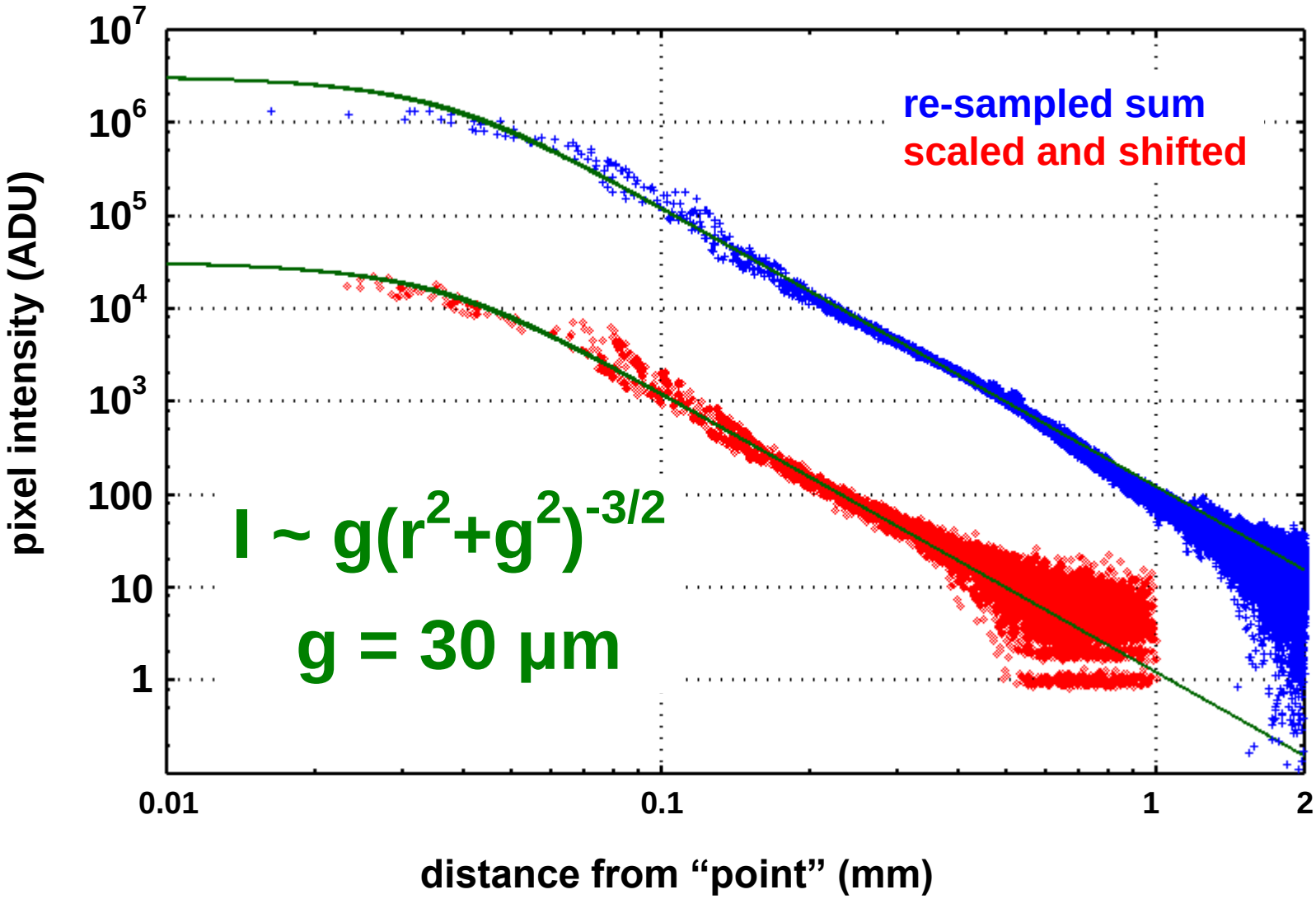
Point Spread Function



Point Spread Function



Point Spread Function



Intensity of a Bragg spot

$$I_{full} \approx |F(hkl)|^2$$

Intensity of a Bragg spot

$$I_{hkl} \approx |F(hkl)|^2$$

Darwin's Formula

$$I(hkl) = I_{beam}\, r_e^2 \frac{V_{xtal}}{V_{cell}} \frac{\lambda^3 L}{\omega V_{cell}} P\, A\, |\, F(hkl)\, |^2$$

I(hkl) - photons/spot (fully-recorded)

I_{beam} - incident (photons/s/m^2)

r_e - classical electron radius (2.818×10^{-15} m)

V_{xtal} - volume of crystal (in m^3)

V_{cell} - volume of unit cell (in m^3)

λ - x-ray wavelength (in meters!)

ω - rotation speed (radians/s)

L - Lorentz factor (speed/speed)

P - polarization factor

$(1+\cos^2(2\theta) - Pfac \cdot \cos(2\Phi)\sin^2(2\theta))/2$

A - absorption factor

$\exp(-\mu_{xtal} \cdot l_{path})$

F(hkl) - structure amplitude (electrons)

C. G. Darwin (1914)

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Background scattering

R. W. James (1947)

$$I_{bg} = I_{beam}\, t\, r_e^2 \frac{N_A \rho V}{Mr} P A \,|\, f(s) \,|^2$$

I_{bg} - scattered photons/steradian

I_{beam} - incident (photons/s/m^2)

t - exposure time (s)

r_e - classical electron radius (2.818×10^{-15} m)

N_A - Avogadro number (6.02×10^{23})

ρ - density of material (g/m^3)

Mr - molecular weight (g/mol)

V - volume of material (in m3)

P - polarization factor

$(1+\cos^2(2\theta) - Pfac \cdot \cos(2\Phi)\sin^2(2\theta))/2$

A - absorption factor

$\exp(-\mu_{xtal} \cdot l_{path})$

f(s) - molecular structure amplitude (electrons)

s - scattering length ($\sin(\theta)/\lambda$)

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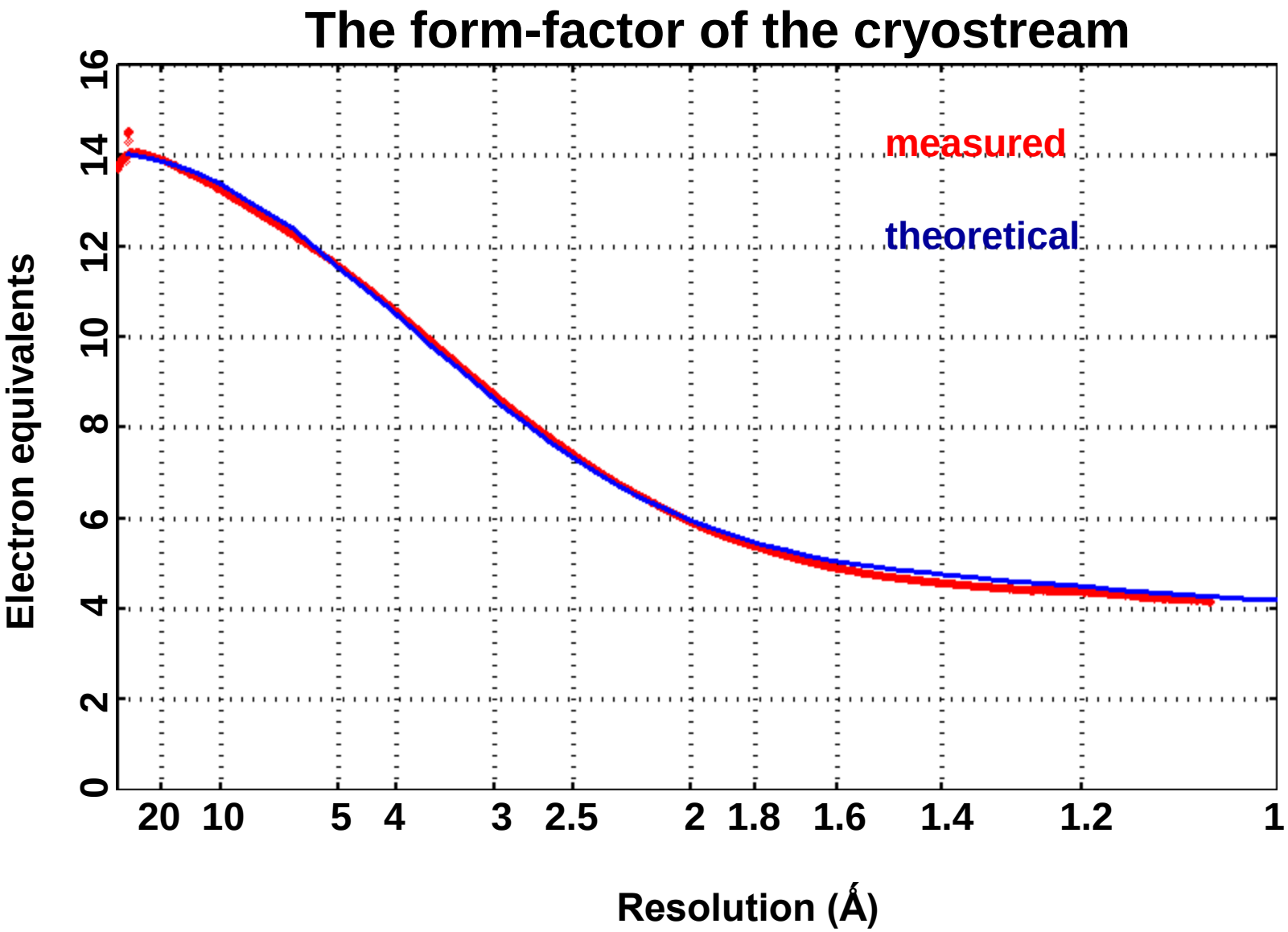
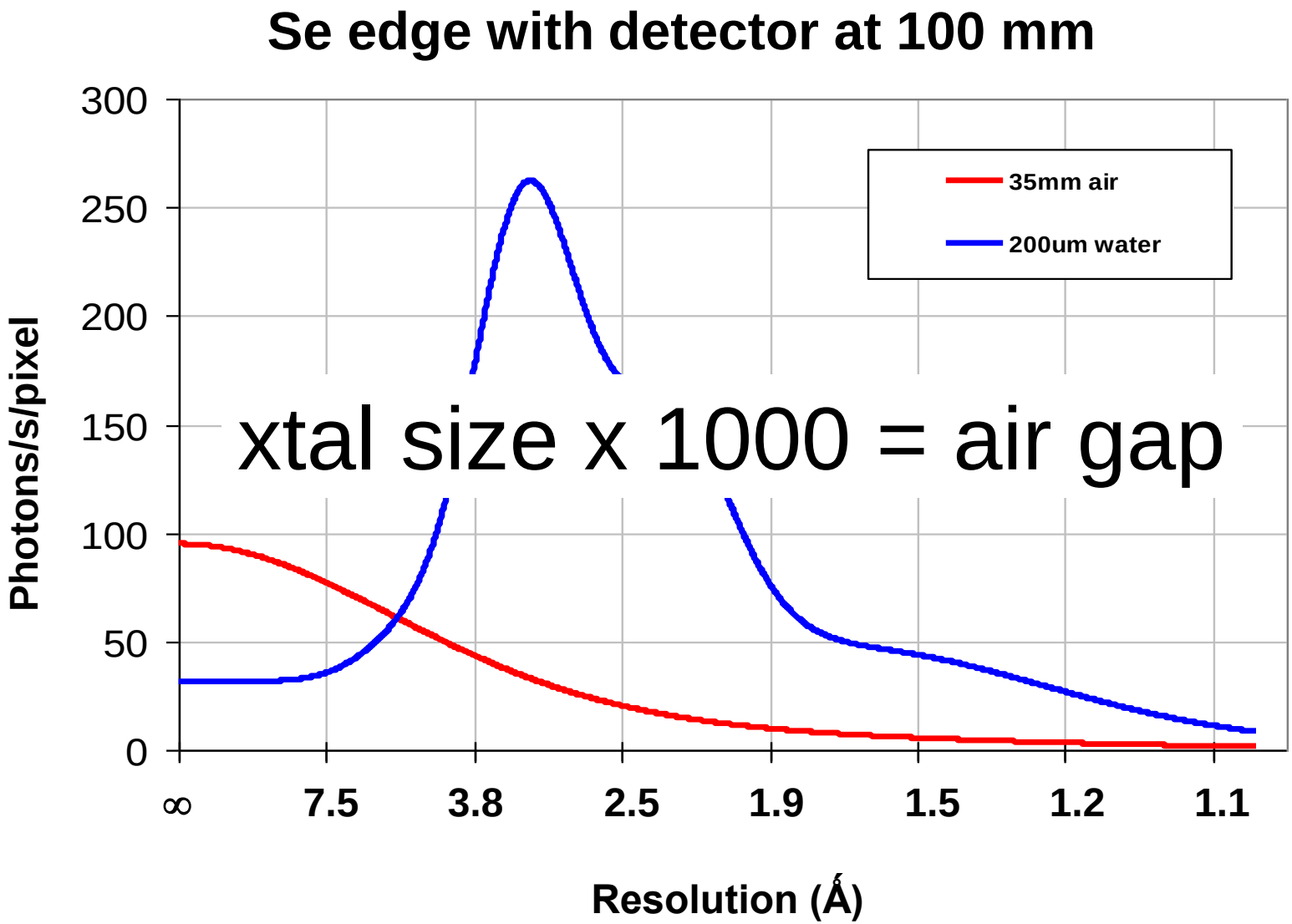


Background scattering



Diffuse scattering

R. W. James (1947)

$$I_{ds} = I_{beam}\, t\, r_e^2 \frac{V_{xtal}}{V_{ASU}}\, P\, A \sum_a |f_a(s)|^2 \left(1-\exp(-2B_a \cdot s^2)\right)$$

I_{ds}	- scattered photons/steradian	P	- polarization factor
I_{beam}	- incident (photons/s/m^2)	A	- absorption factor
t	- exposure time (s)	a	- particular atom in the ASU
r_e	- classical electron radius (2.818×10^{-15} m)	$f_a(s)$	- atomic structure amplitude (electrons)
V_{xtal}	- volume of crystal (in m^3)	s	- scattering length ($\sin(\theta)/\lambda$)
V_{ASU}	- asymmetric unit (in m^3)	B_a	- atomic B factor

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V_{xtal}	- volume of crystal (in m^3)	s	- scattering length (sin(θ)/λ)
V_{ASU}	- asymmetric unit (in m^3)	B_a	- atomic B factor

Compton scattering

R. W. James (1947)

$$I_{compton} = I_{beam}\, t\, r_e^2 \frac{V_{xtal}}{V_{ASU}} \frac{P\,A}{1+\kappa\,(1-\cos(\theta))^2} \sum_a Z_a - |f_a(s)|$$

$I_{compton}$	- scattered photons/steradian
I_{beam}	- incident (photons/s/m^2)
t	- exposure time (s)
r_e	- classical electron radius (2.818x10^{-15} m)
V_{xtal}	- volume of crystal (in m^3)
V_{ASU}	- asymmetric unit (in m^3)
P	- polarization factor
A	- absorption factor
a	- particular atom in the ASU
θ	- Bragg angle
κ	- photon energy (keV) / 511 keV
Z_a	- atomic number
$f_a(s)$	- atomic structure amplitude (electrons)
s	- scattering length ($\sin(\theta)/\lambda$)

Compton scattering

R. W. James (1947)

$$I_{compton} = I_{beam}\, t\, r_e^2 \frac{V_{xtal}}{V_{ASU}} \frac{P\,A}{1+\kappa\,(1-\cos(\theta))^2} \sum_a Z_a \cdot |f_a(s)|$$

$I_{compton}$	- scattered photons/steradian
I_{beam}	- incident (photons/s/m^2)
t	- exposure time (s)
r_e	- classical electron radius (2.818×10^{-15} m)
V_{xtal}	- volume of crystal (in m^3)
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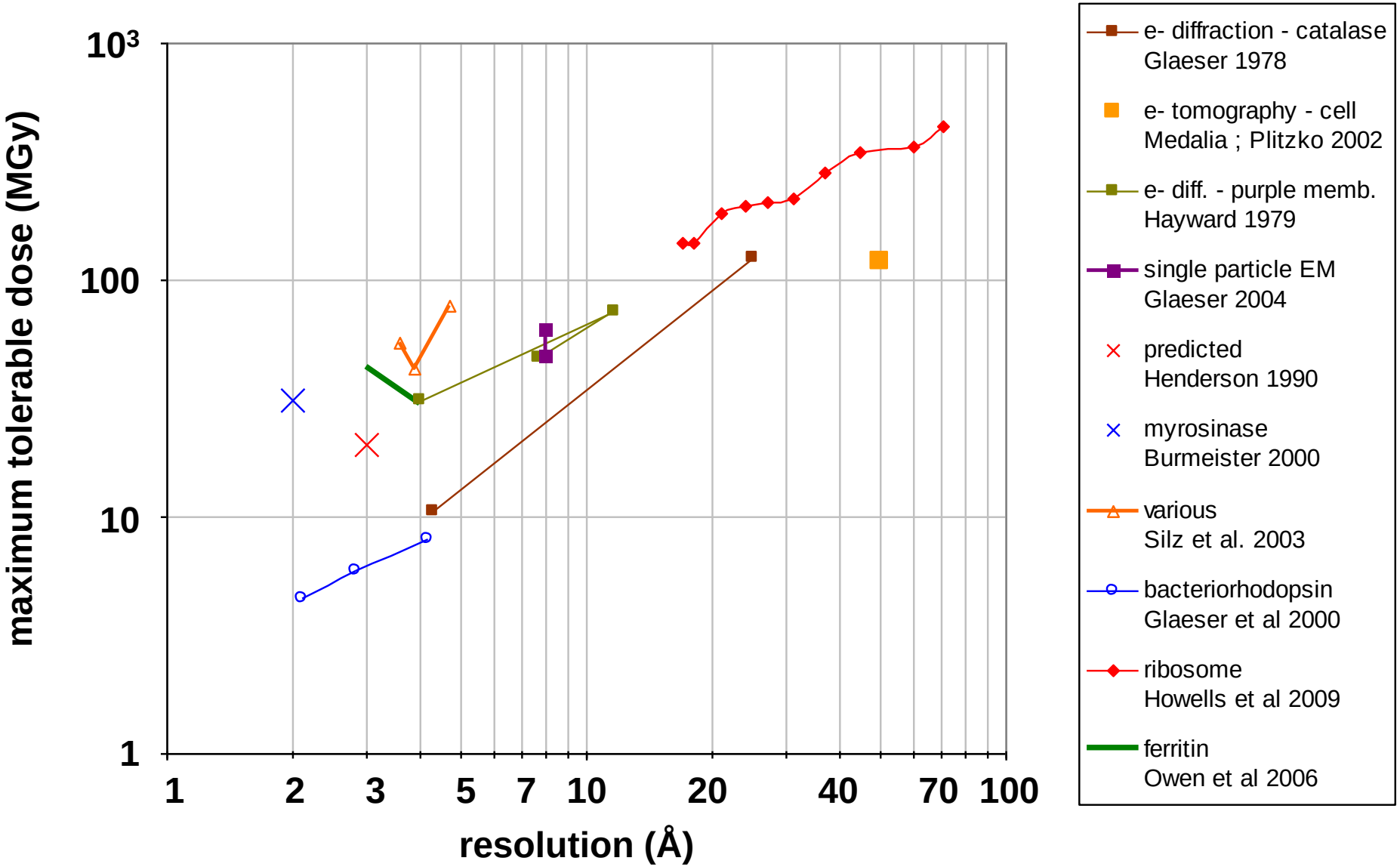
Z_a	- atomic number
$f_a(s)$	- atomic structure amplitude (electrons)
s	- scattering length ($\sin(\theta)/\lambda$)

Radiation Damage Model

$$\mathbf{dose = I_{beam}\ t\ E\ (1-\exp(-\mu_{xtal} T_{xtal}))\ /\ \rho}$$

dose	- absorbed dose (Gy)
$\mathbf{I_{beam}}$	- incident (photons/s/m^2)
E	- photon energy (J/photon)
t	- exposure time (s)
$\boldsymbol{\mu_{xtal}}$	- absorption coefficient (in 1/m)
$\mathbf{T_{xtal}}$	- thickness of crystal (in m)
ρ	- crystal density (kg/m^3)

Howells *et al.* (2009)
J. Electron. Spectrosc. Relat. Phenom. **170** 4-12



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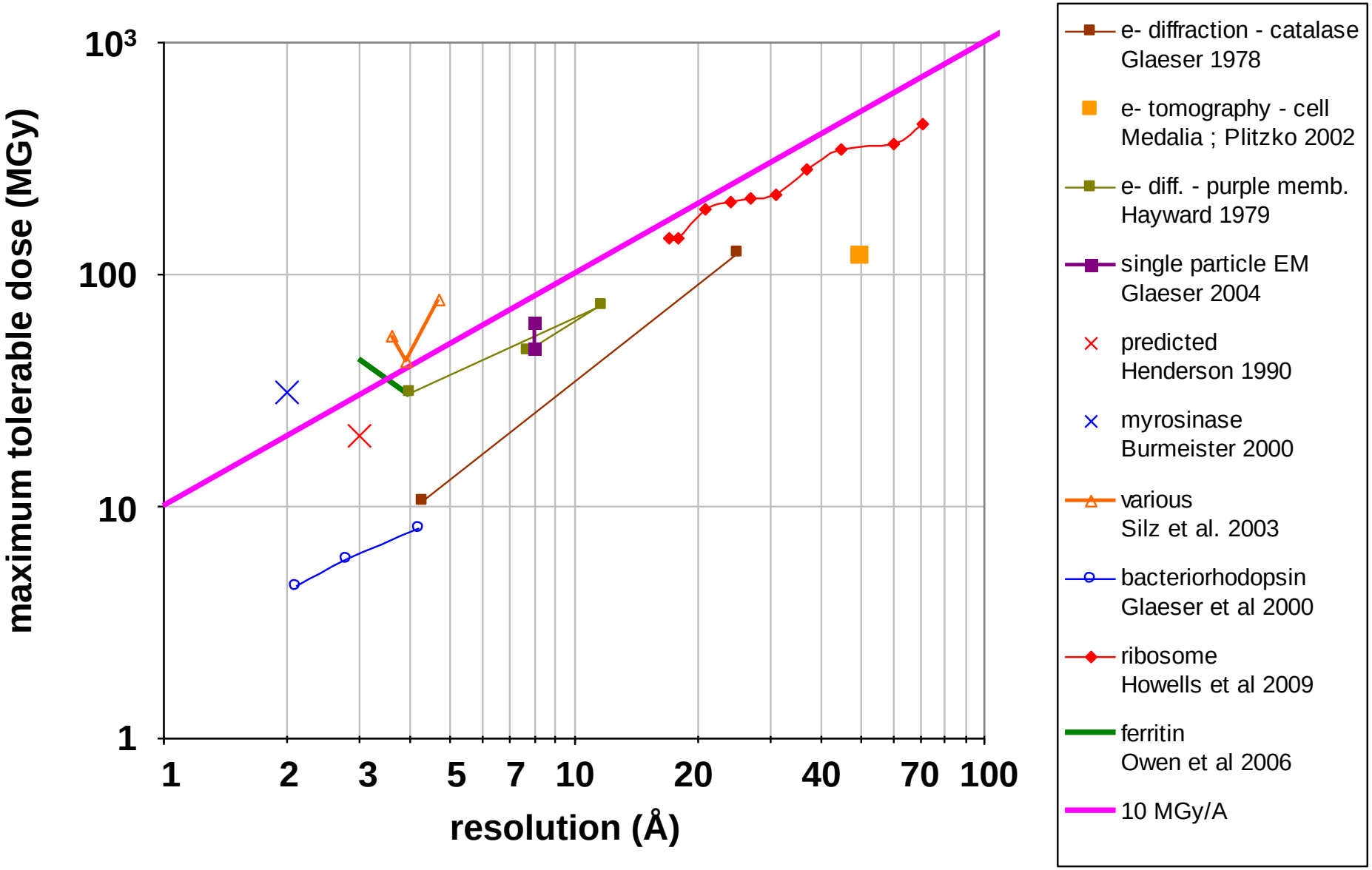


Radiation Damage Model

global (lattice) damage

$$|F_{used}| = |F_{undam}| \exp\left(-\ln(2) \frac{dose}{d \cdot H}\right)$$

F_{used}	- structure factor used for spot
F_{undam}	- structure factor of undamaged crystal
dose	- absorbed dose (MGy)
H	- 10 MGy/Å
d	- resolution of spot (Å)

Radiation Damage Model

global (lattice) damage

$$\mathbf{F = F_0 \exp(- A \cdot s)}$$

F	- structure factor used for spot
$\mathbf{F_0}$	- structure factor of undamaged crystal
A	- something Debye said was zero
s	- 0.5/**d**
d	- resolution of spot (Å)

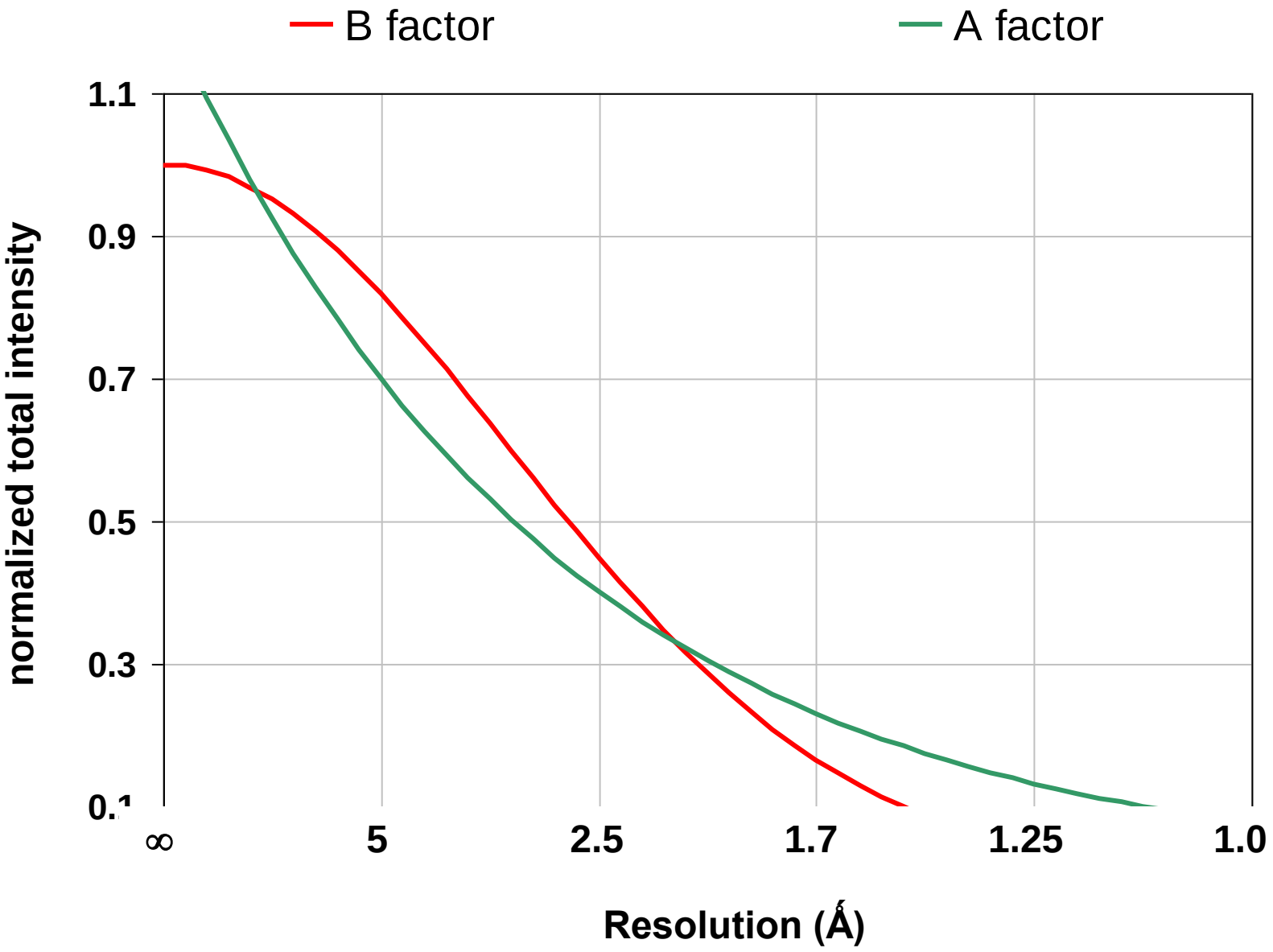
Radiation Damage Model

global (lattice) damage

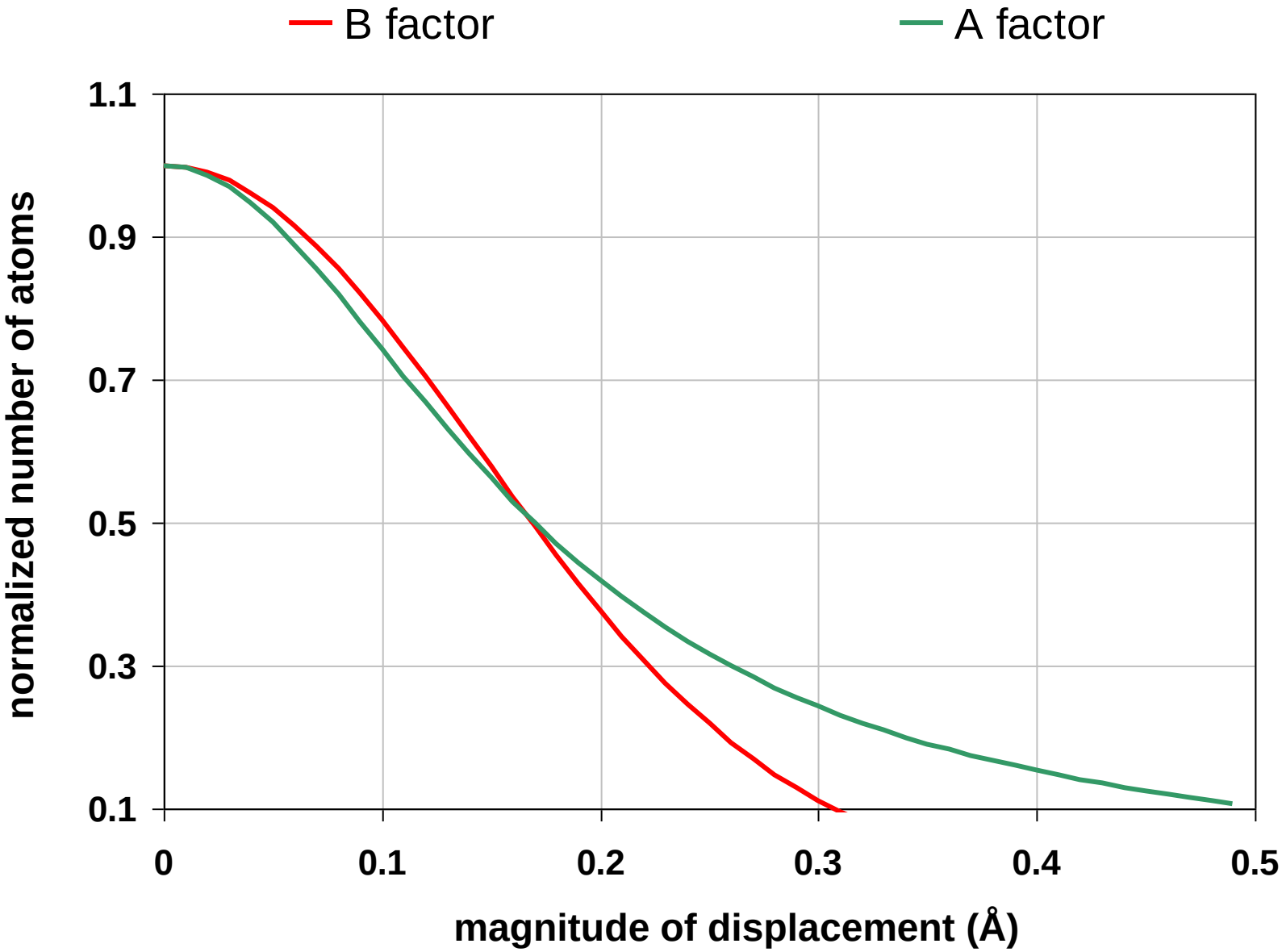
$$\mathbf{F = F_0 \exp(- A \cdot s - B \cdot s^2 - C \cdot s^3 - \ldots)}$$

A	- something Debye said was zero
B	- canonical Debye-Waller factor
C	- something else Debye said was zero
s	- 0.5/**d**
d	- resolution of spot (Å)

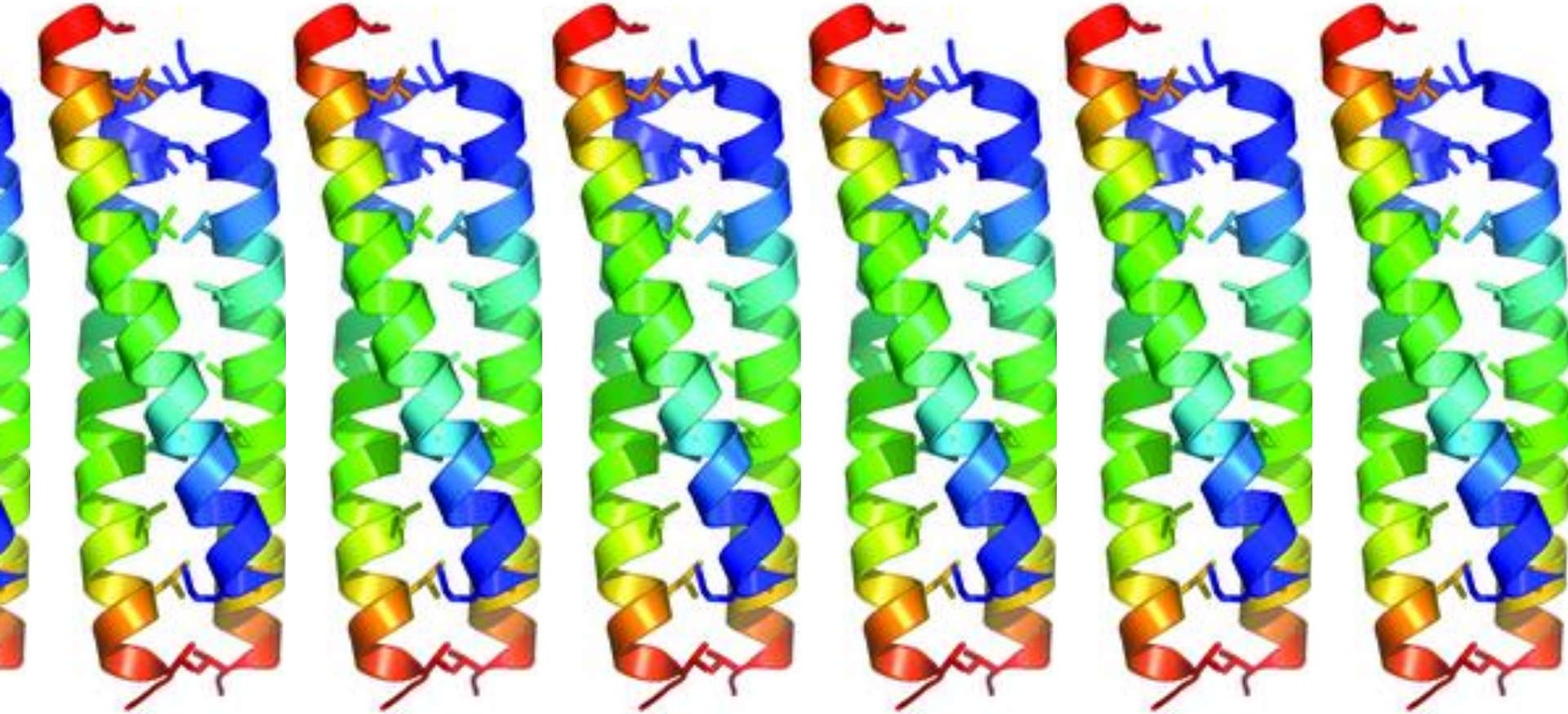
Radiation Damage Model



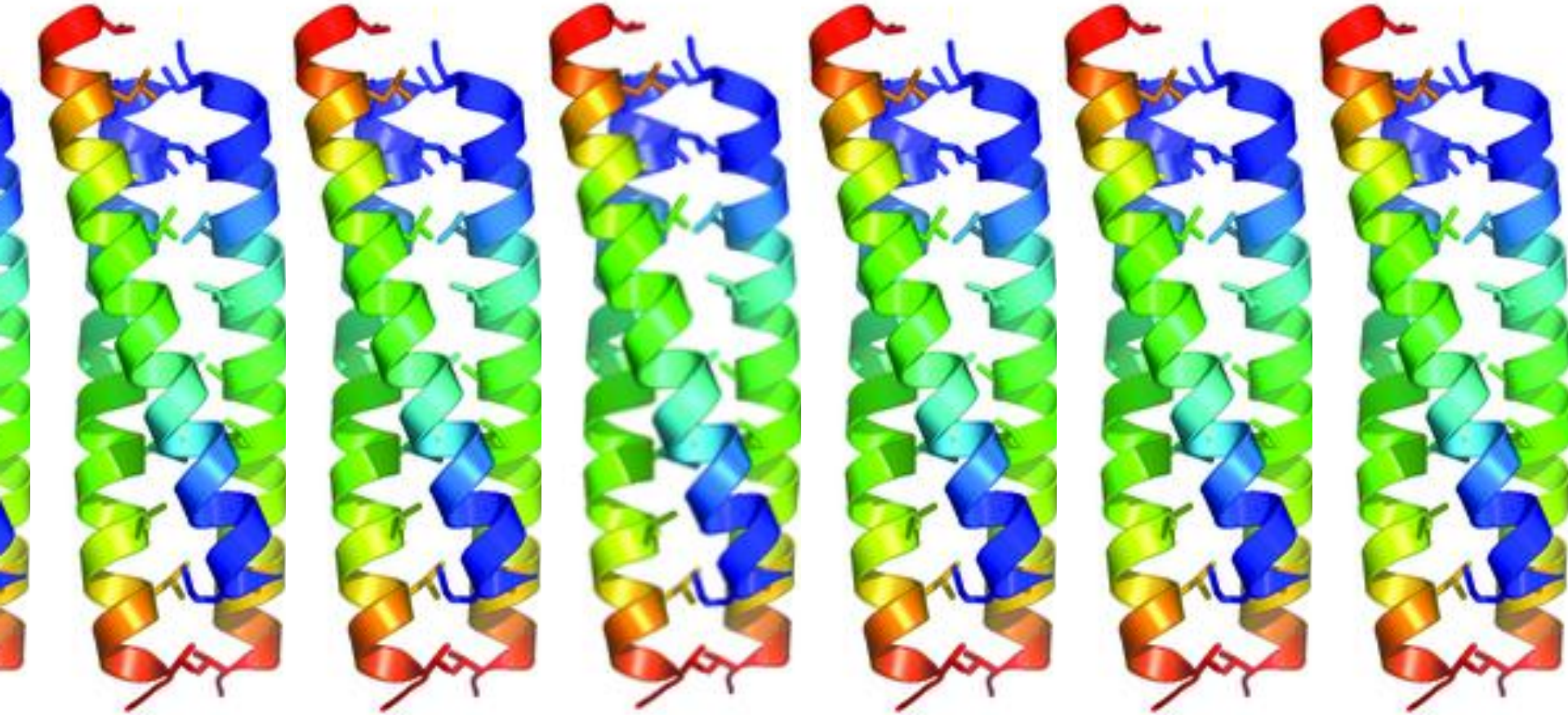
Radiation Damage Model



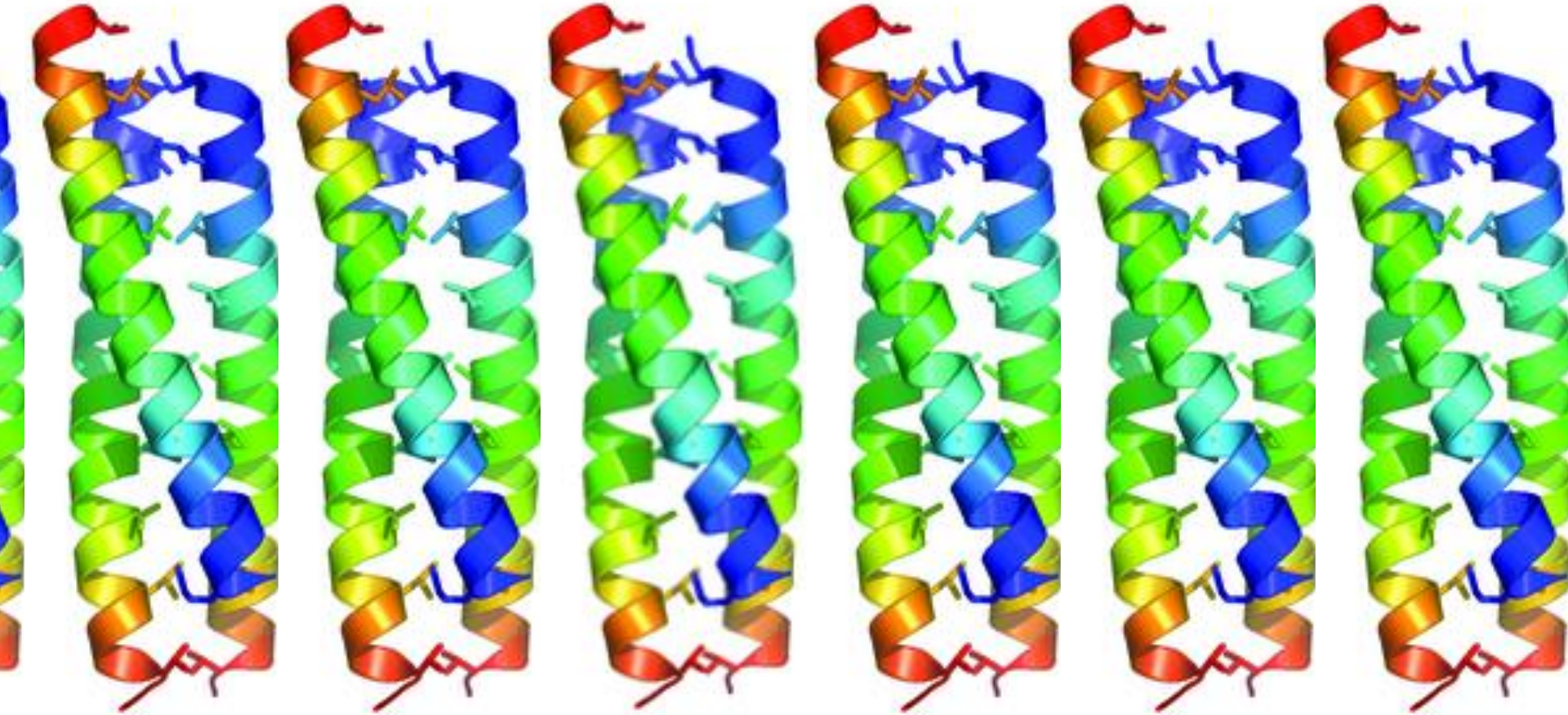
Radiation Damage Model



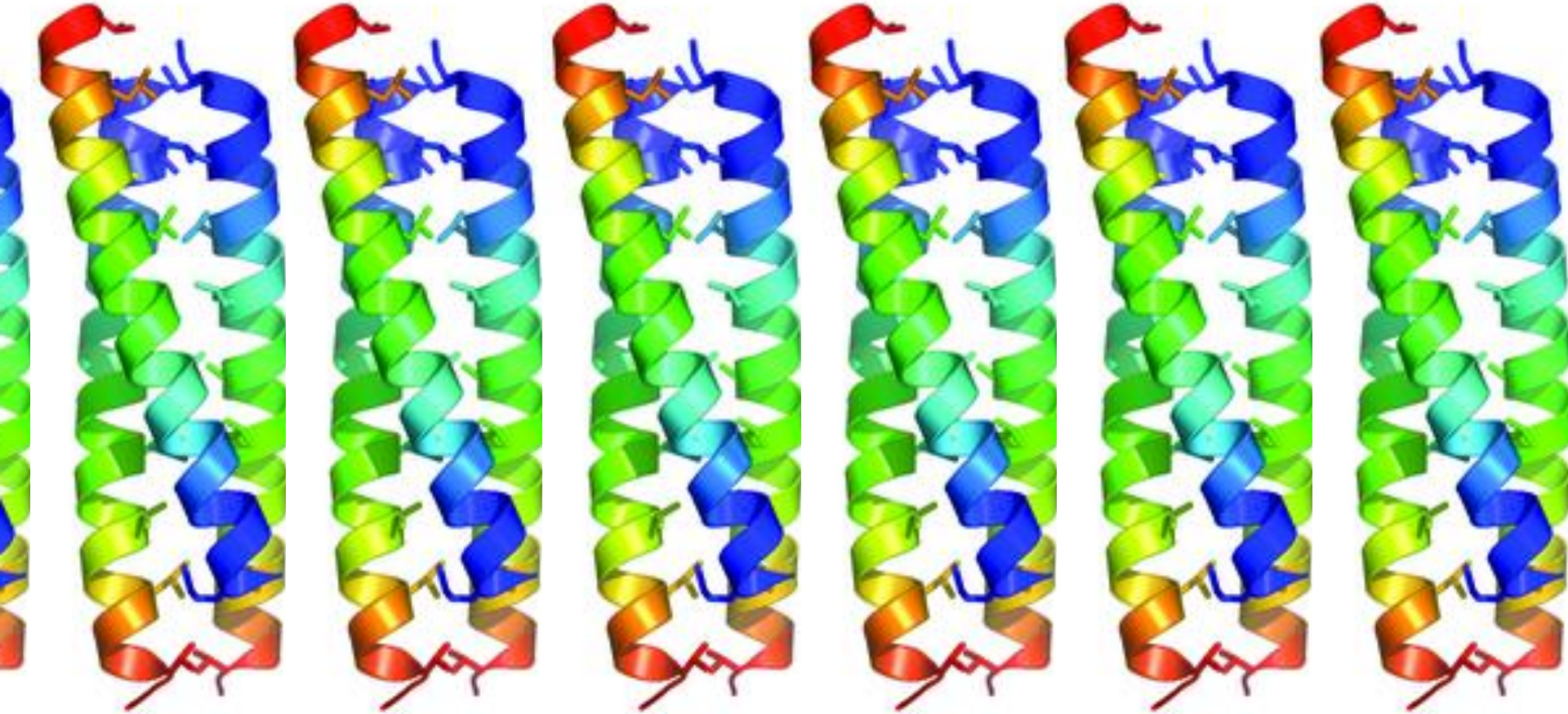
Radiation Damage Model



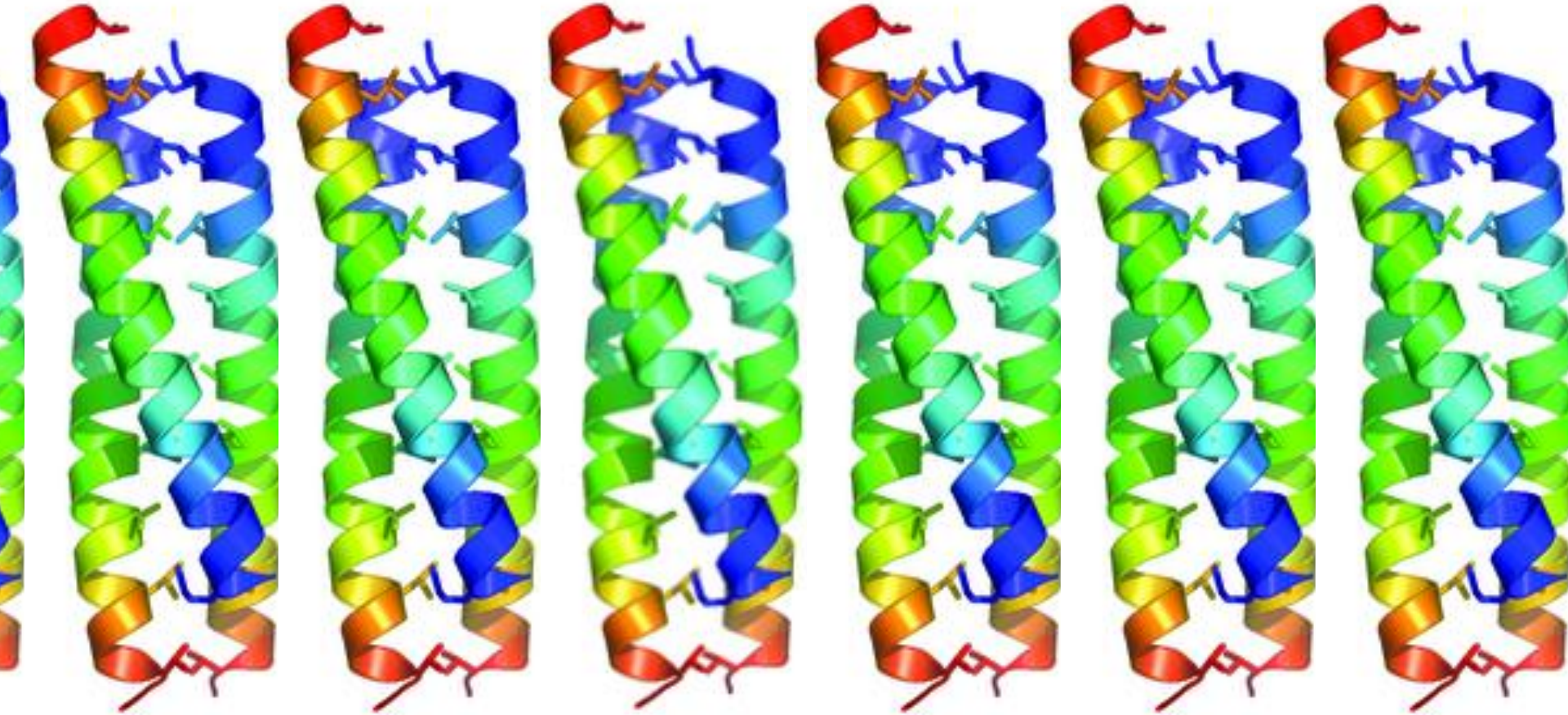
Radiation Damage Model



Radiation Damage Model

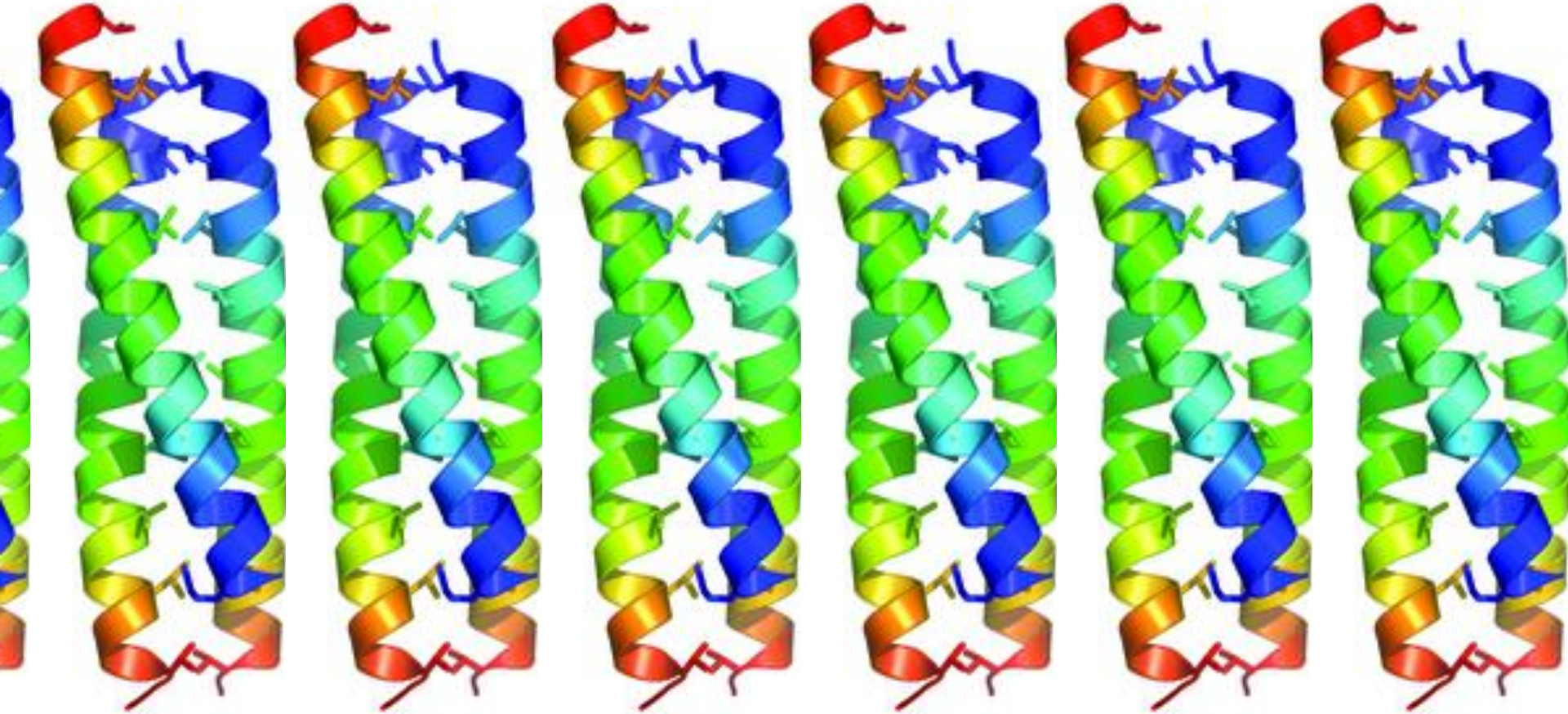


Radiation Damage Model



Kanzaki 1957

Radiation Damage Model



Kanzaki 1957

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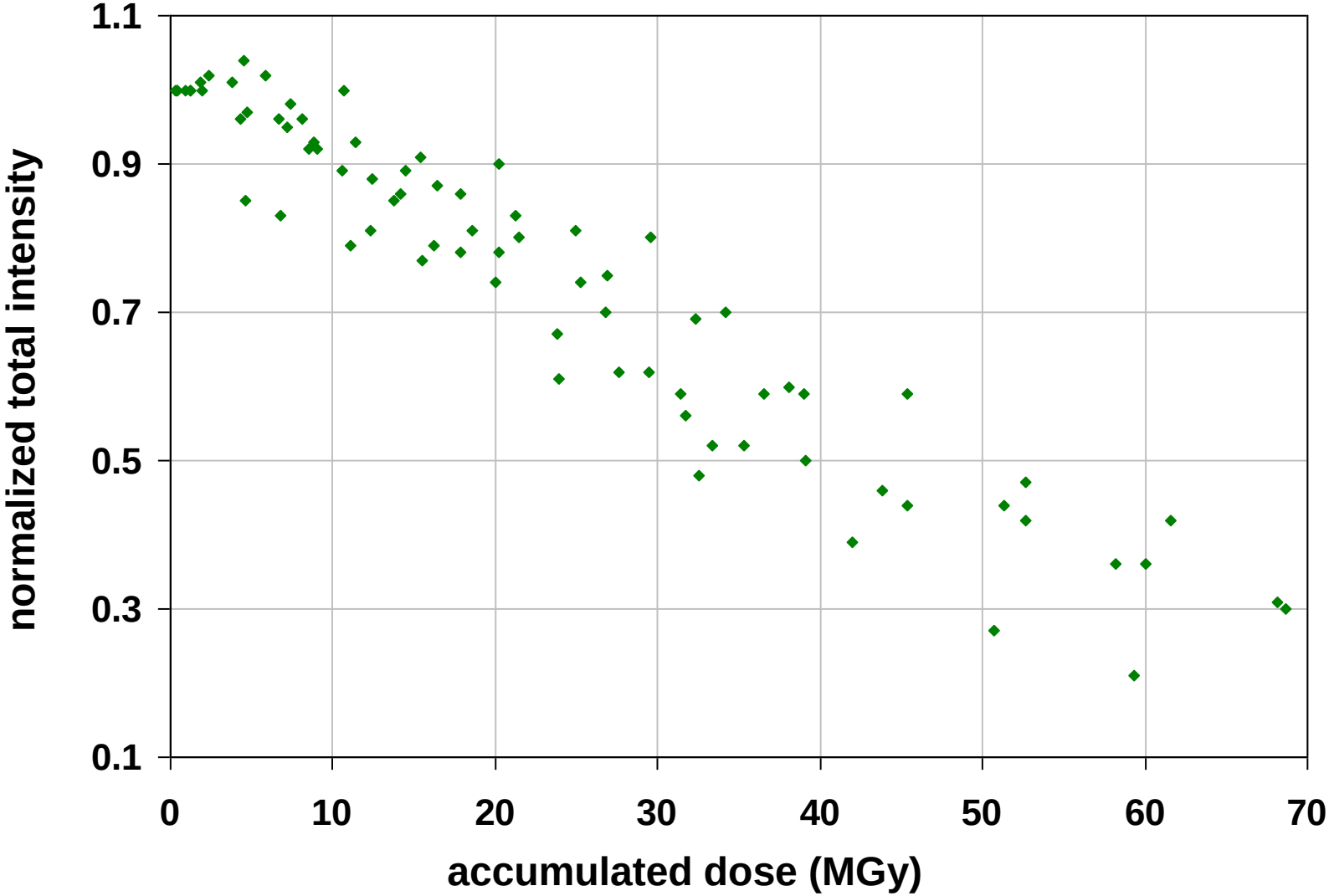
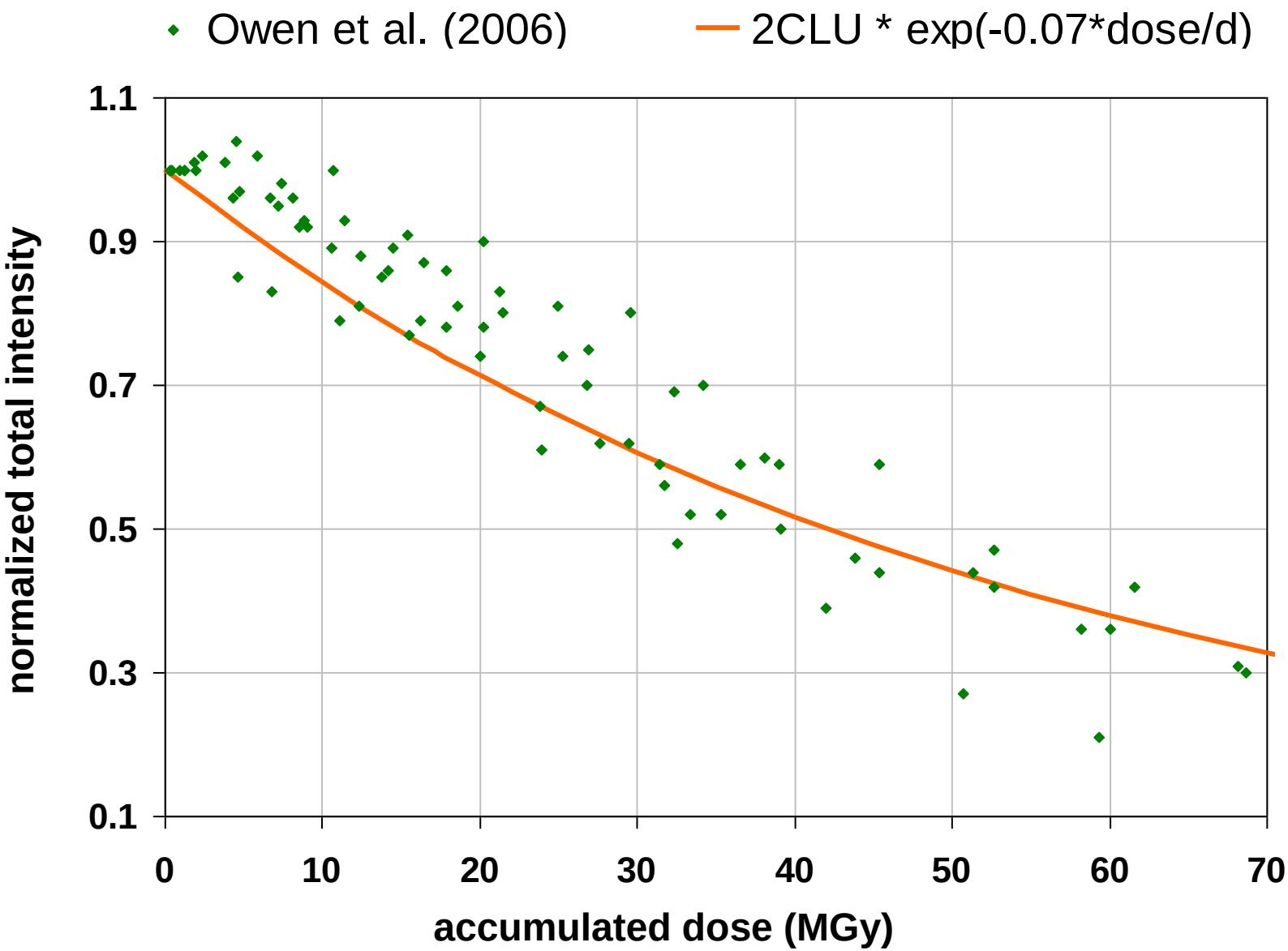
dose	- absorbed dose (MGy)
H	- 10 MGy/Å
d	- resolution of spot (Å)

Radiation Damage Model

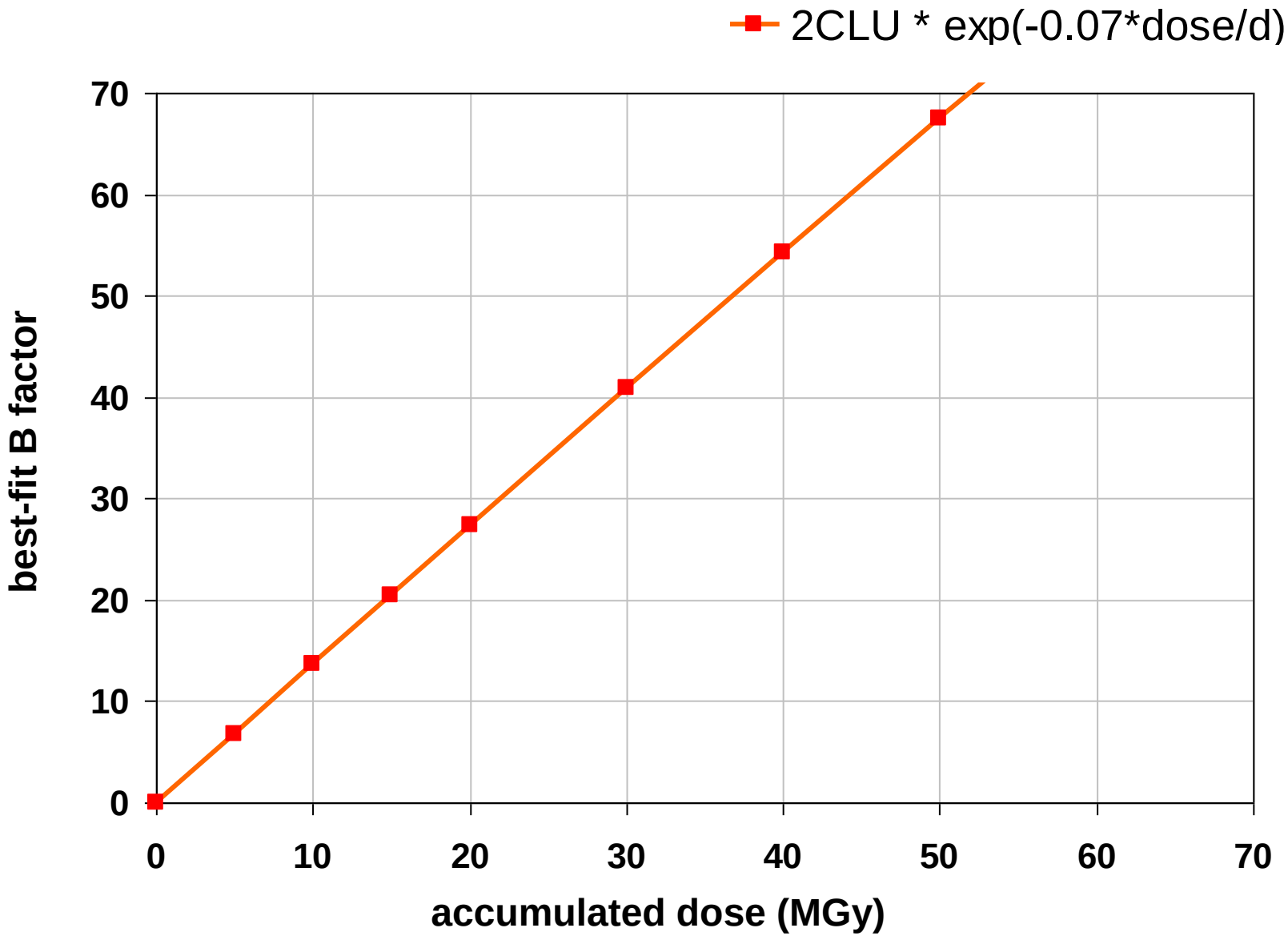
- Owen et al. (2006)



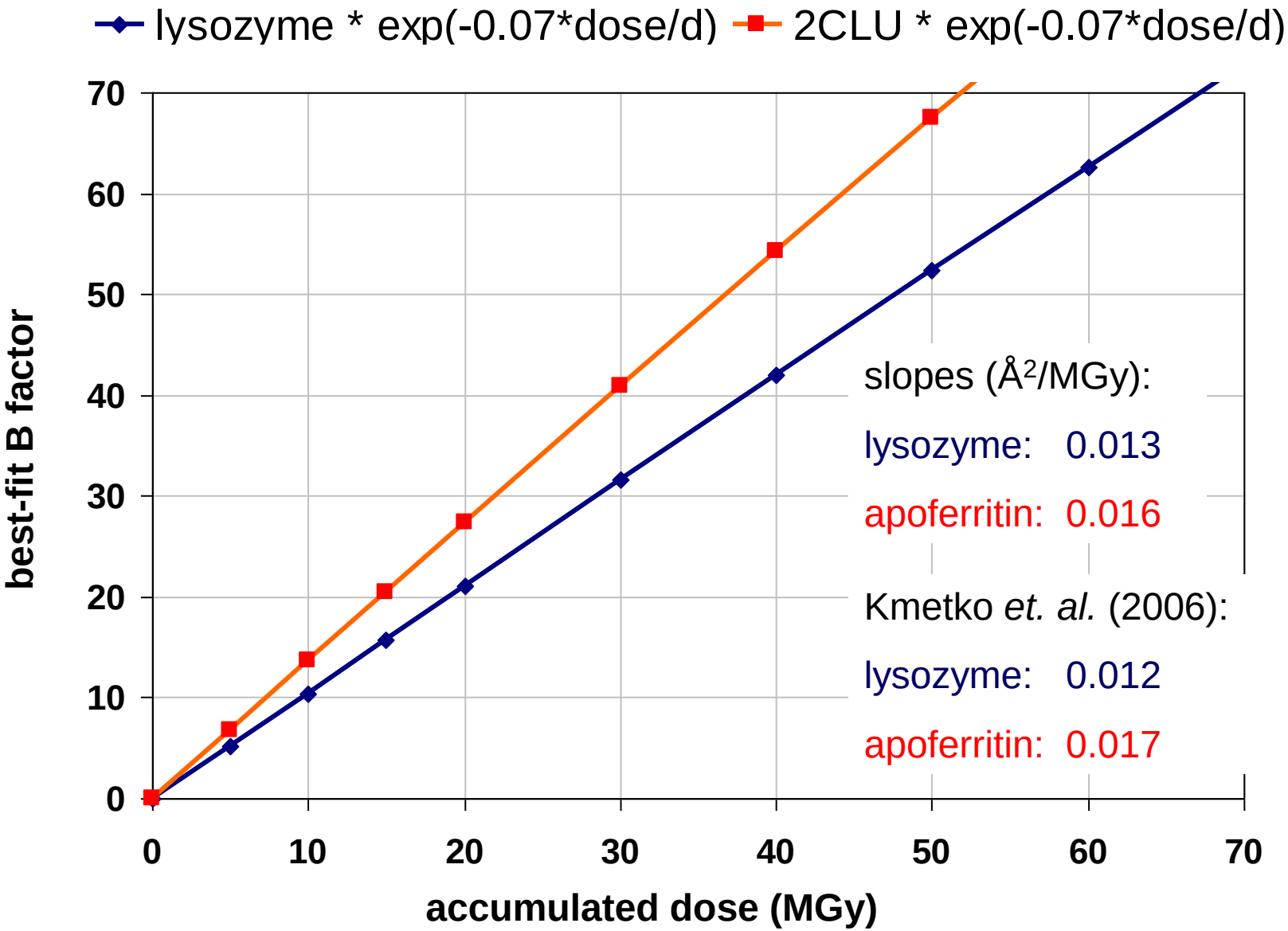
Radiation Damage Model



Radiation Damage Model



Radiation Damage Model

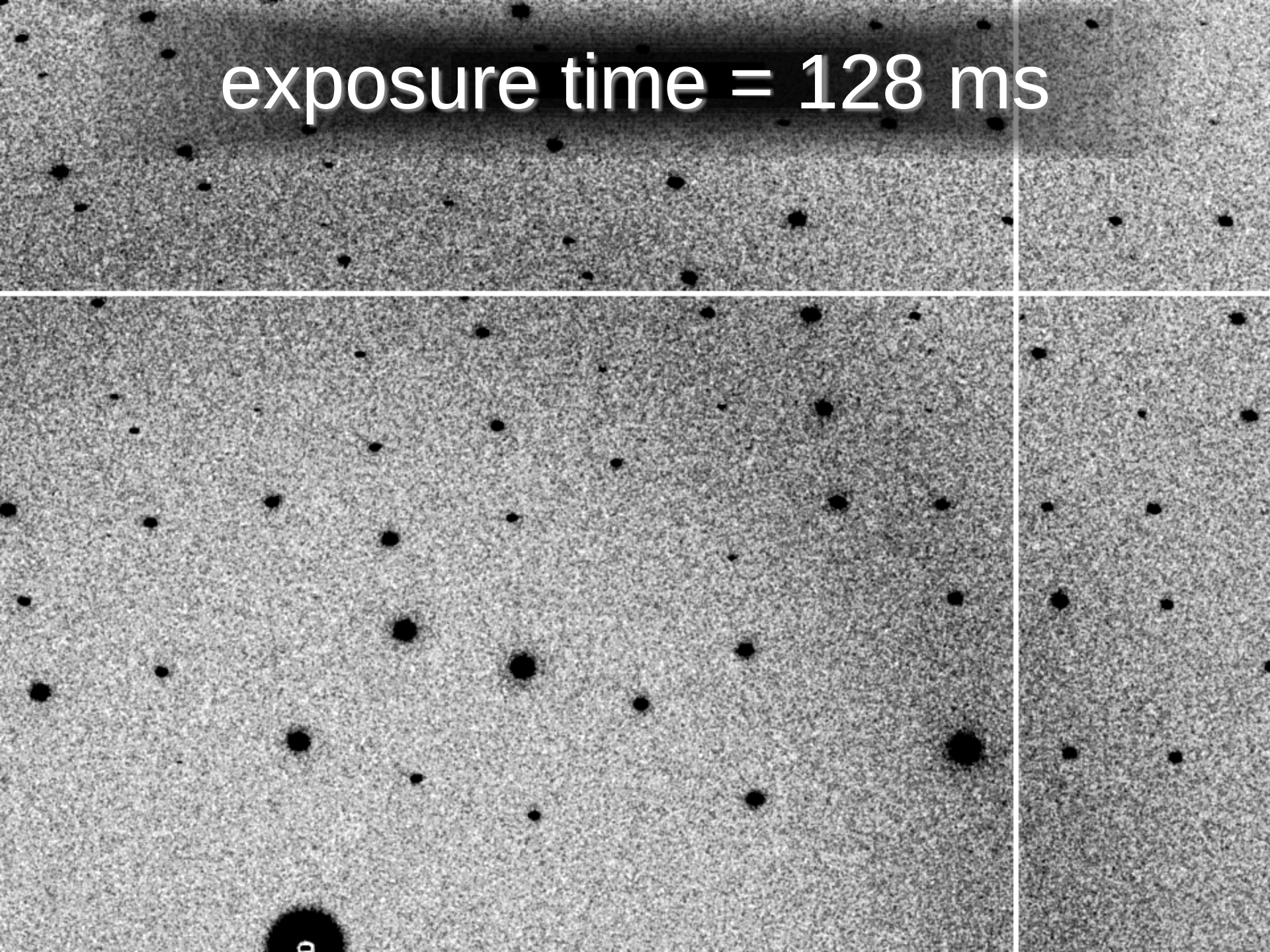


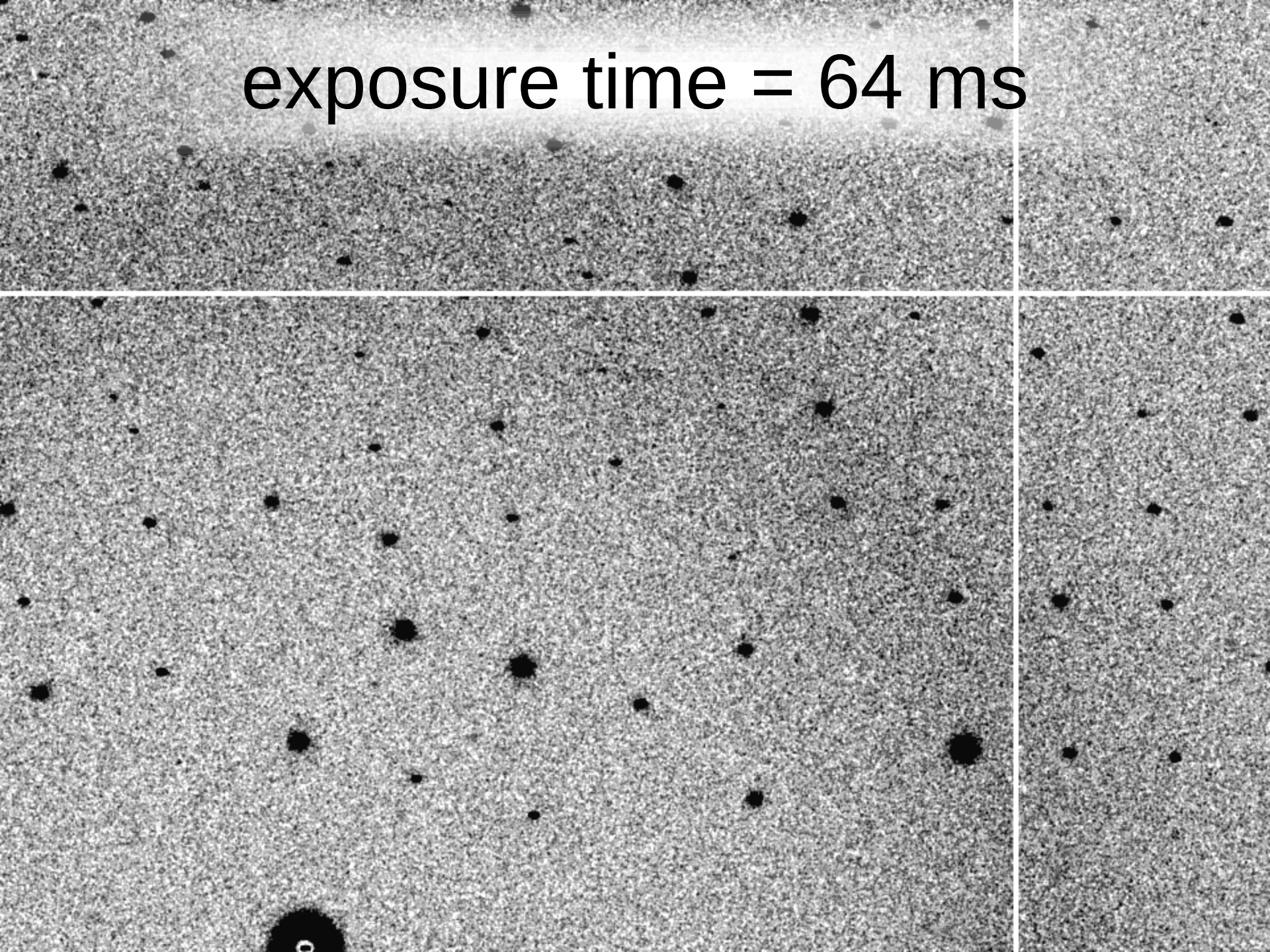
Development Snapshot

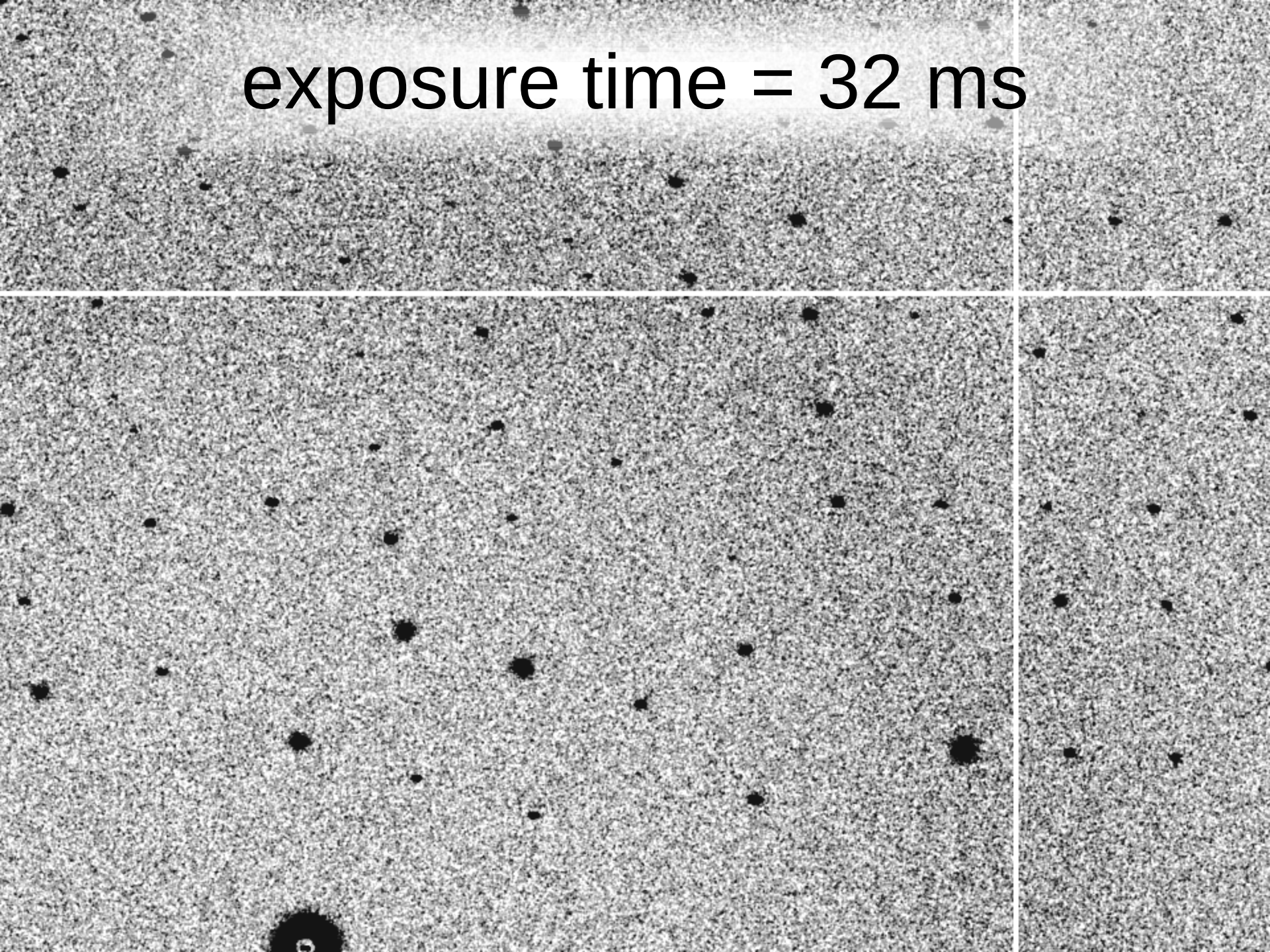
http://bl831.als.lbl.gov/~jamesh/mlfsom/development_snapshot.tar.gz

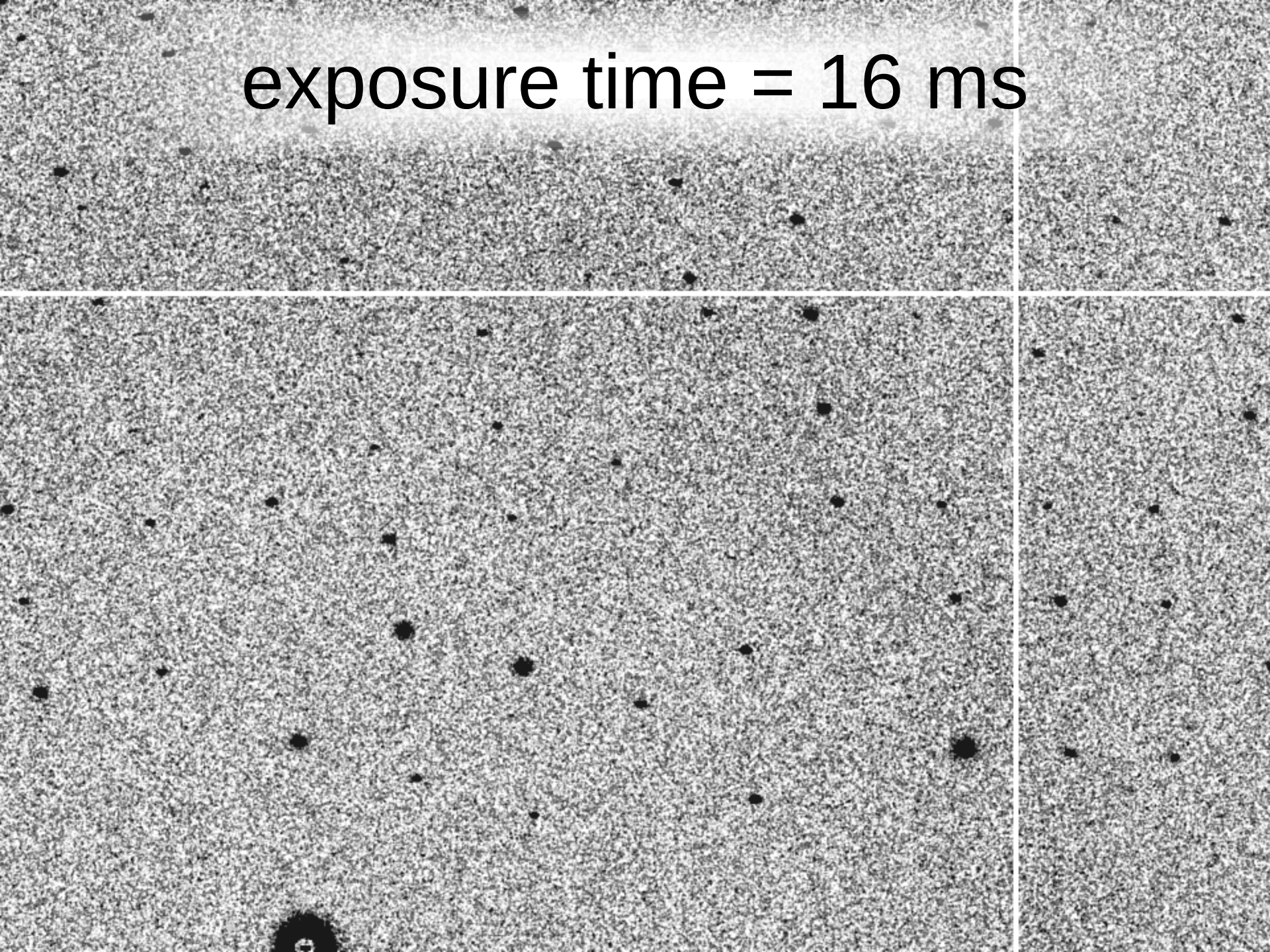
http://bl831.als.lbl.gov/~jamesh/powerpoint/BNL_2009.ppt

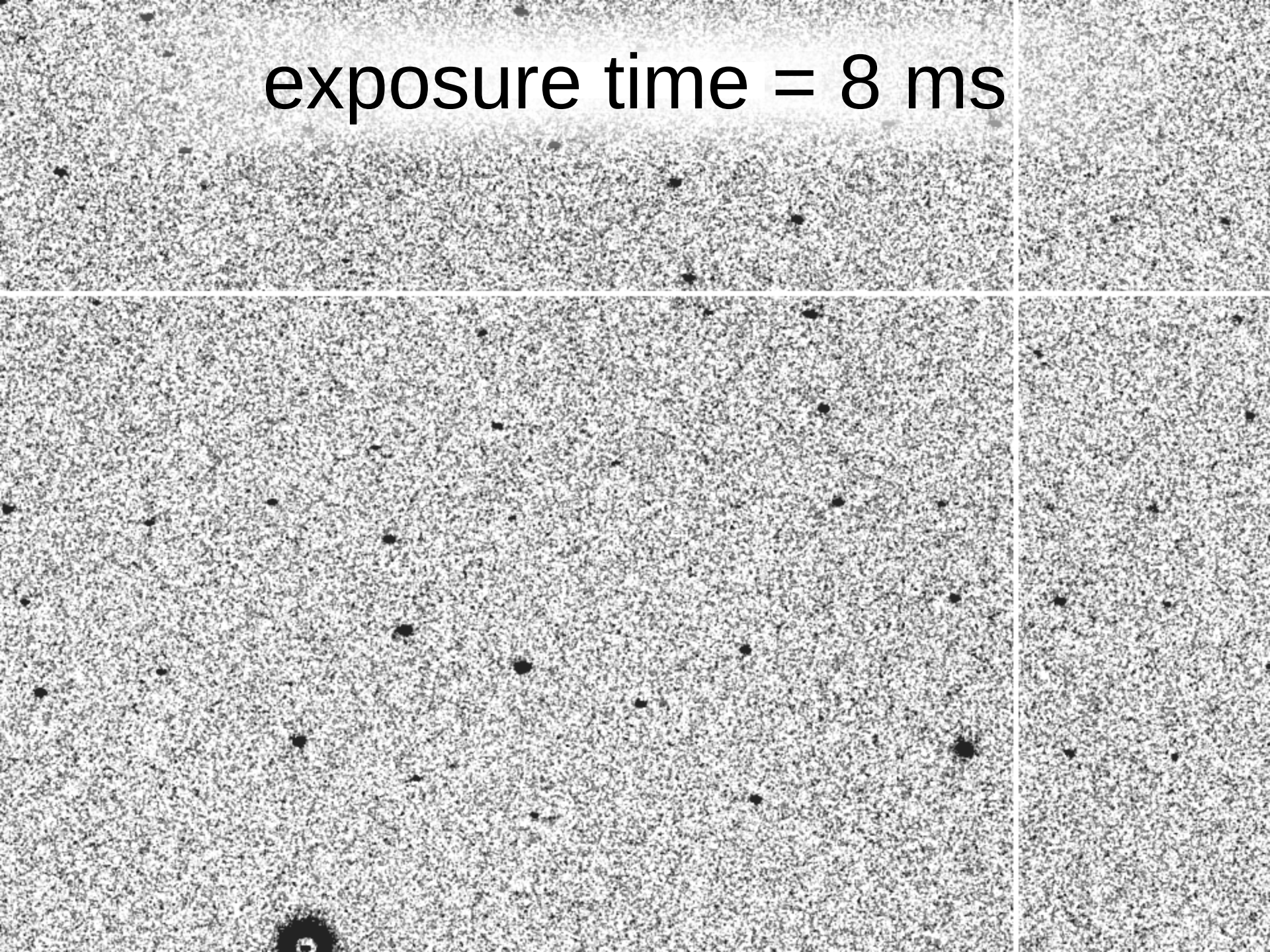
What is the
best exposure time?


exposure time = 128 ms


exposure time = 64 ms


exposure time = 32 ms


exposure time = 16 ms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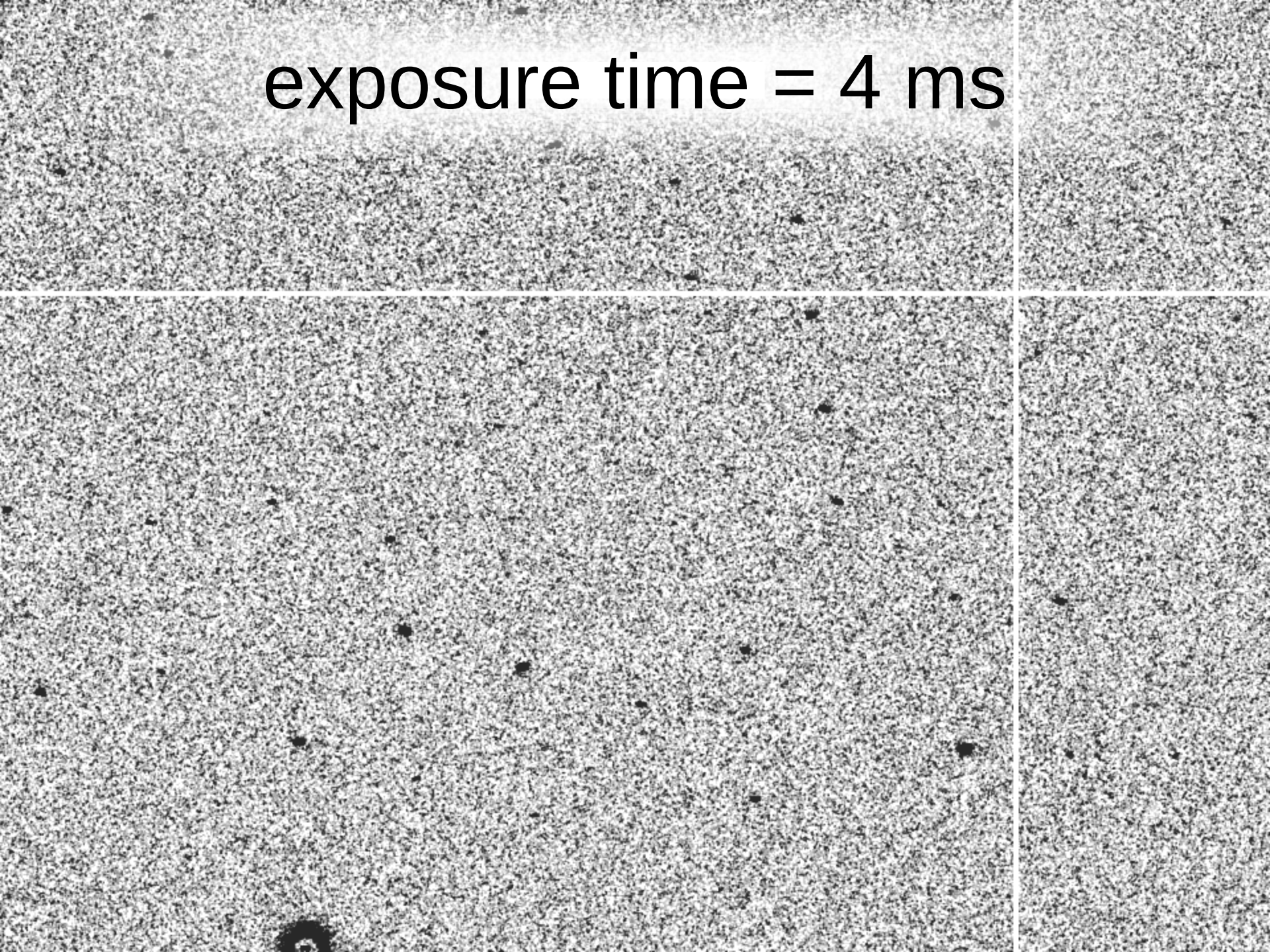
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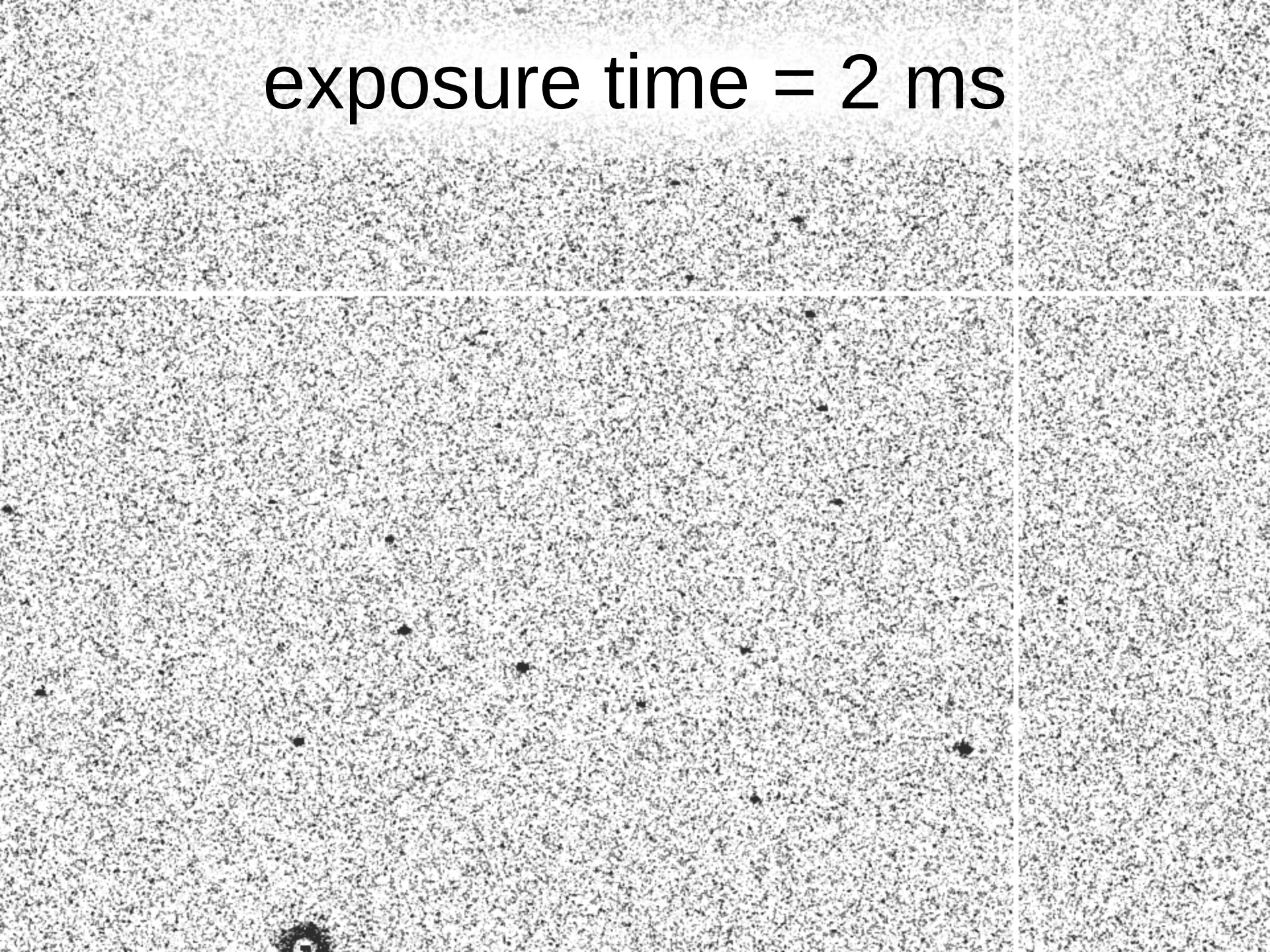
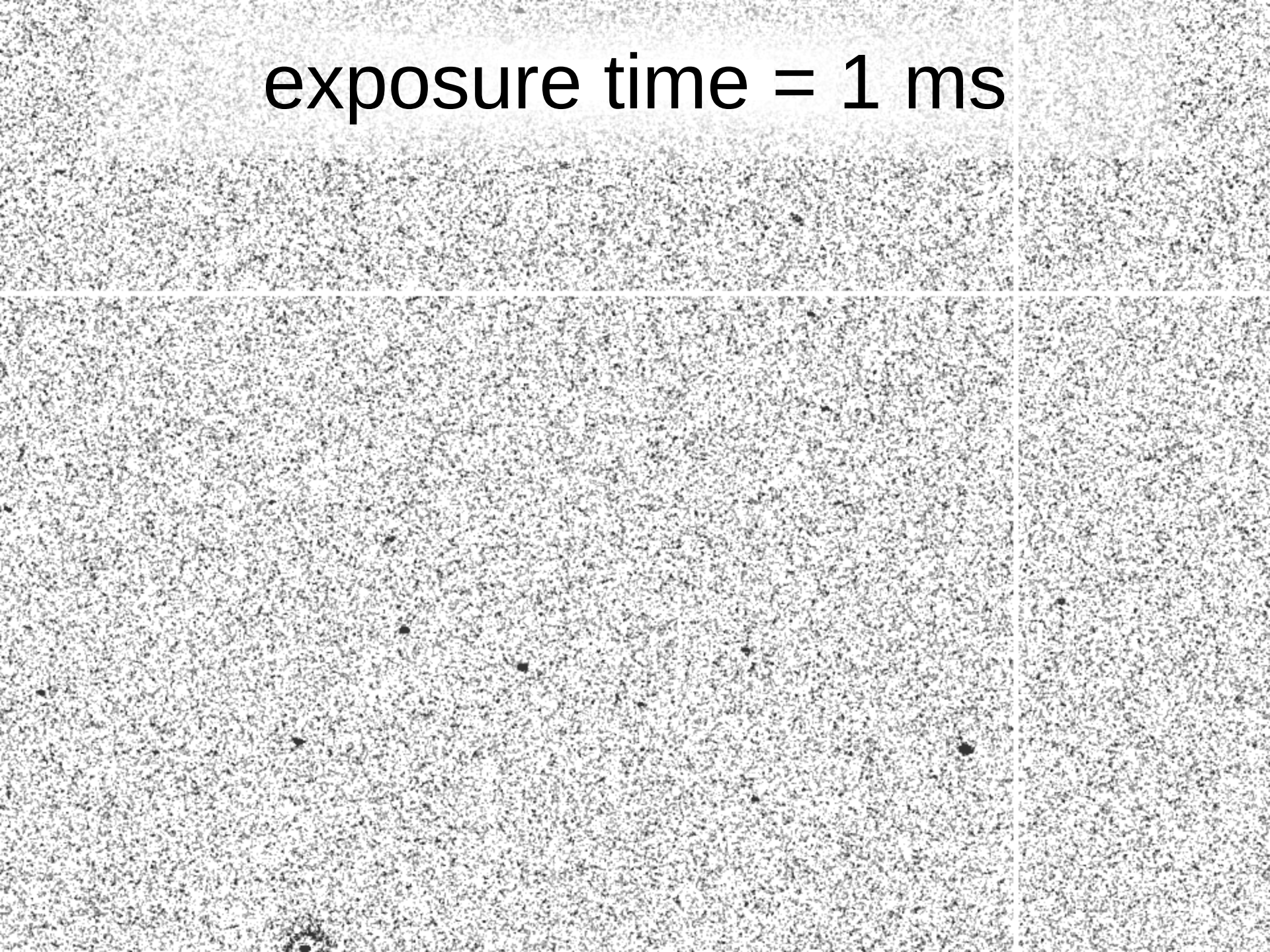
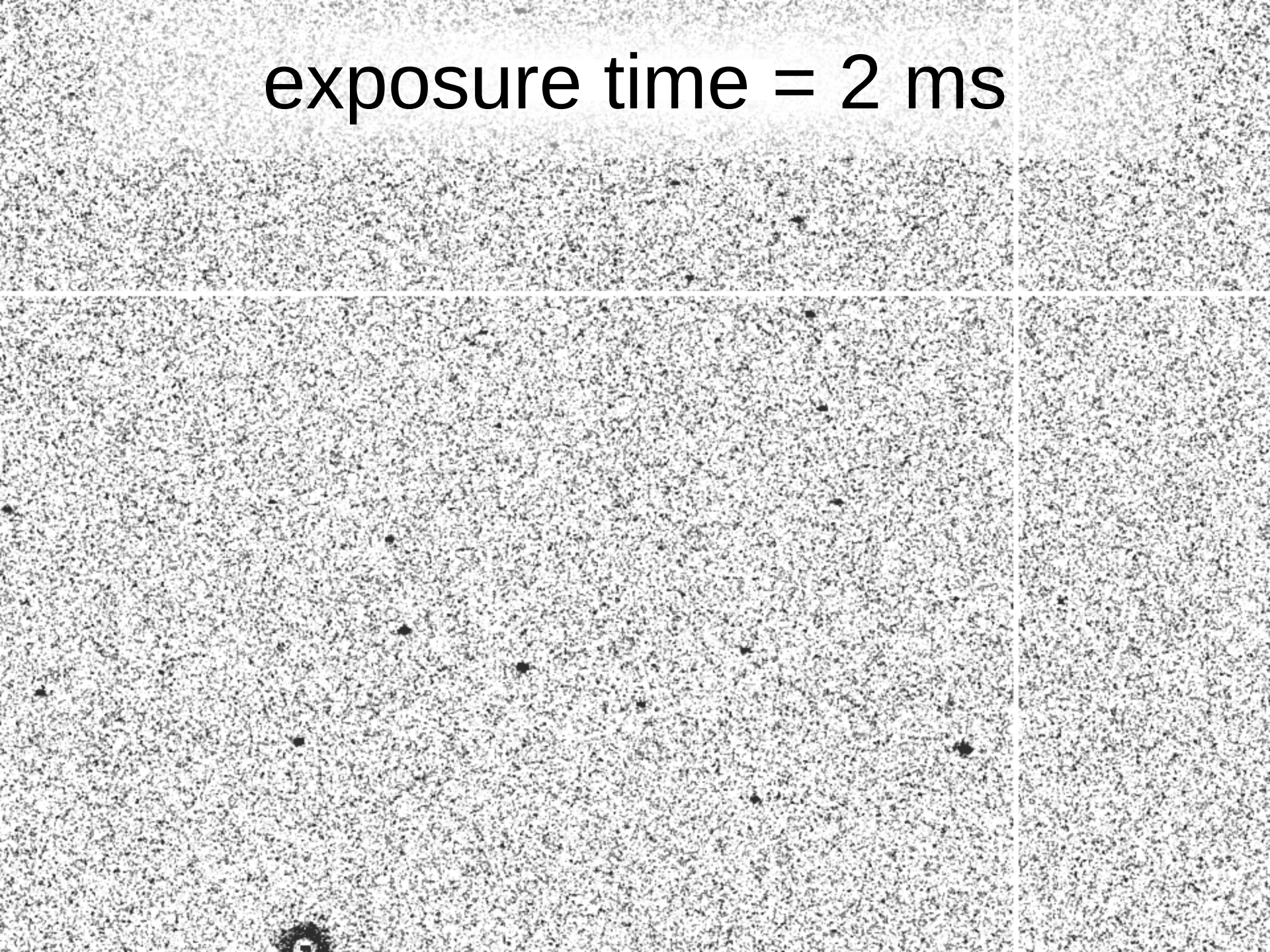
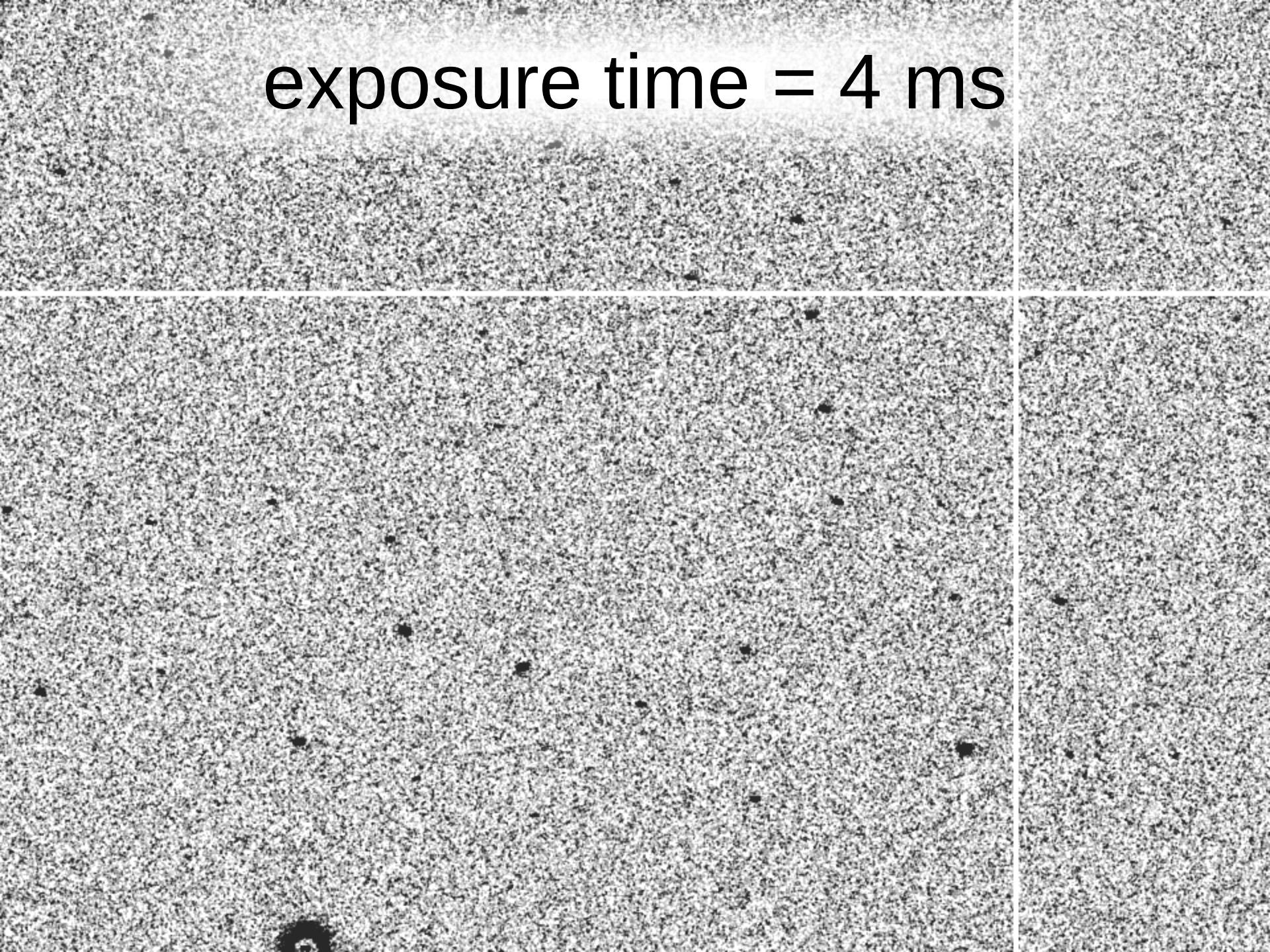

exposure time = 2 ms


exposure time = 1 ms


exposure time = 2 ms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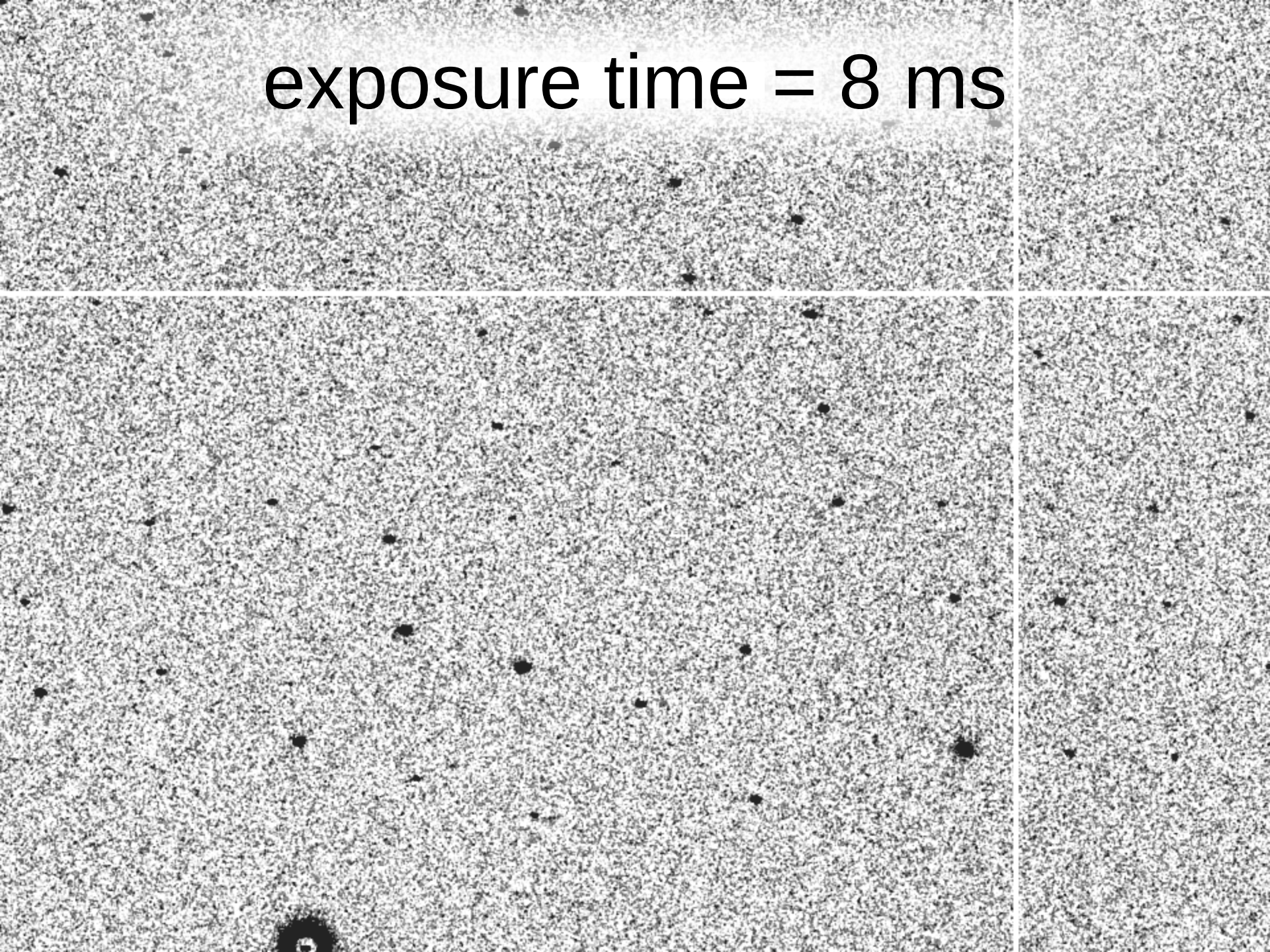
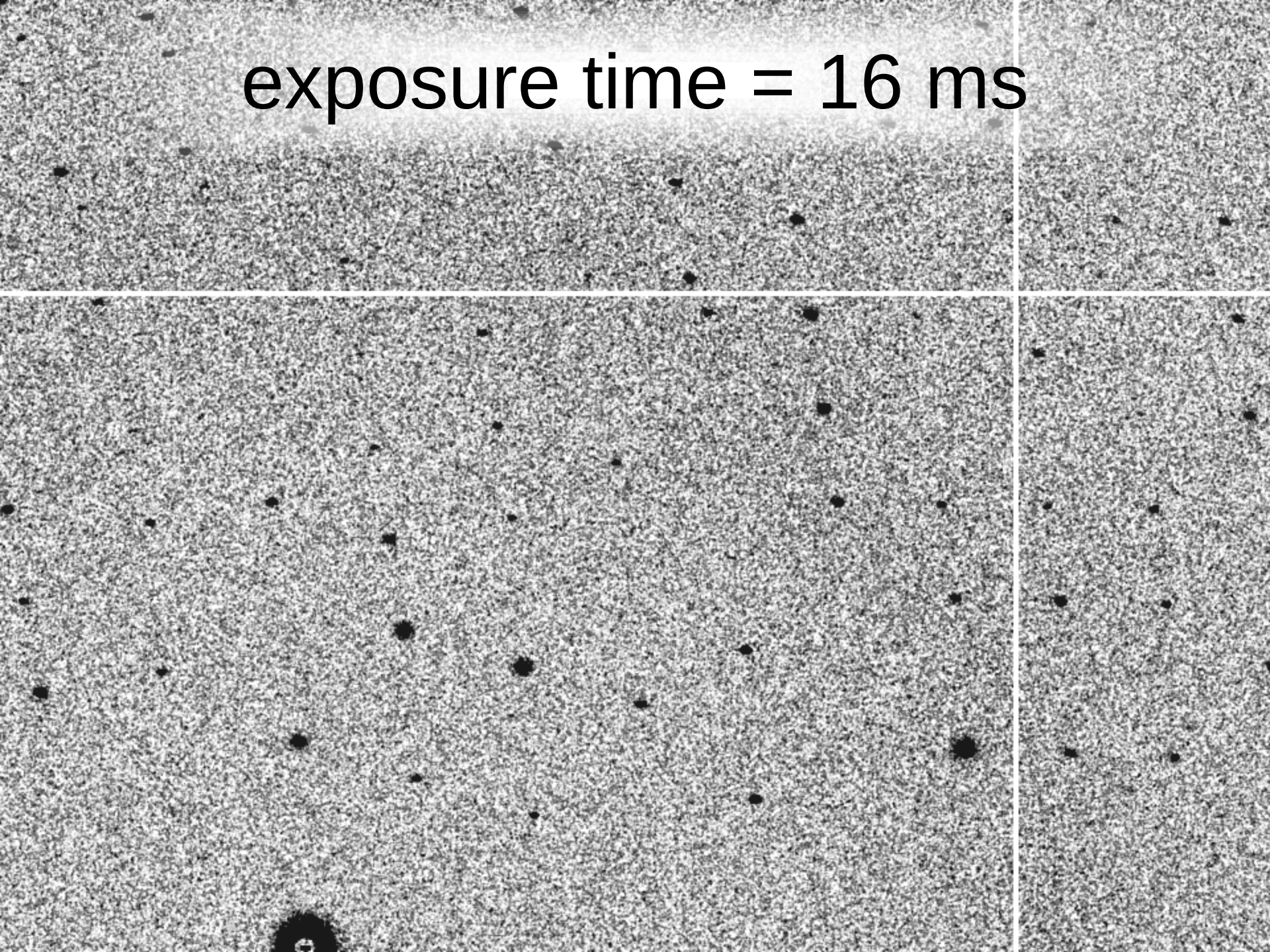
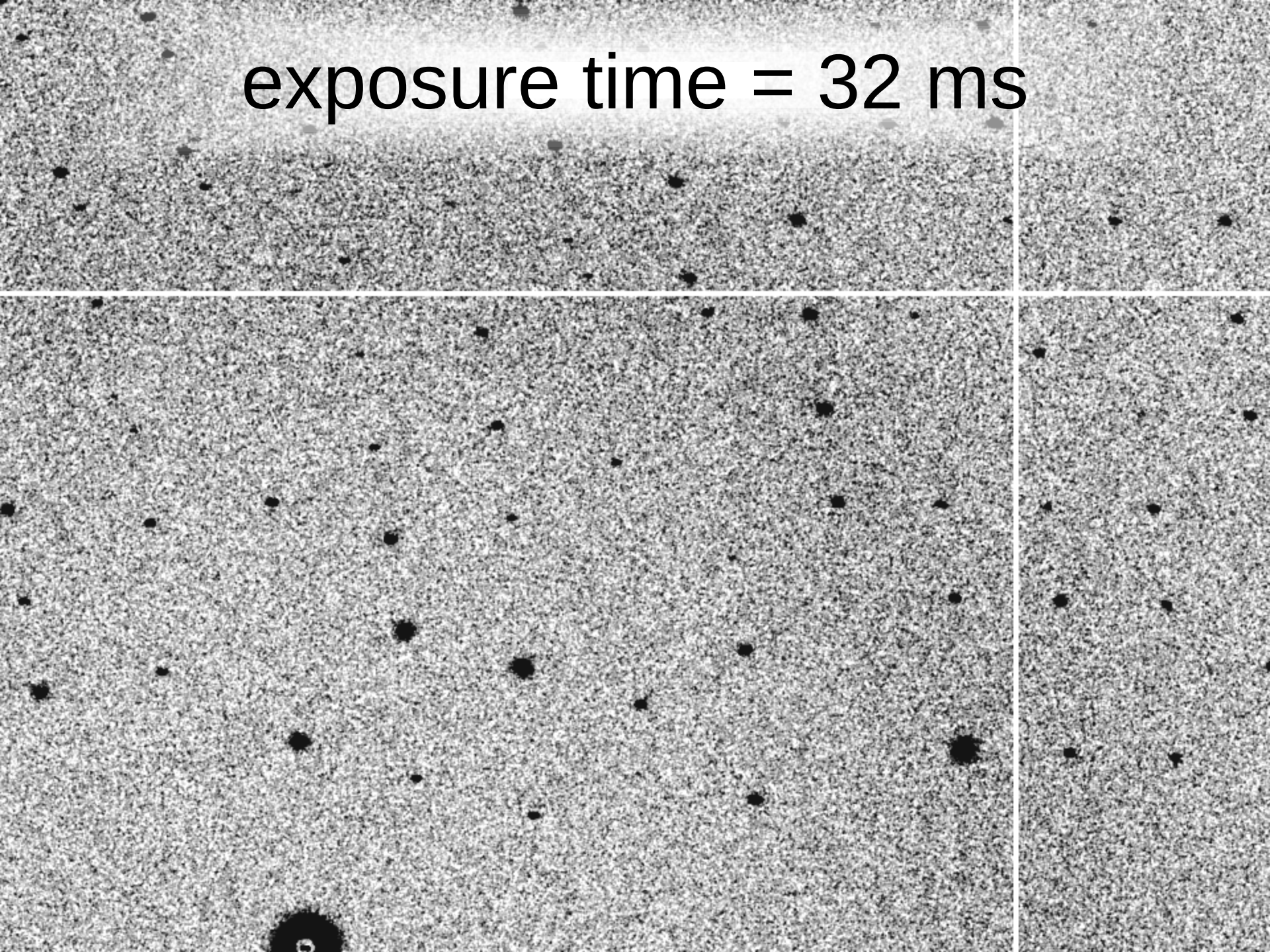
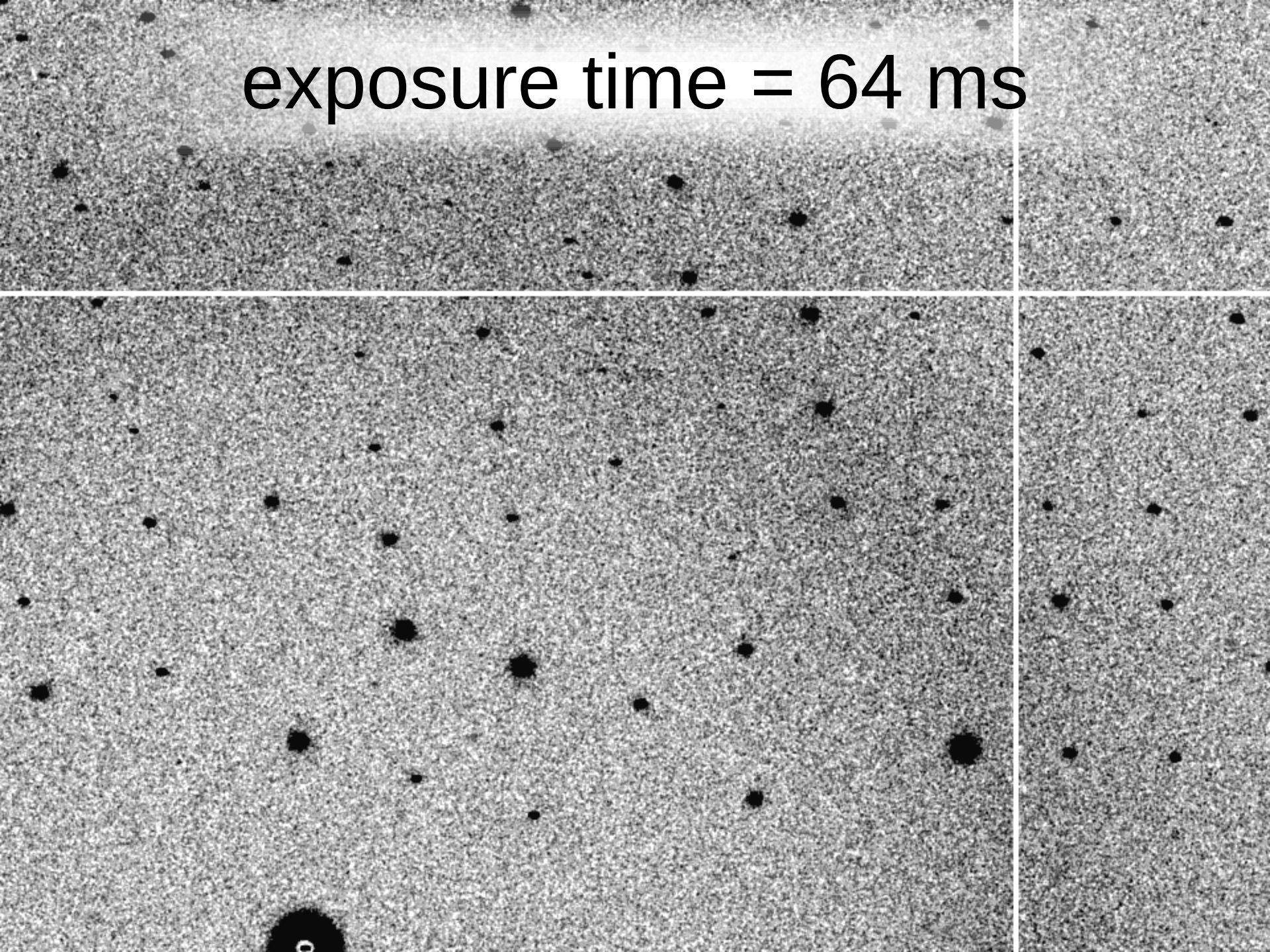
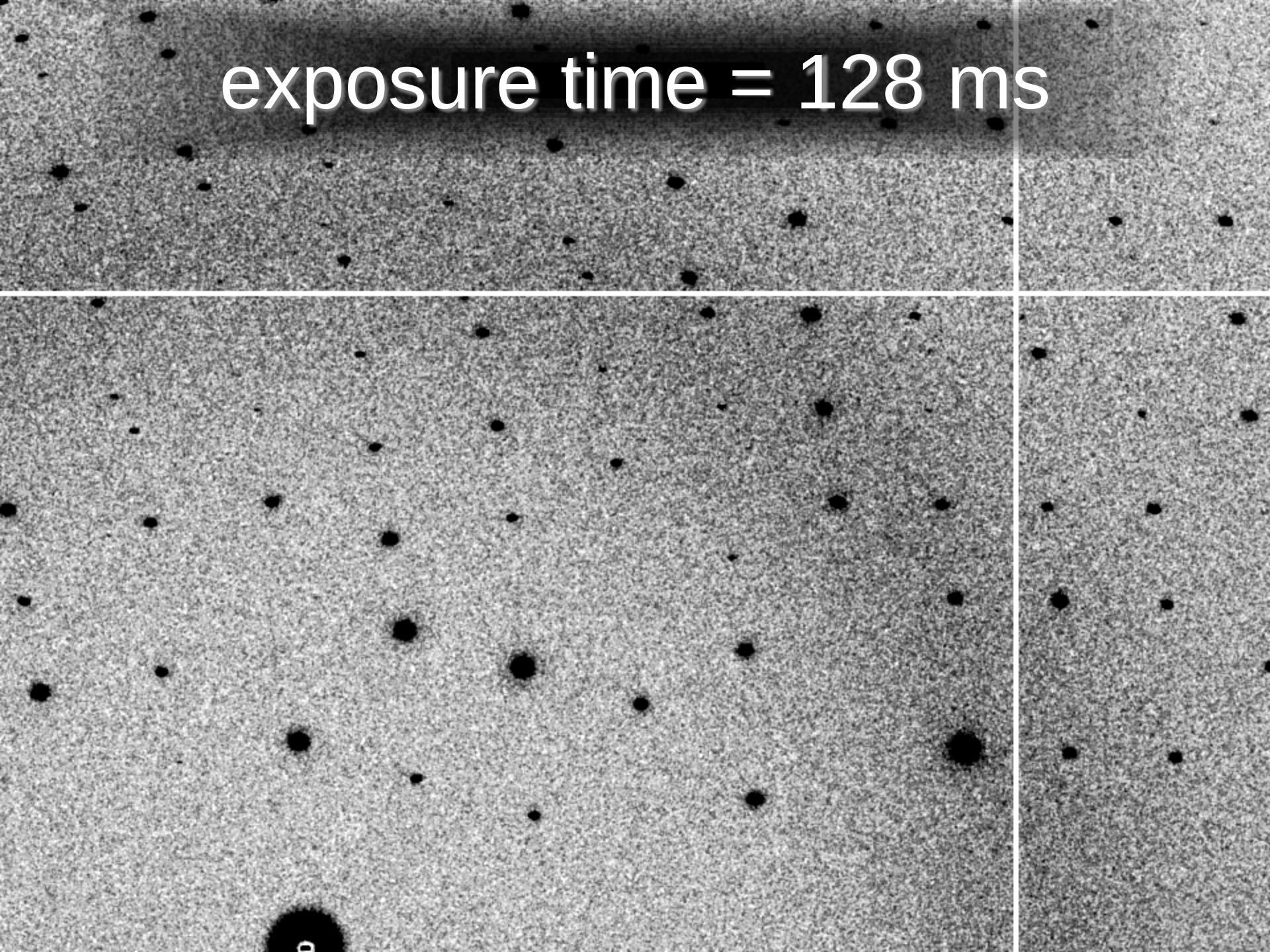
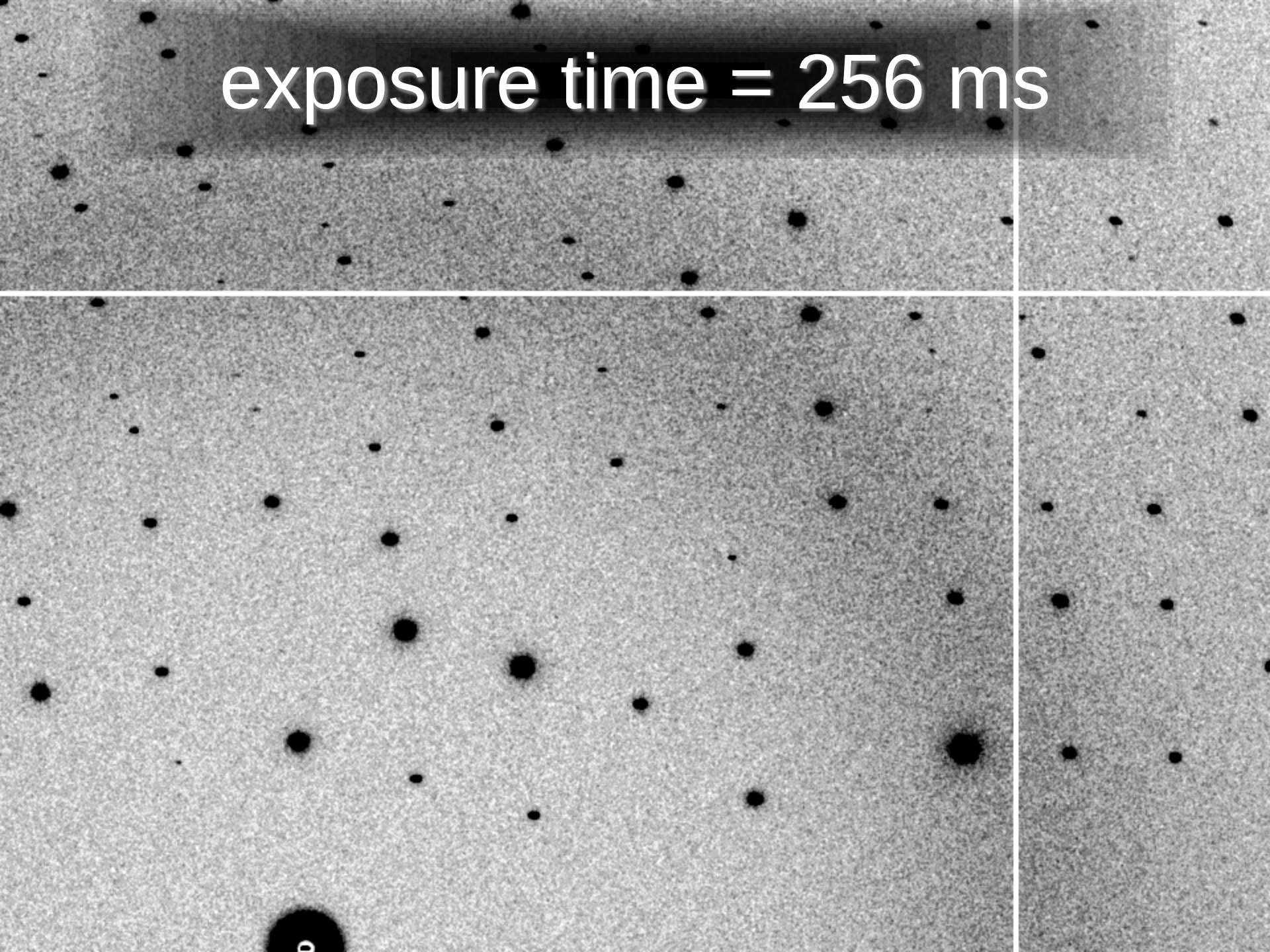

exposure time = 8 ms

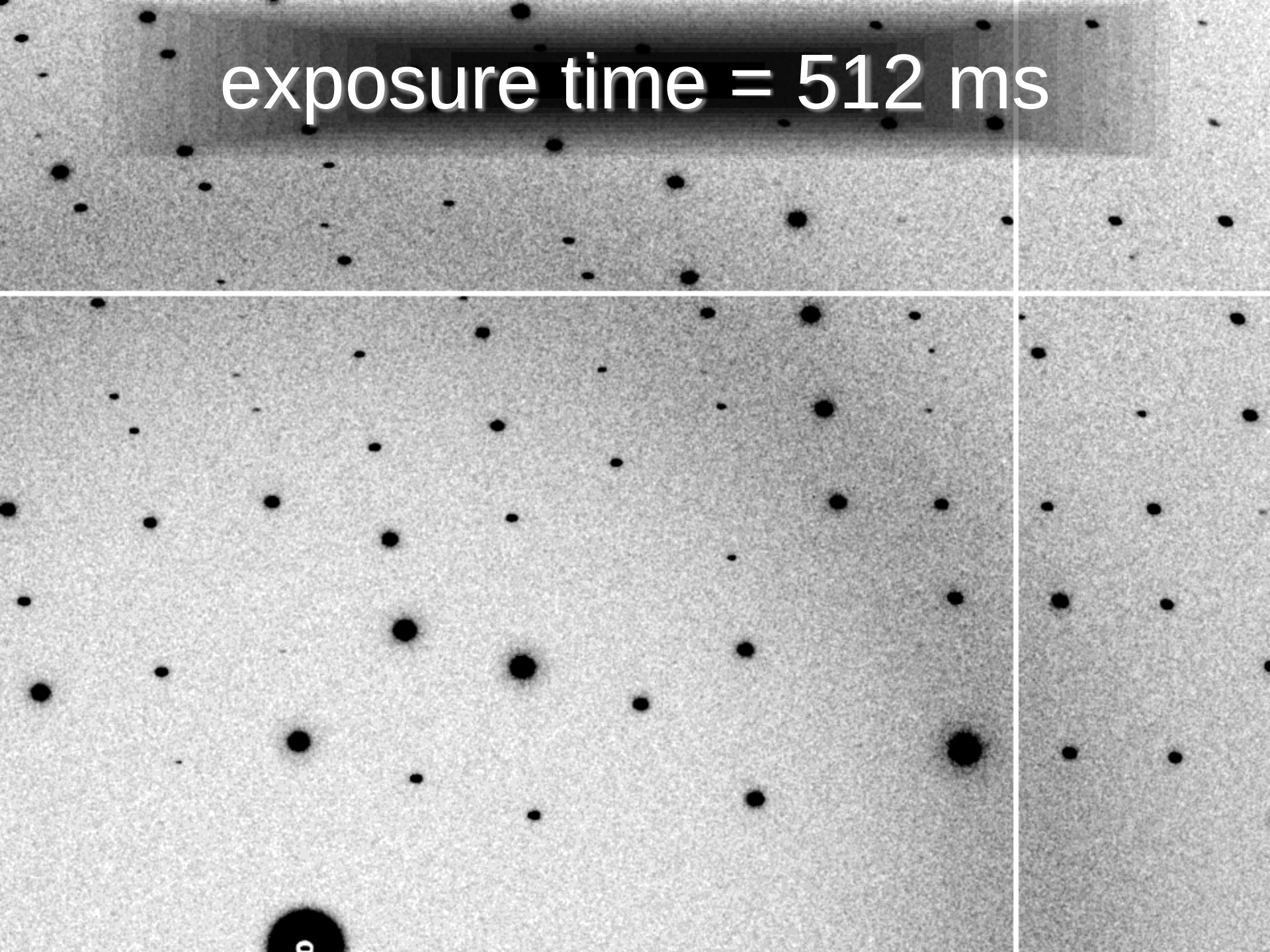

exposure time = 16 ms


exposure time = 32 ms


exposure time = 64 ms


exposure time = 128 ms


exposure time = 256 ms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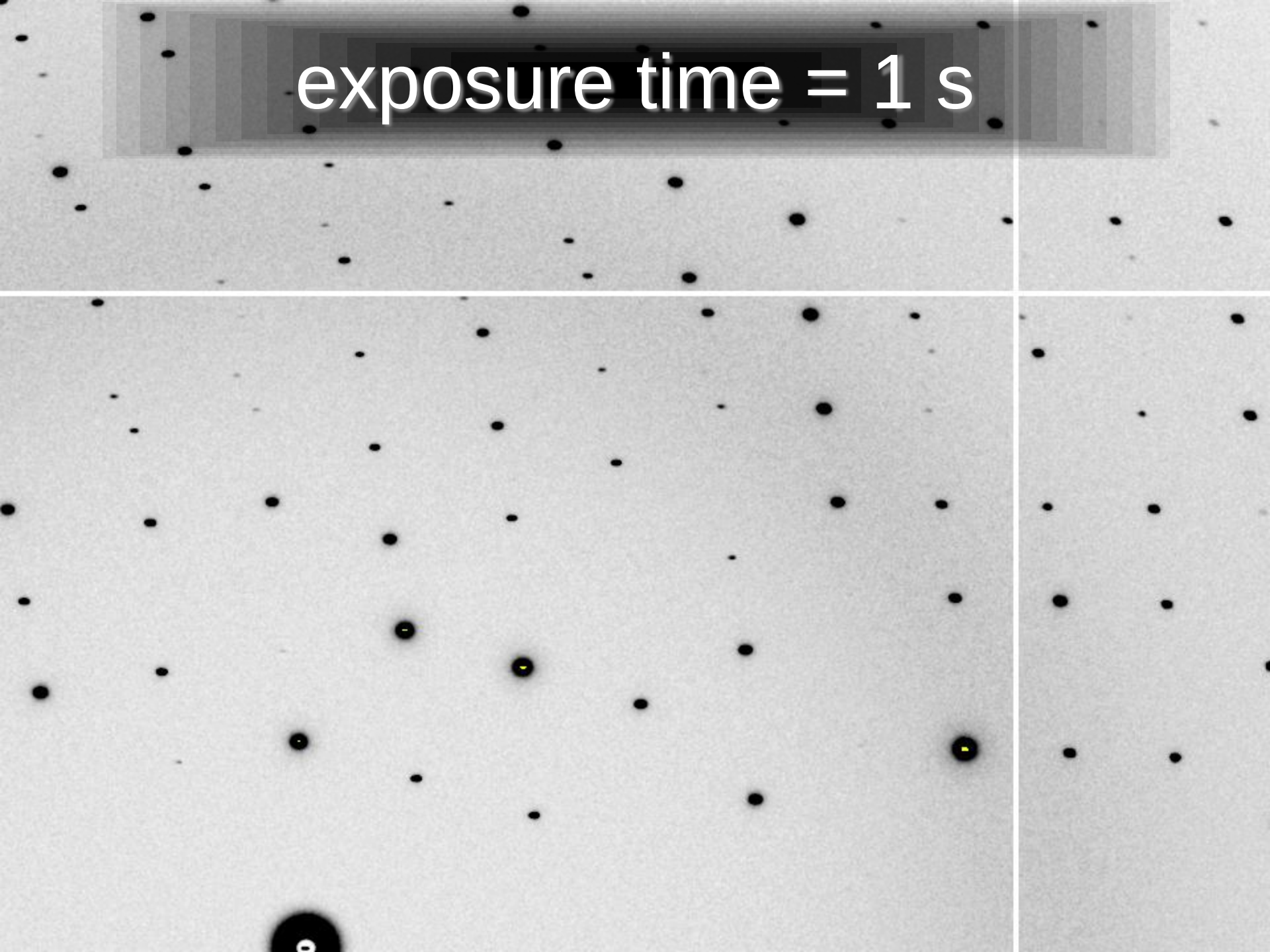
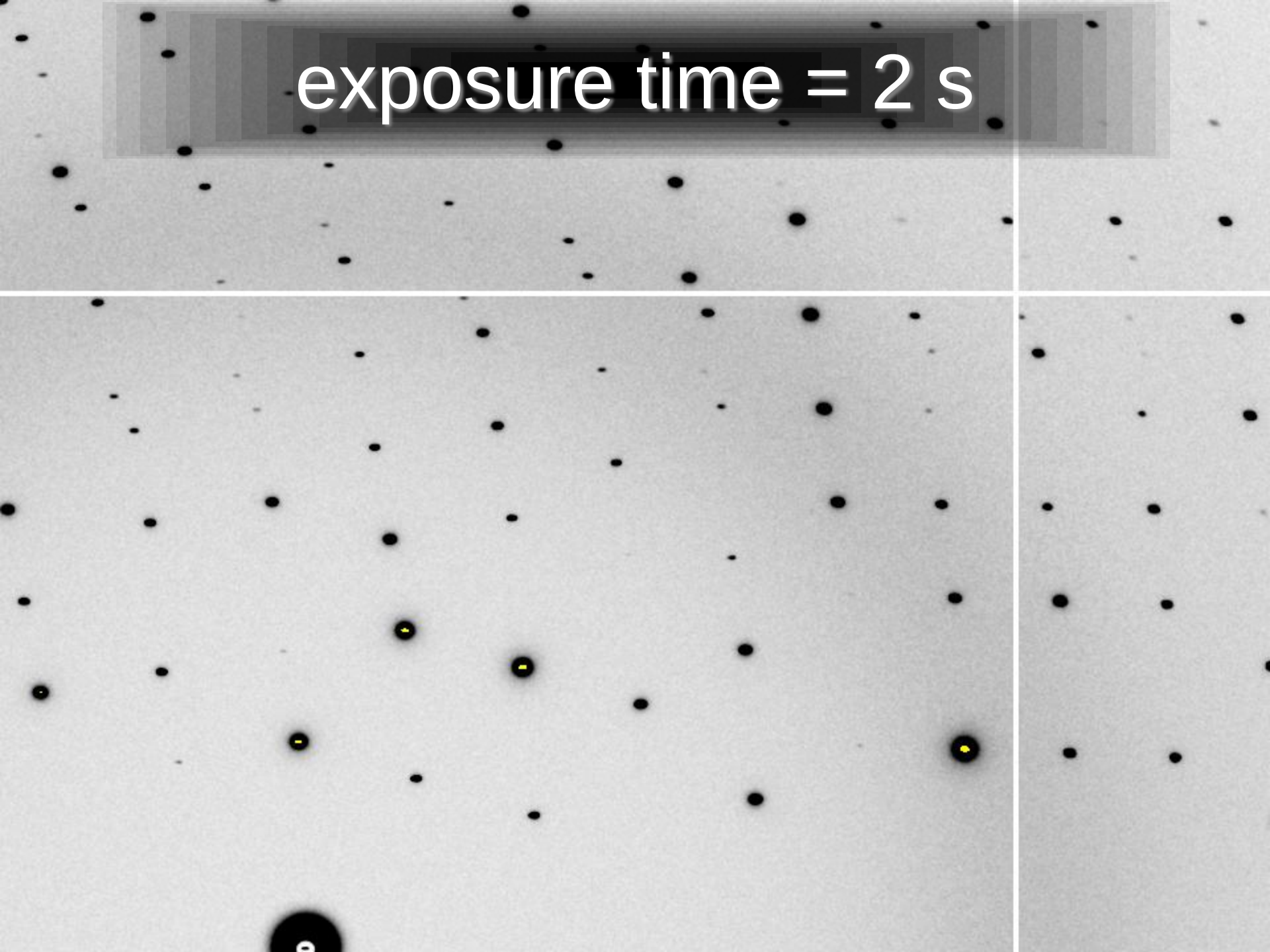
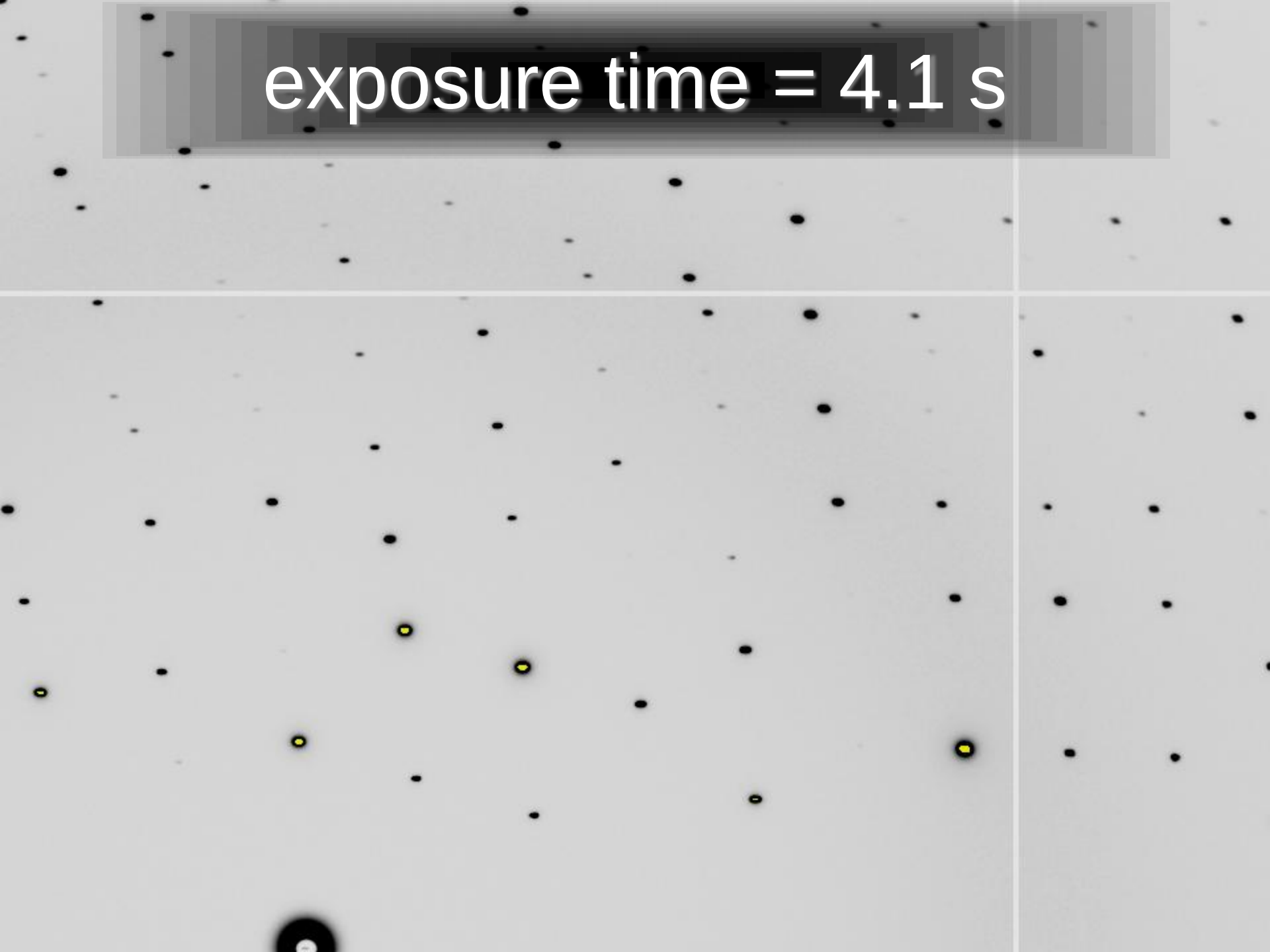
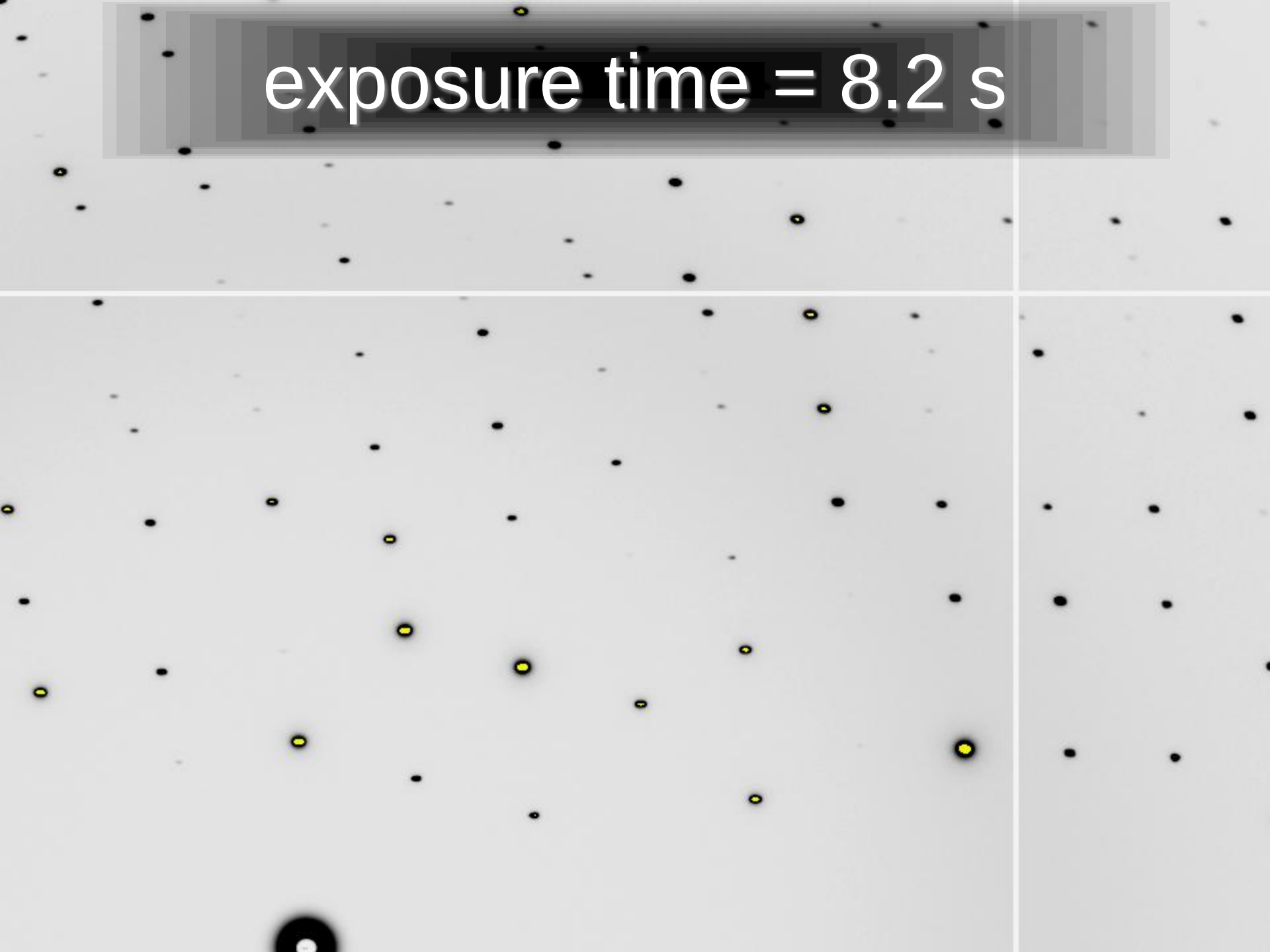
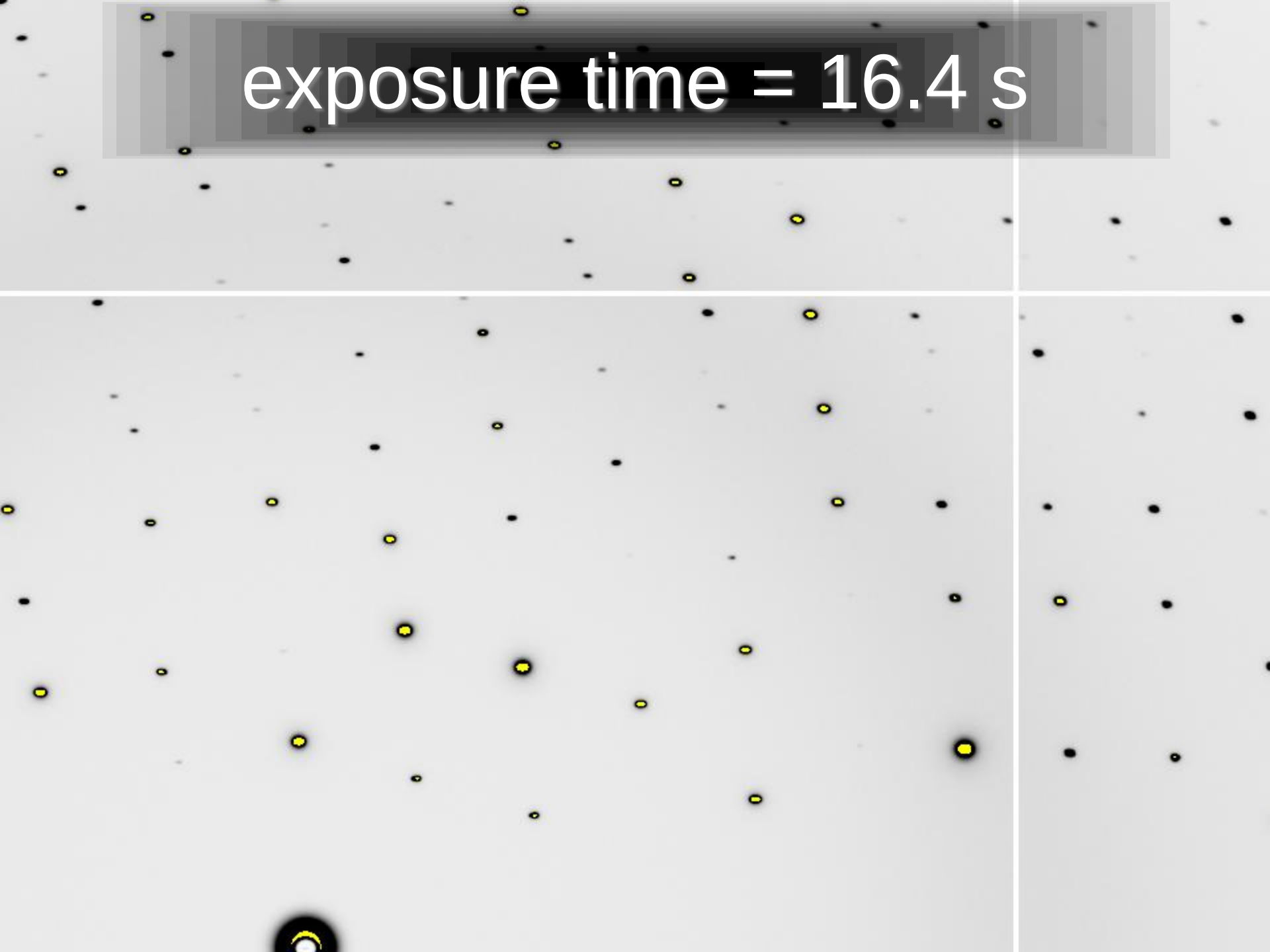
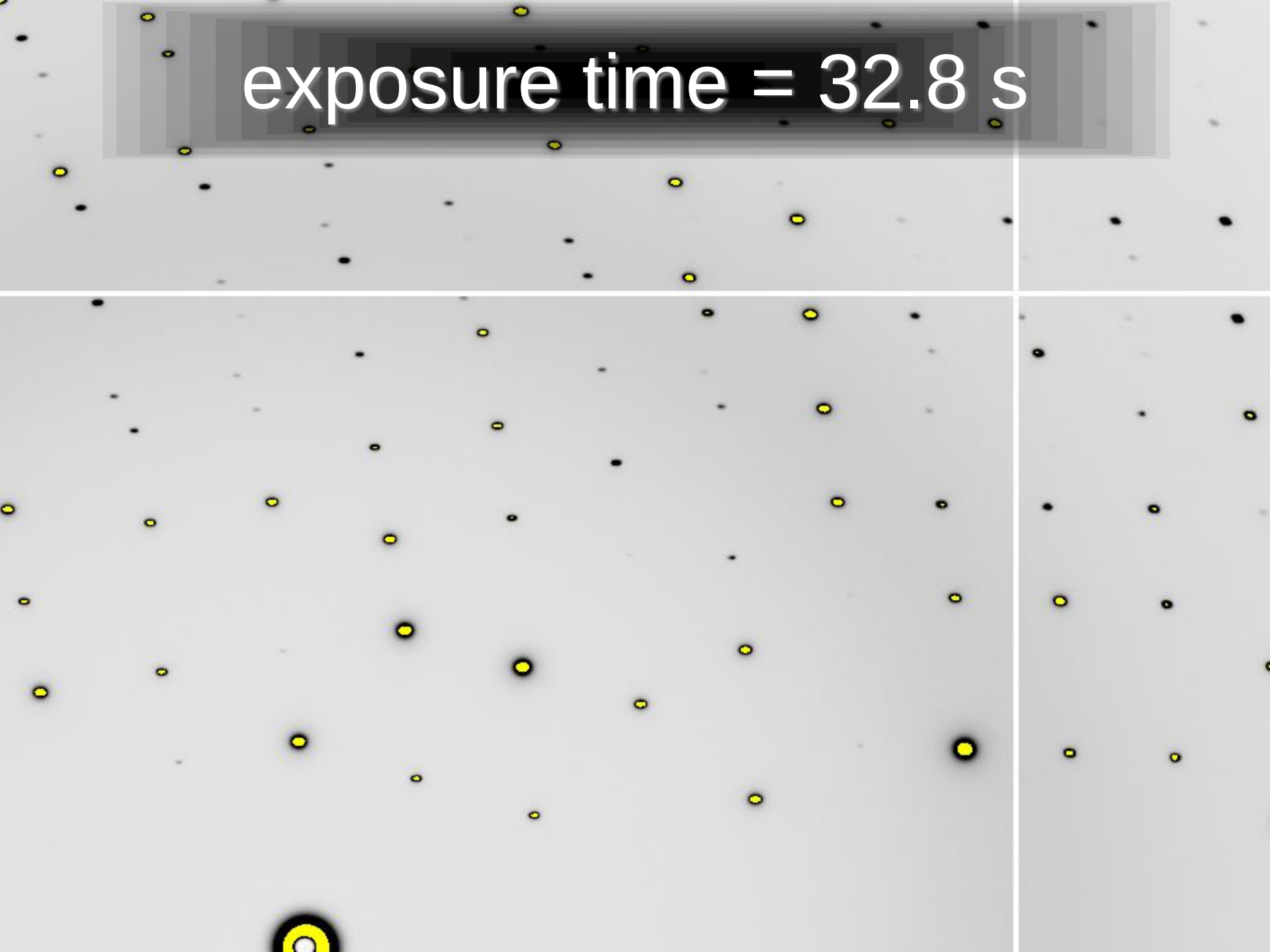

exposure time = 1 s

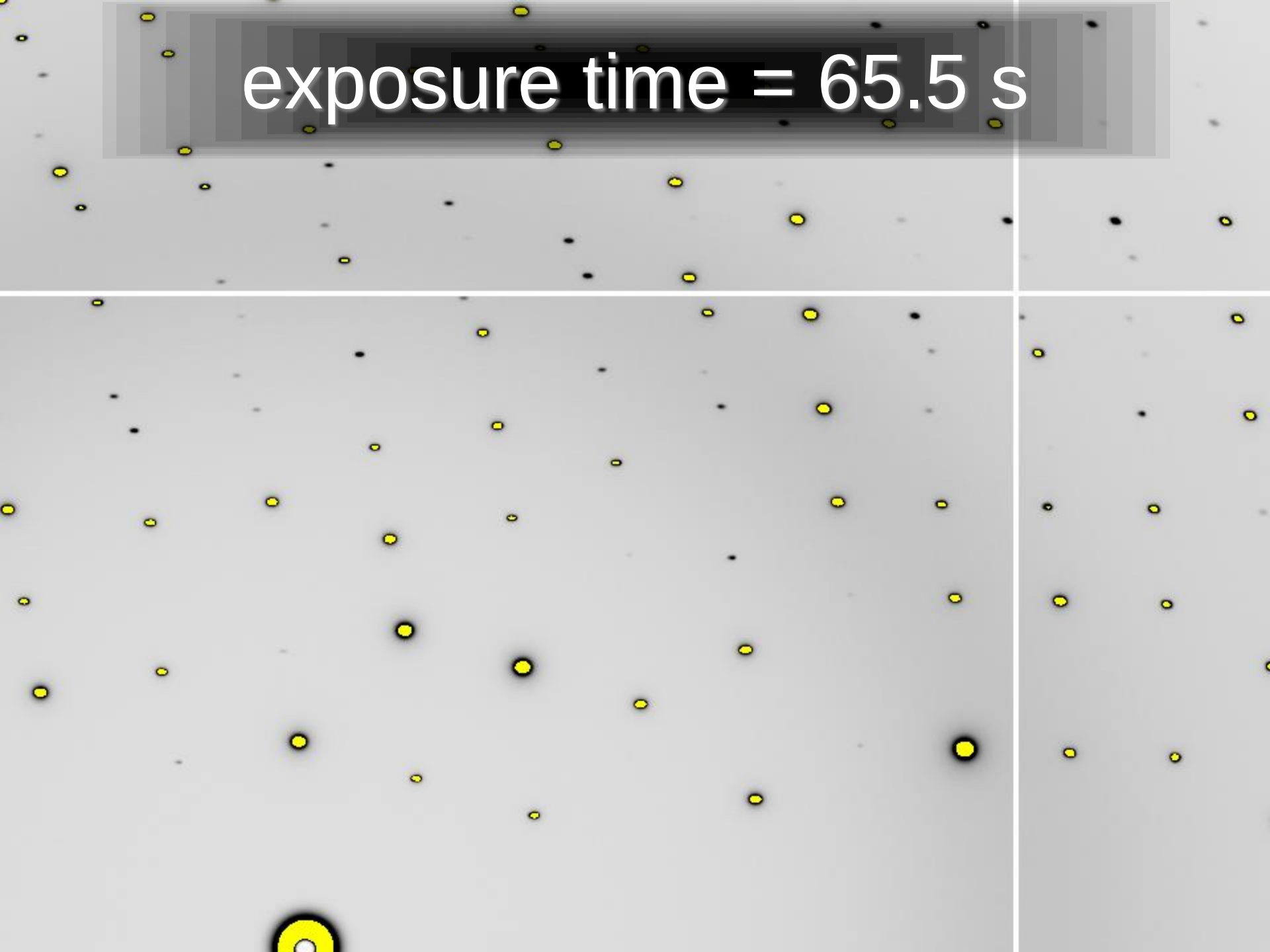

exposure time = 2 s

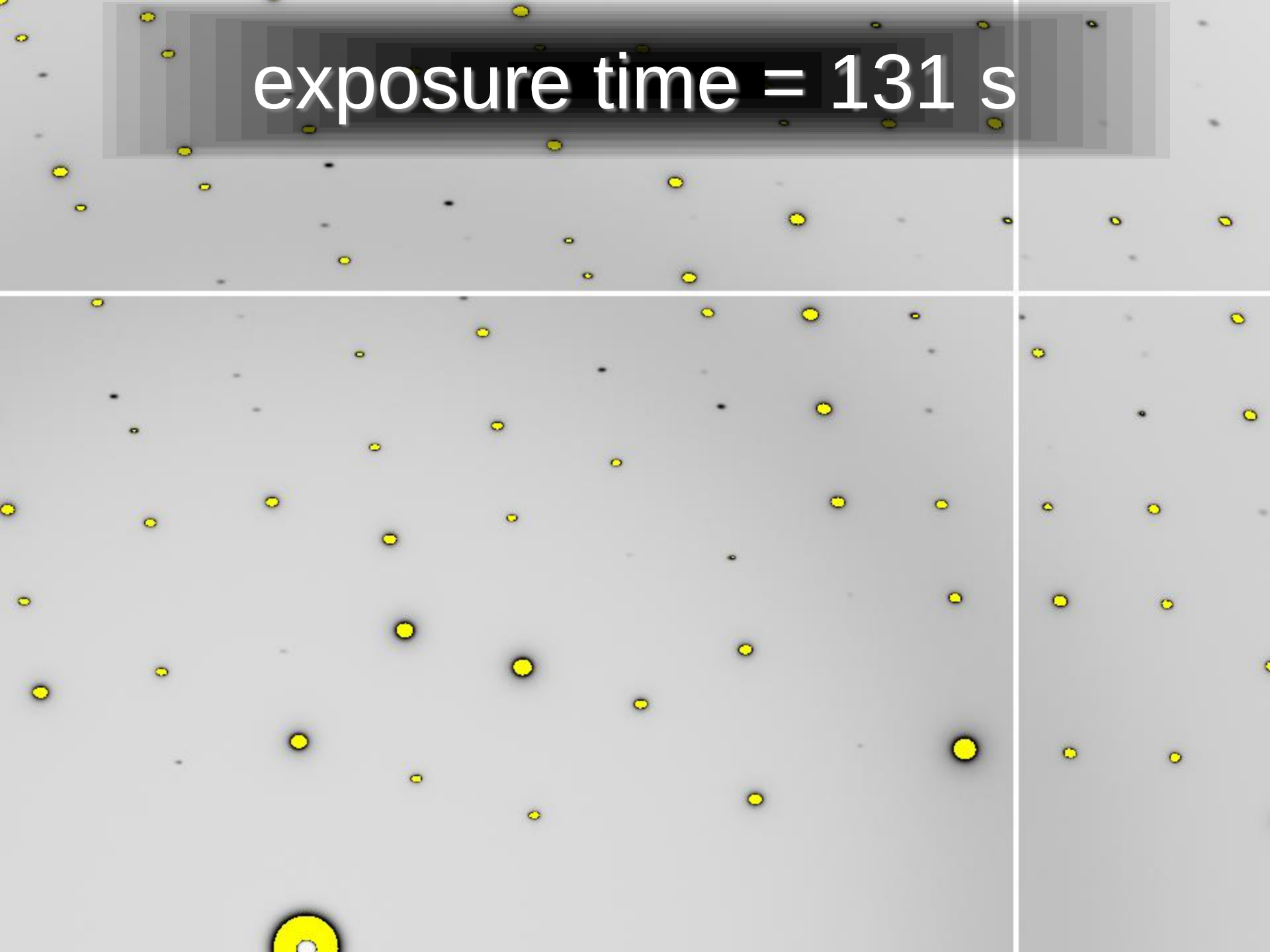

exposure time = 4.1 s

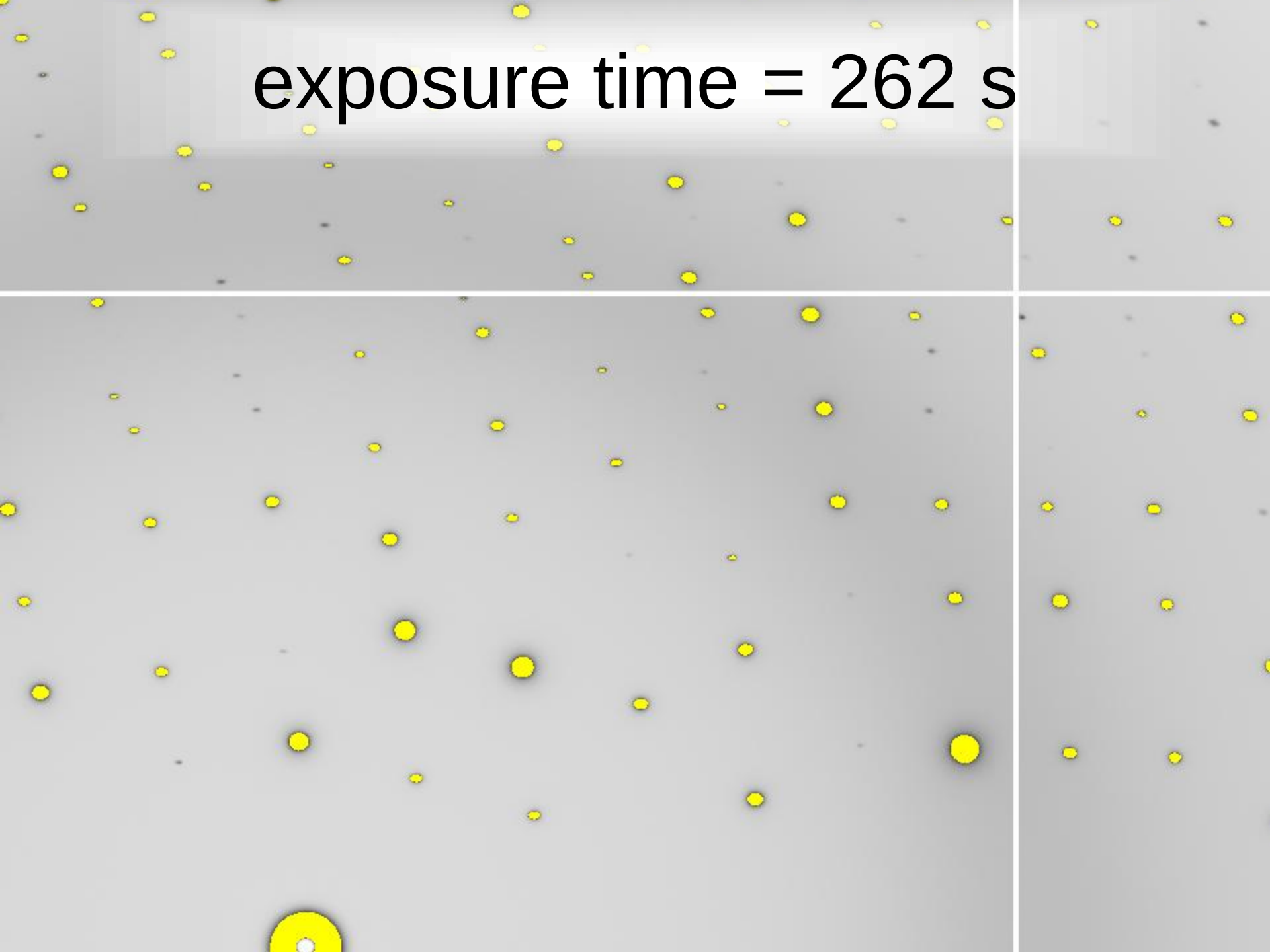

exposure time = 8.2 s


exposure time = 16.4 s

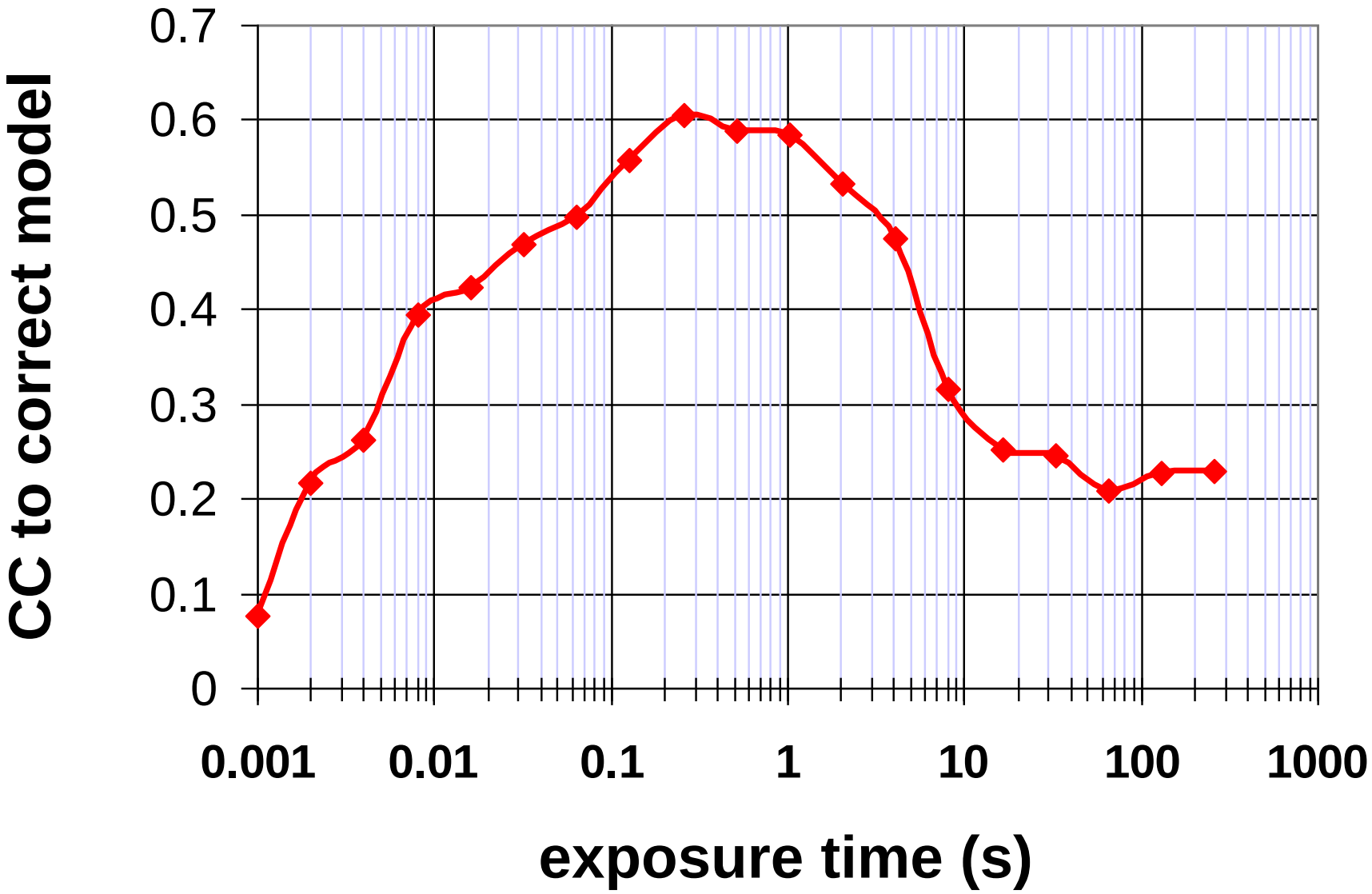

exposure time = 32.8 s


exposure time = 65.5 s

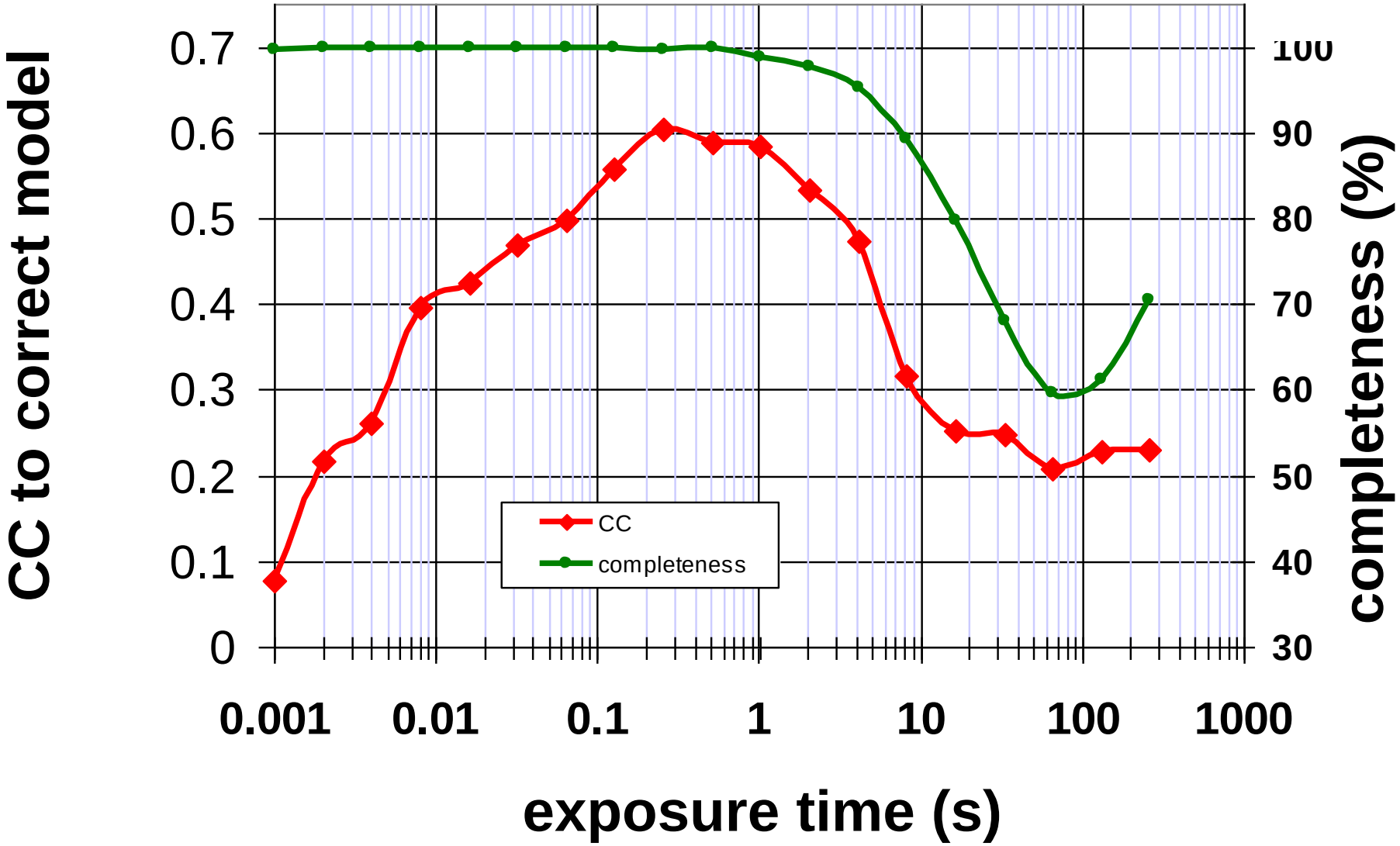

exposure time = 131 s


exposure time = 262 s

Exposure time



Exposure time



Darwin's Formula

$$I(hkl) = I_{beam}\, r_e^2 \frac{V_{xtal}}{V_{cell}} \frac{\lambda^3 L}{\omega V_{cell}} P\, A\, |\, F(hkl)\, |^2$$

I(hkl) - photons/spot (fully-recorded)

I_{beam} - incident (photons/s/m^2)

r_e - classical electron radius (2.818×10^{-15} m)

V_{xtal} - volume of crystal (in m^3)

V_{cell} - volume of unit cell (in m^3)

λ - x-ray wavelength (in meters!)

ω - rotation speed (radians/s)

L - Lorentz factor (speed/speed)

P - polarization factor

$(1+\cos^2(2\theta) - Pfac \cdot \cos(2\Phi)\sin^2(2\theta))/2$

A - absorption factor

$\exp(-\mu_{xtal} \cdot l_{path})$

F(hkl) - structure amplitude (electrons)

C. G. Darwin (1914)

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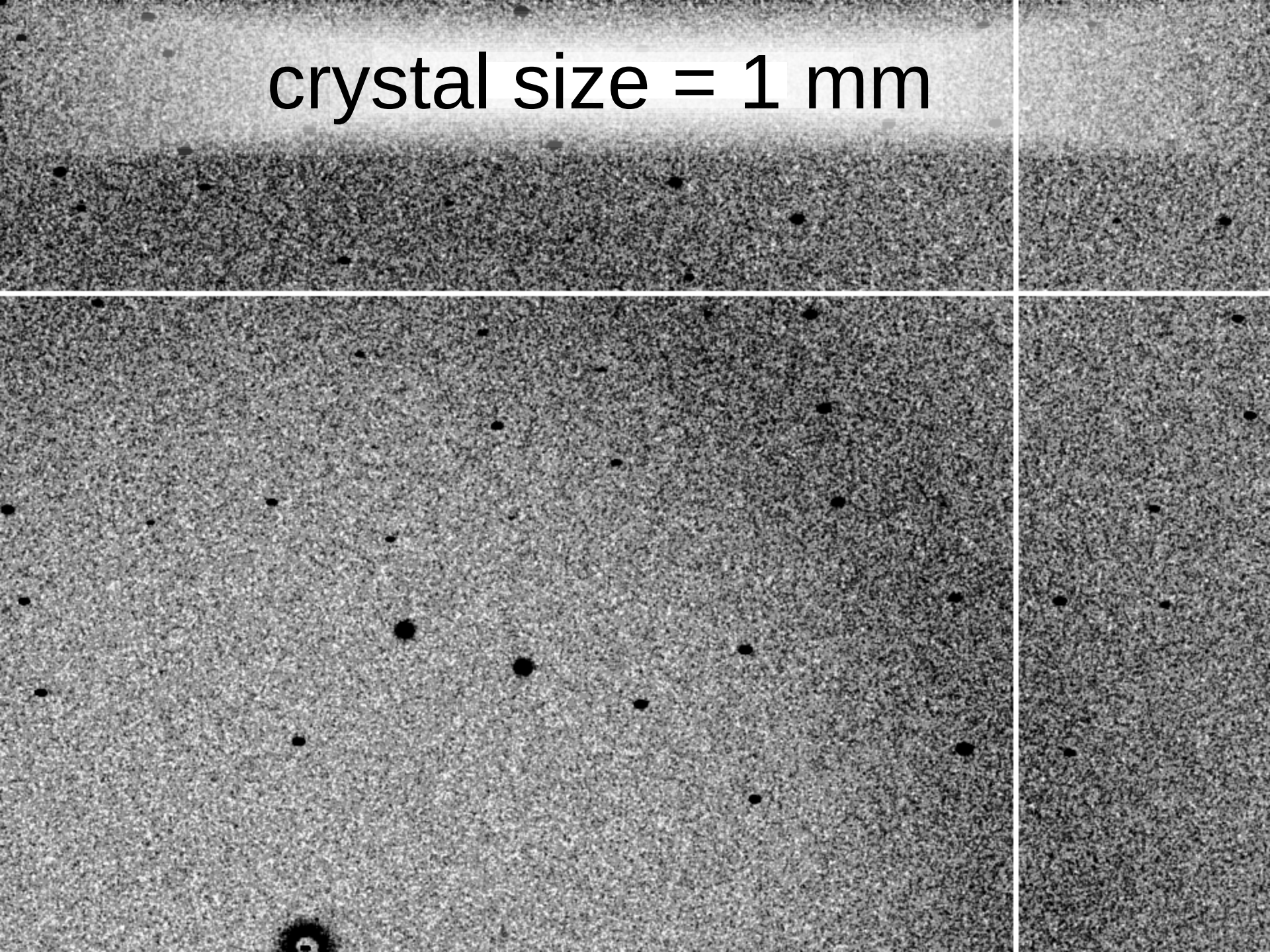
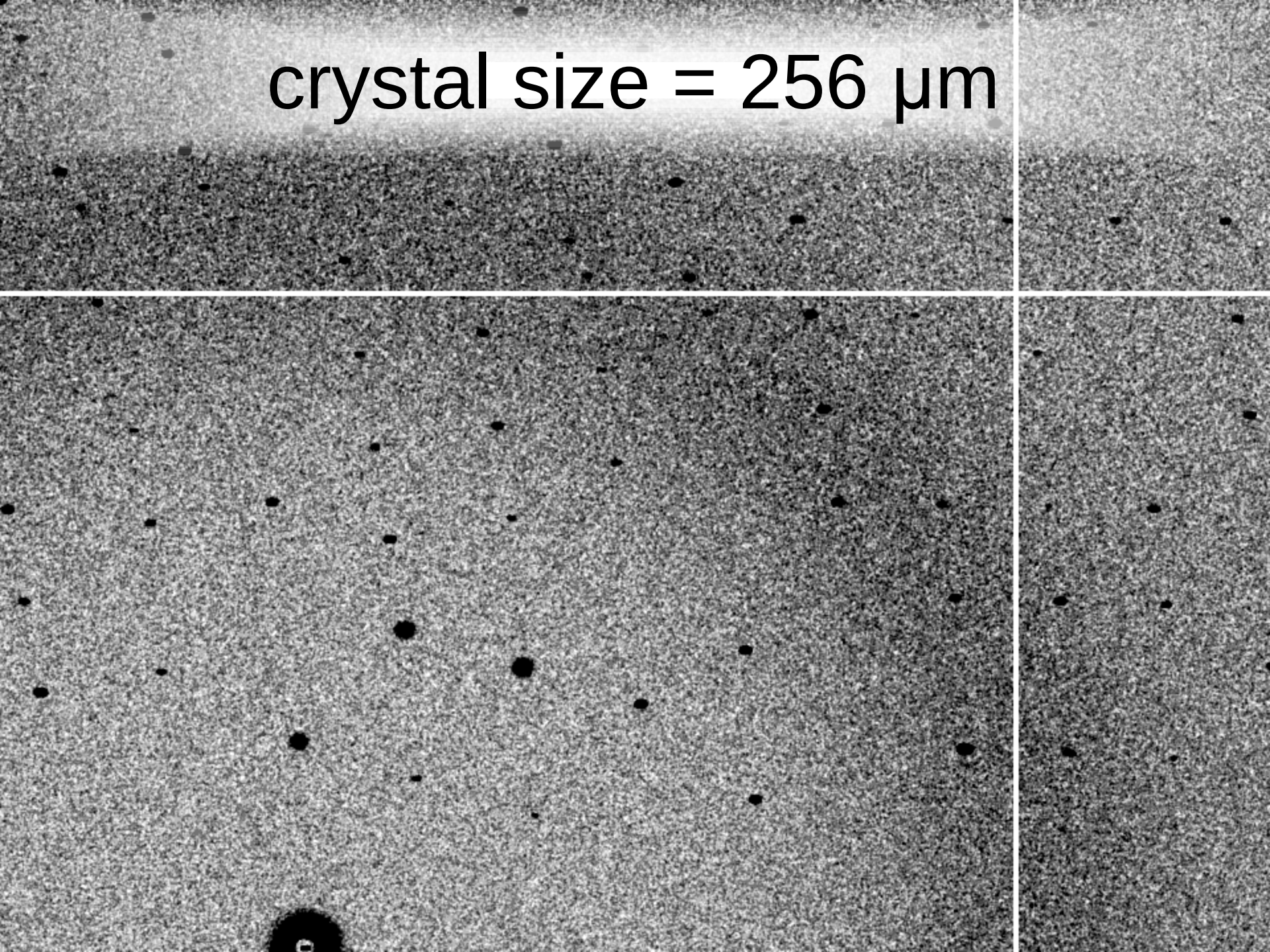
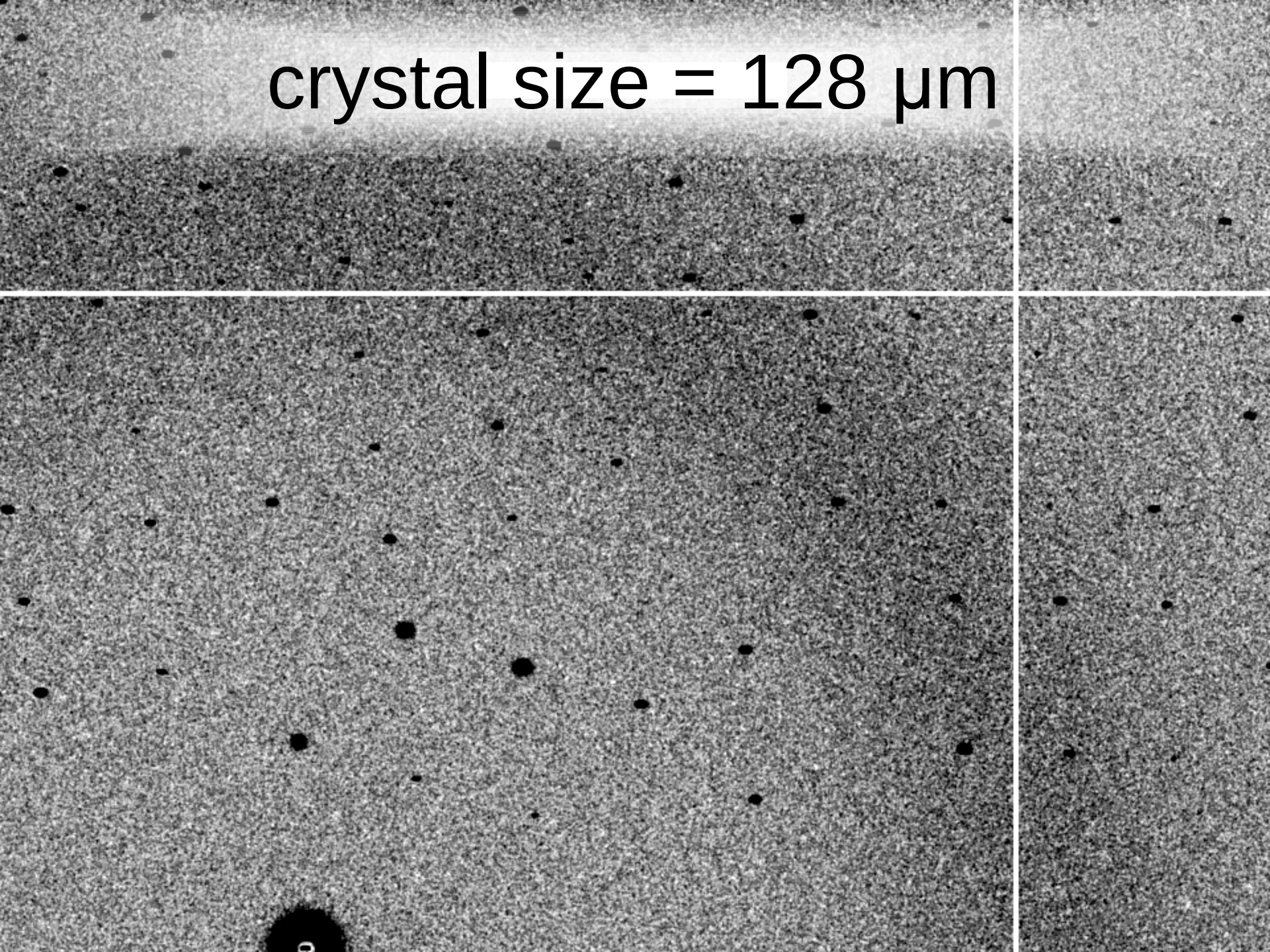
C. G. Darwin (1914)

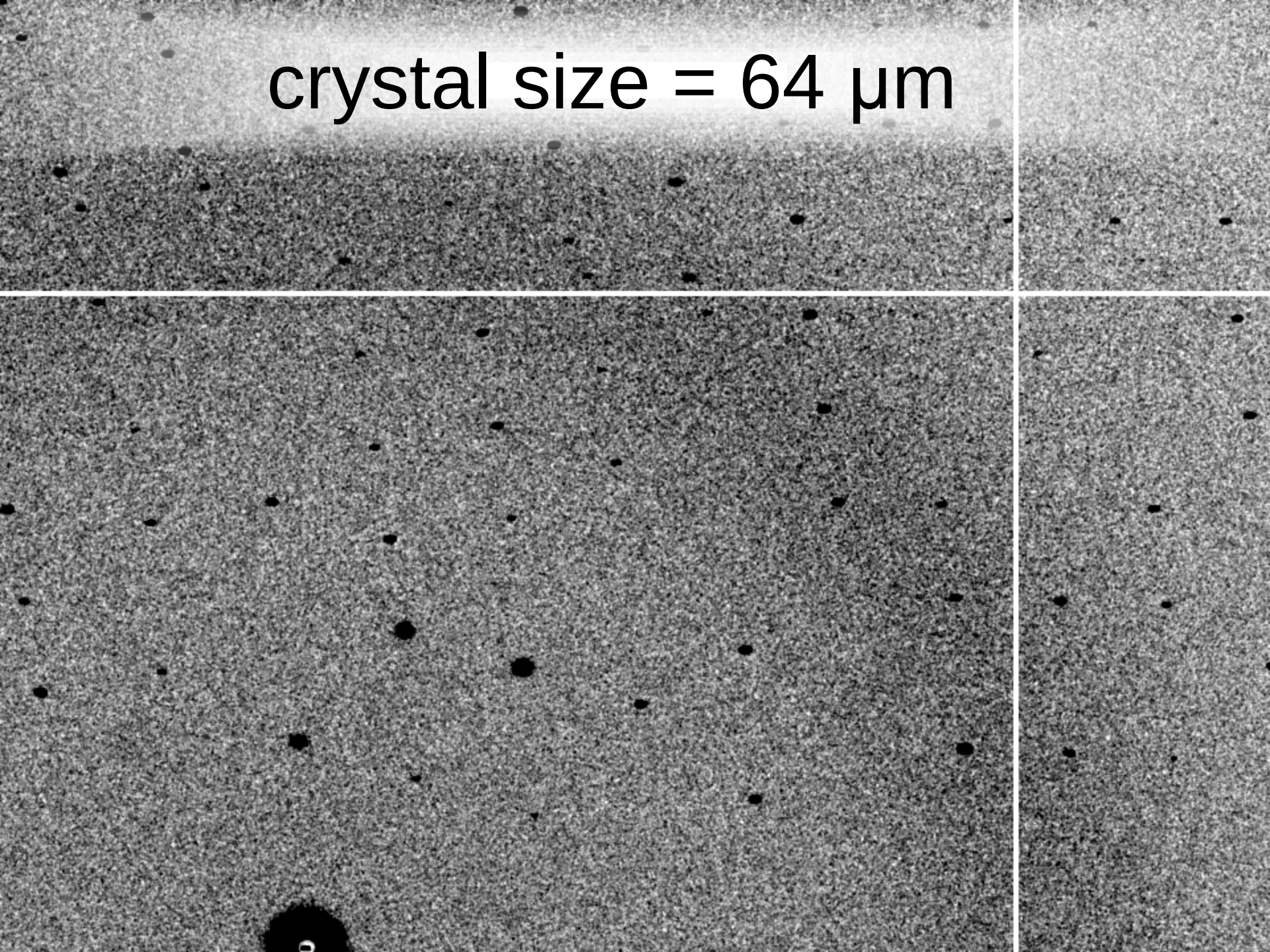
How small can the crystal be?

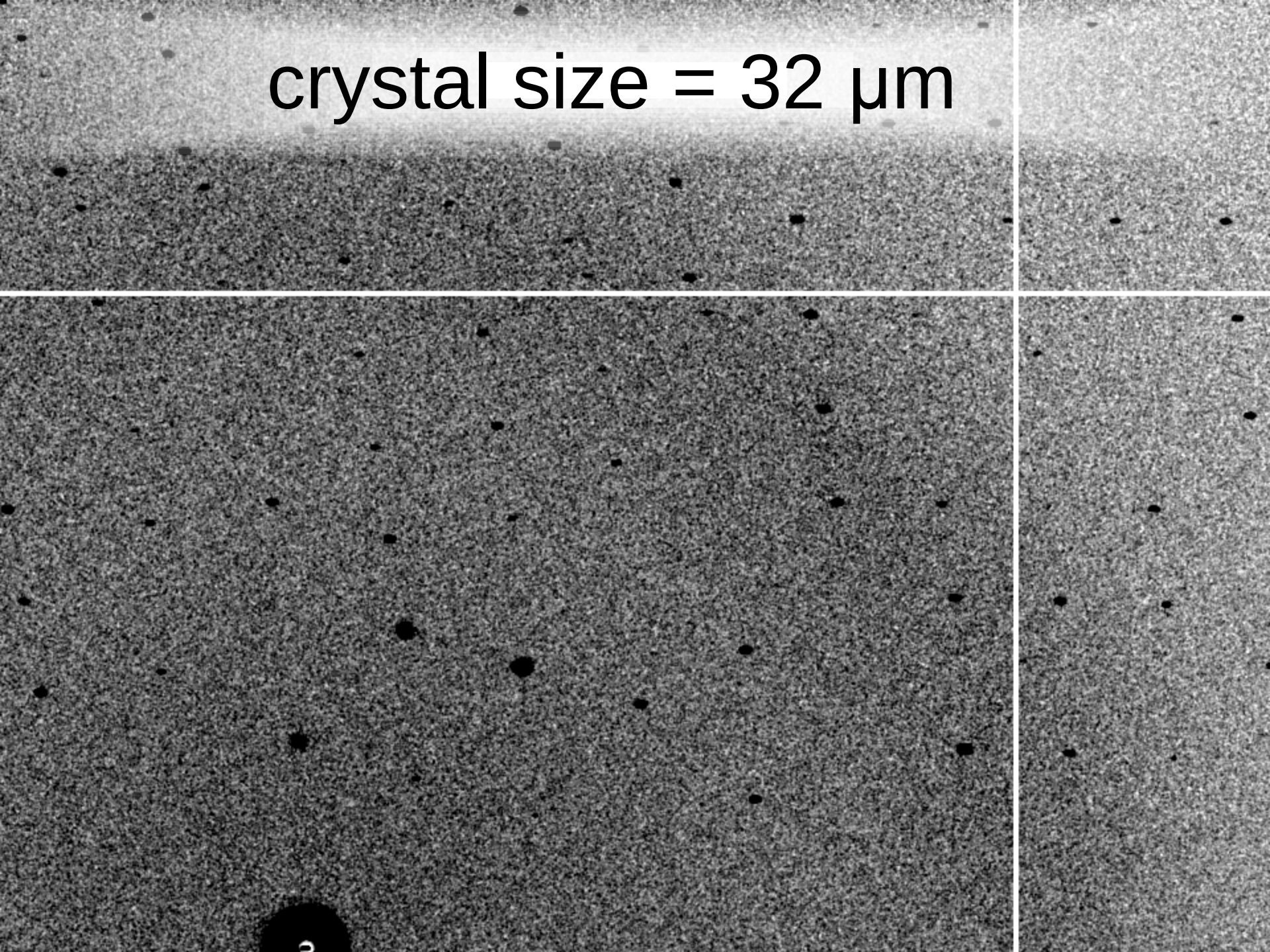

crystal size = 1 mm

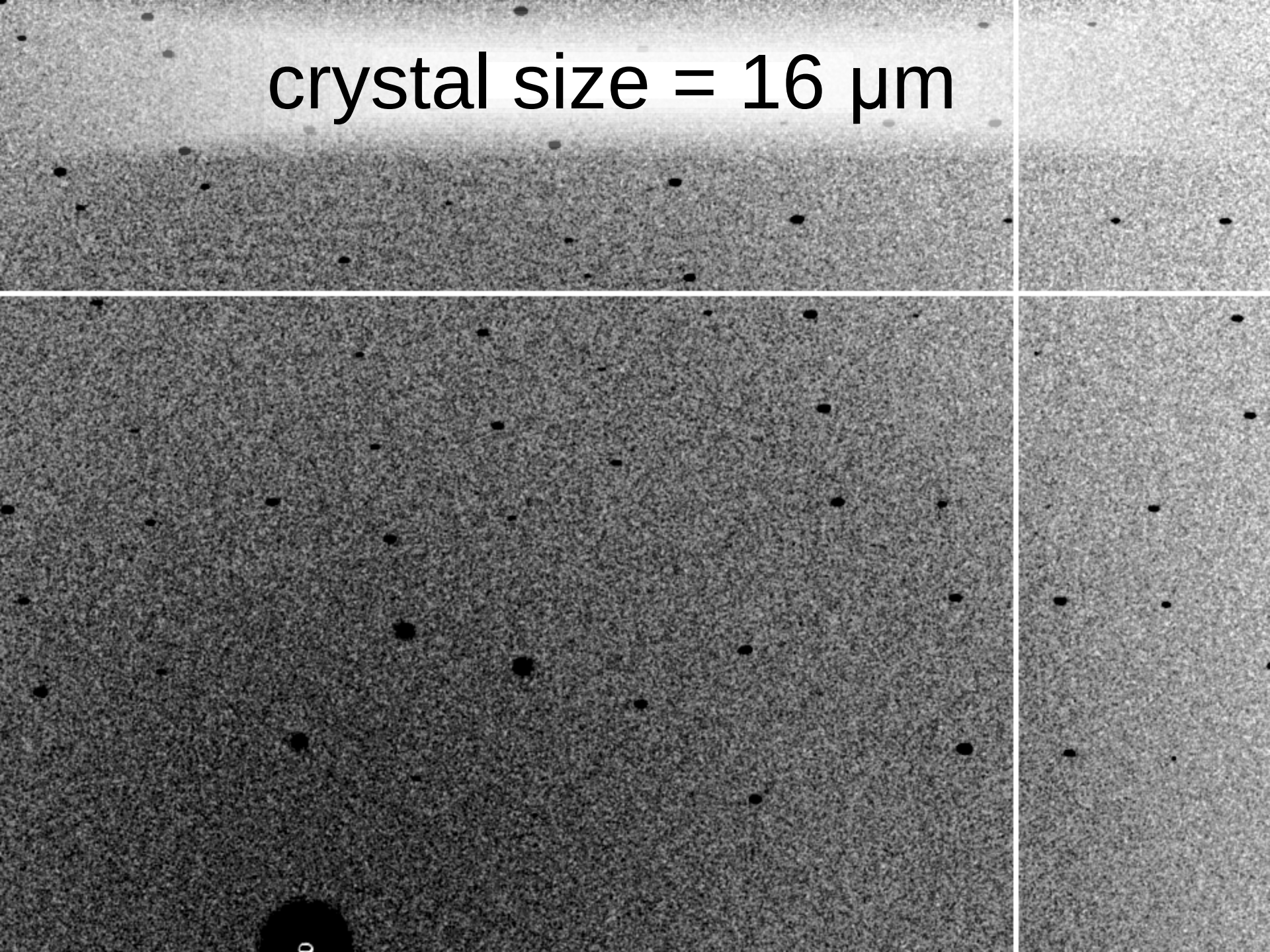
crystal size = 512 µm

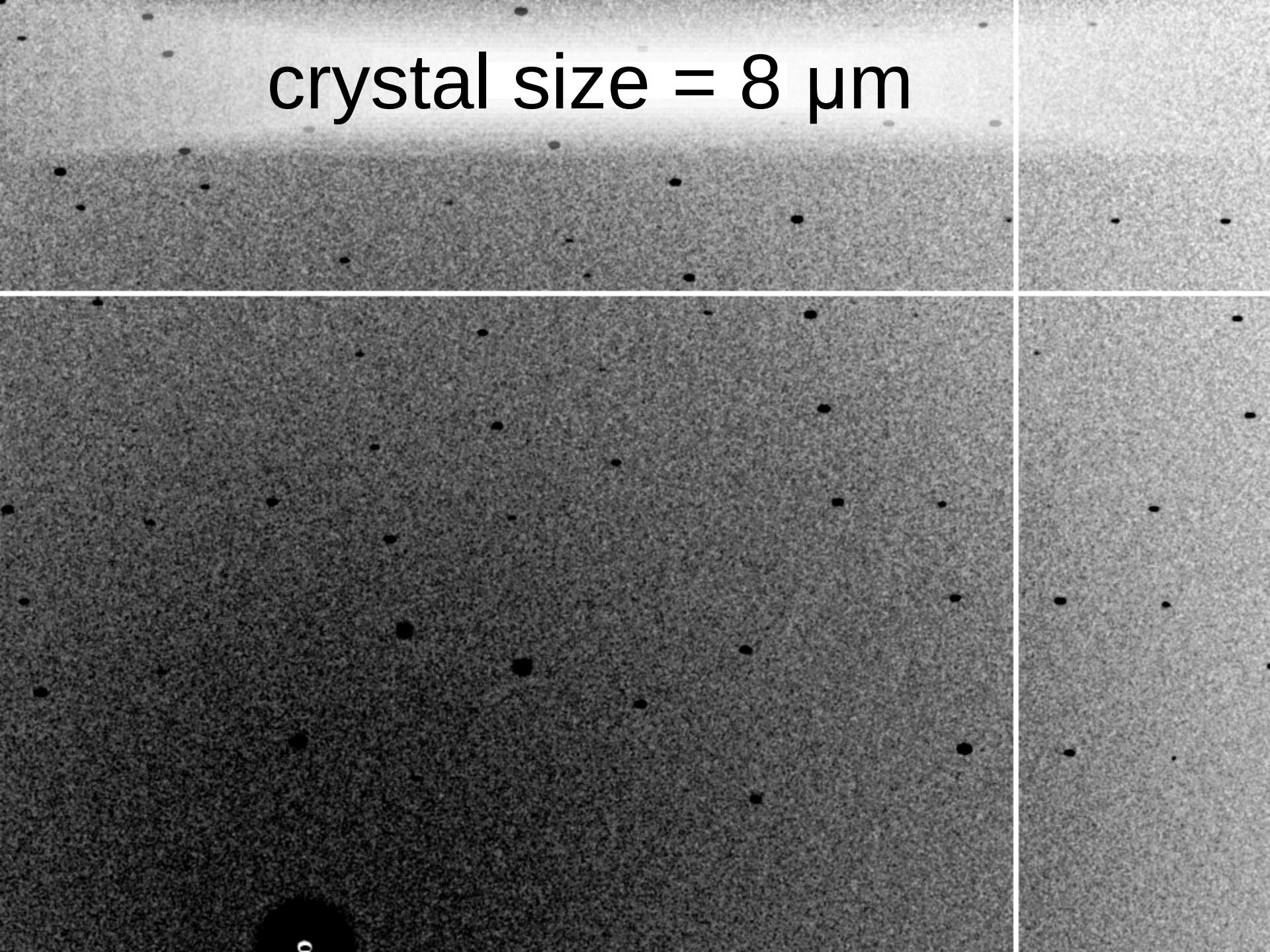

crystal size = 256 μm

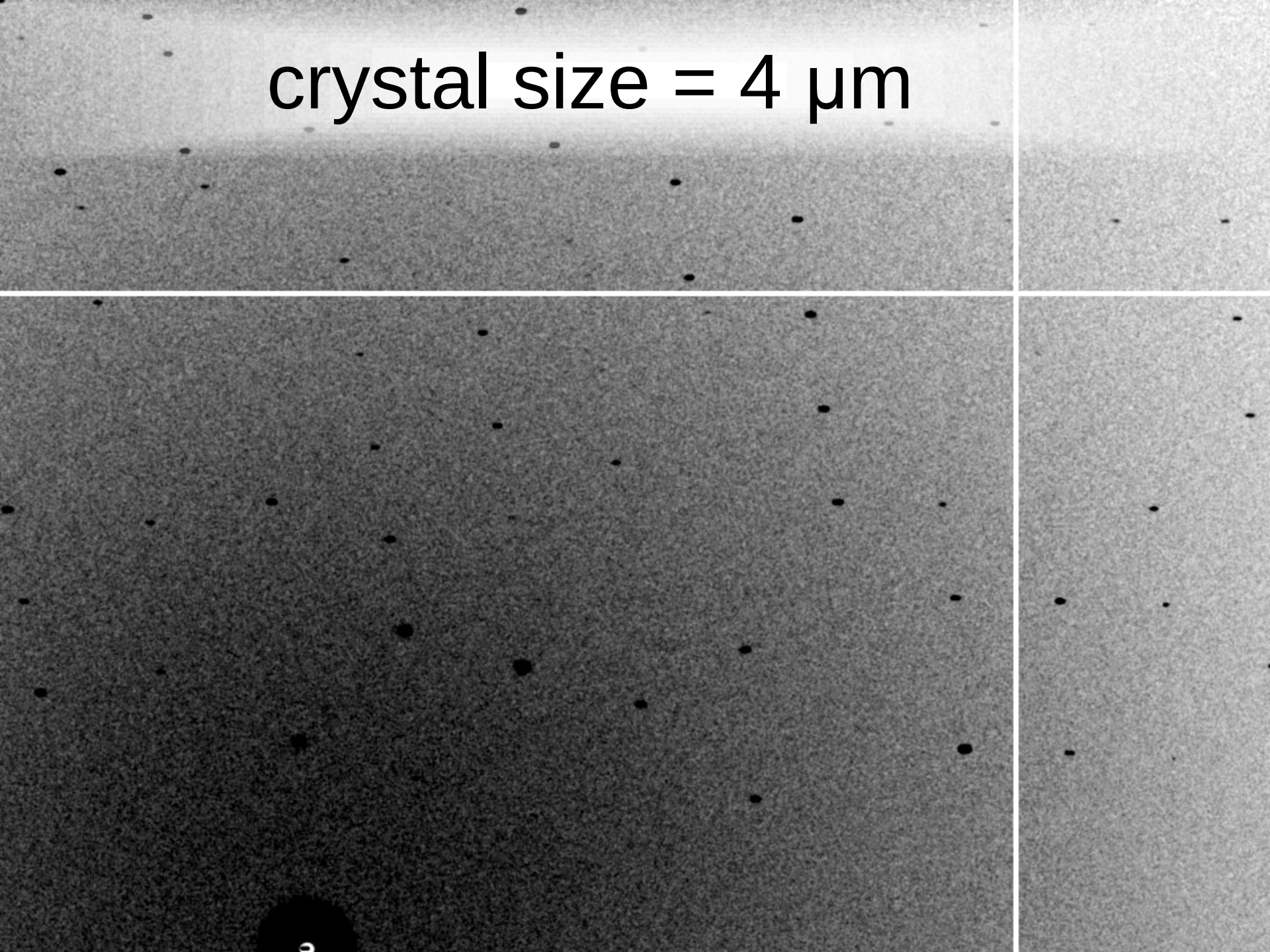

crystal size = 128 μm


crystal size = 64 μm

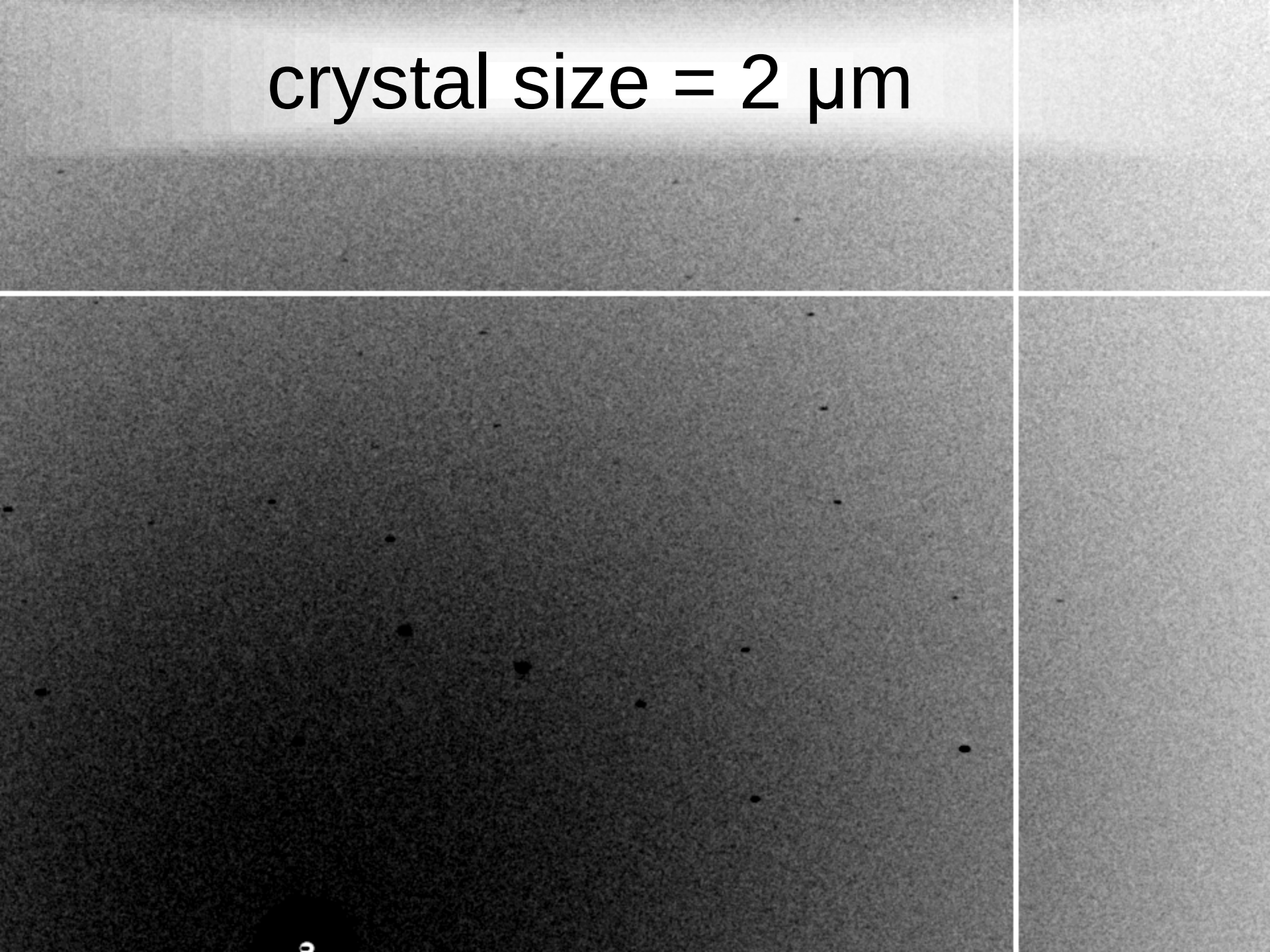

crystal size = 32 μm


crystal size = 16 μm

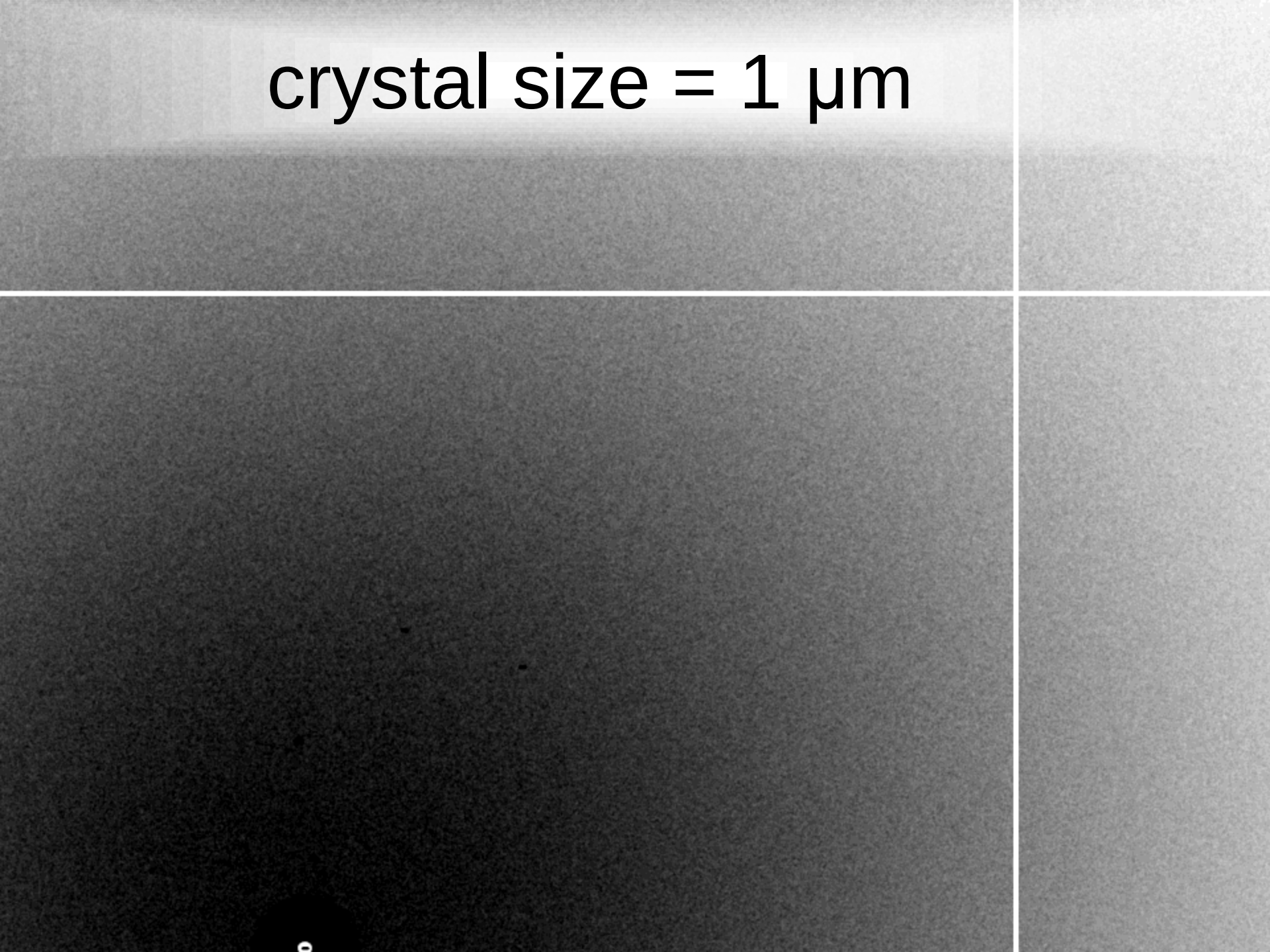

crystal size = 8 μm

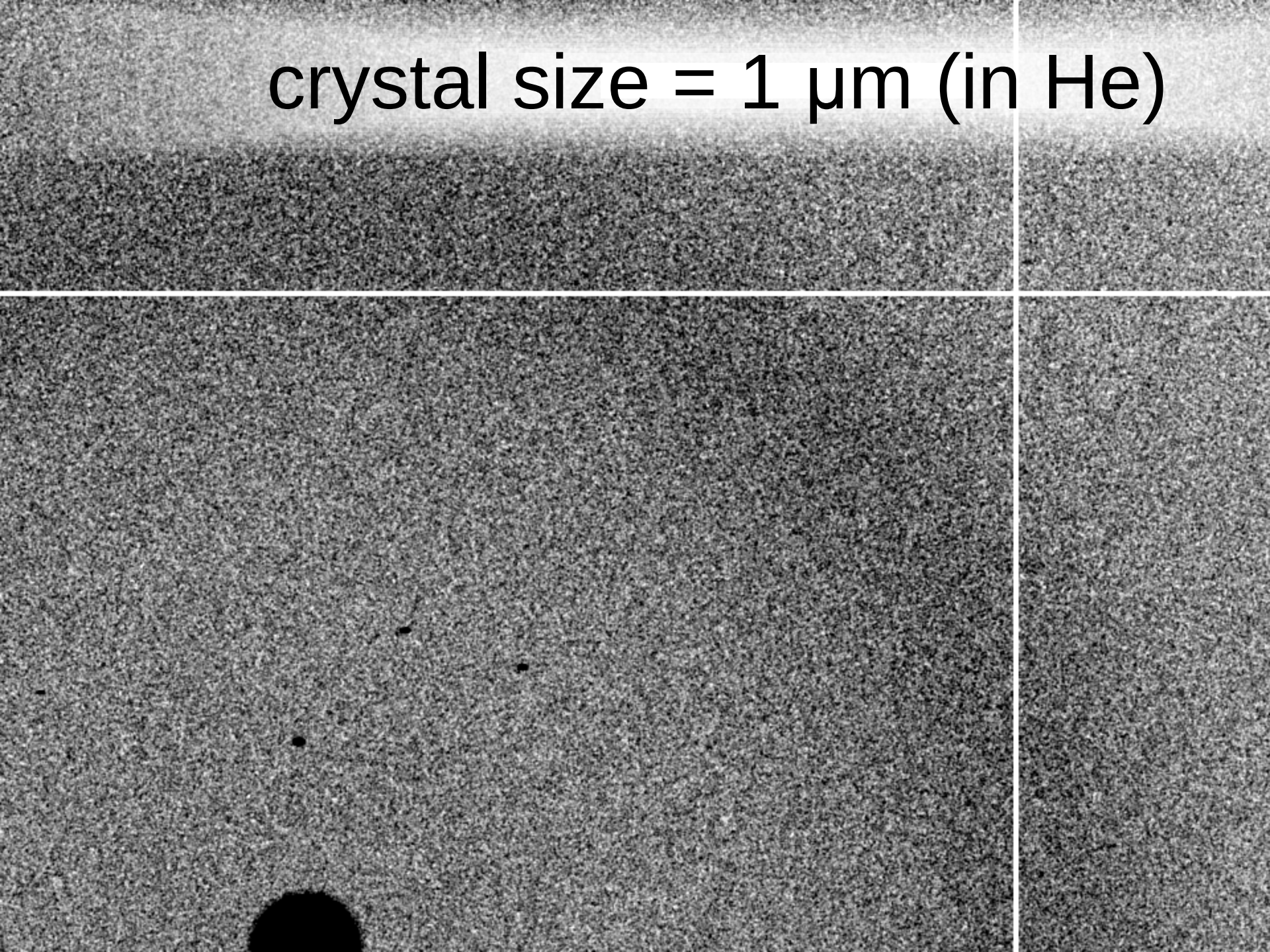

crystal size = 4 μm

crystal size = 2 μm

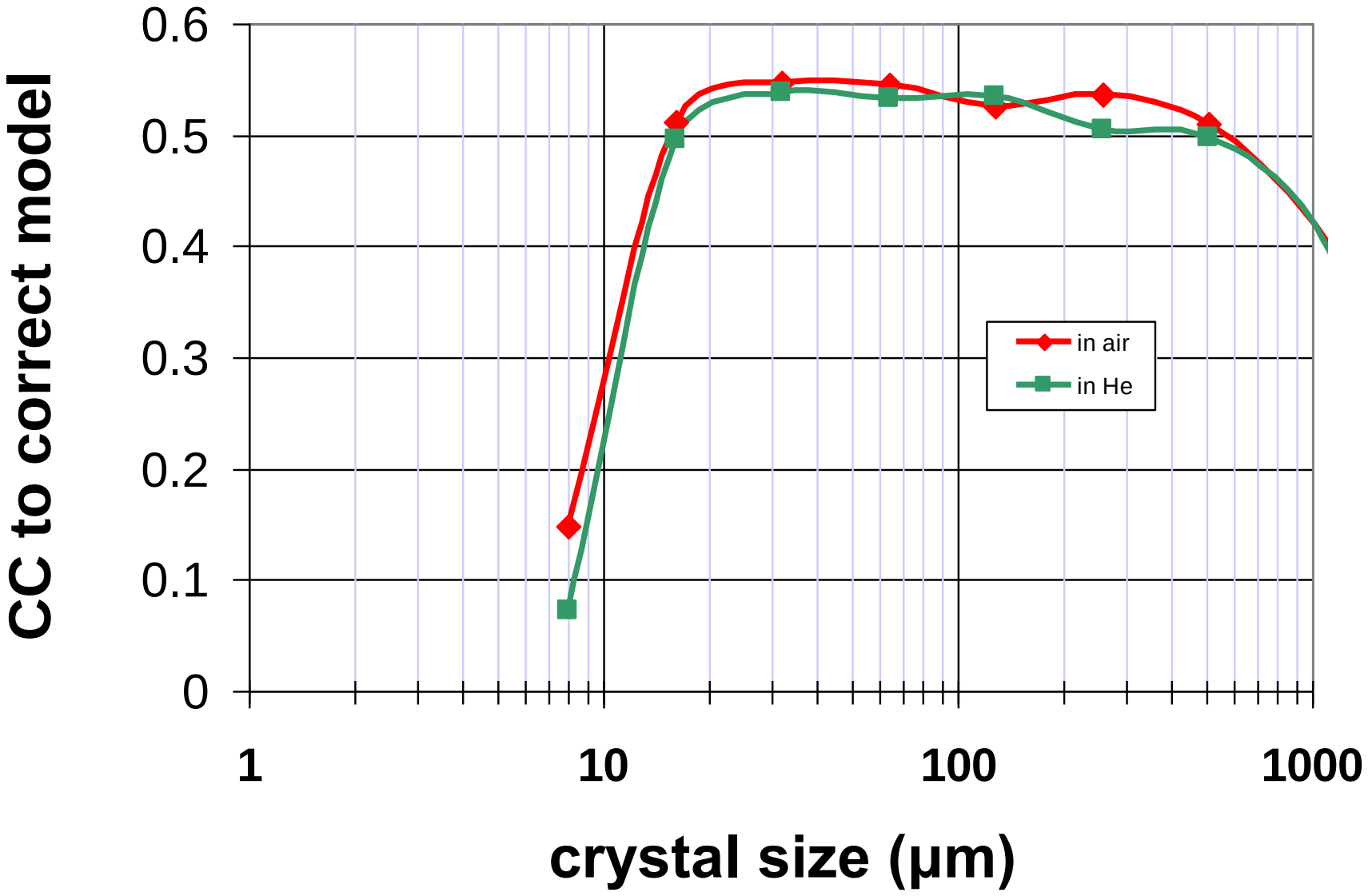


crystal size = 1 μm




crystal size = 1 μm (in He)

Crystal Size



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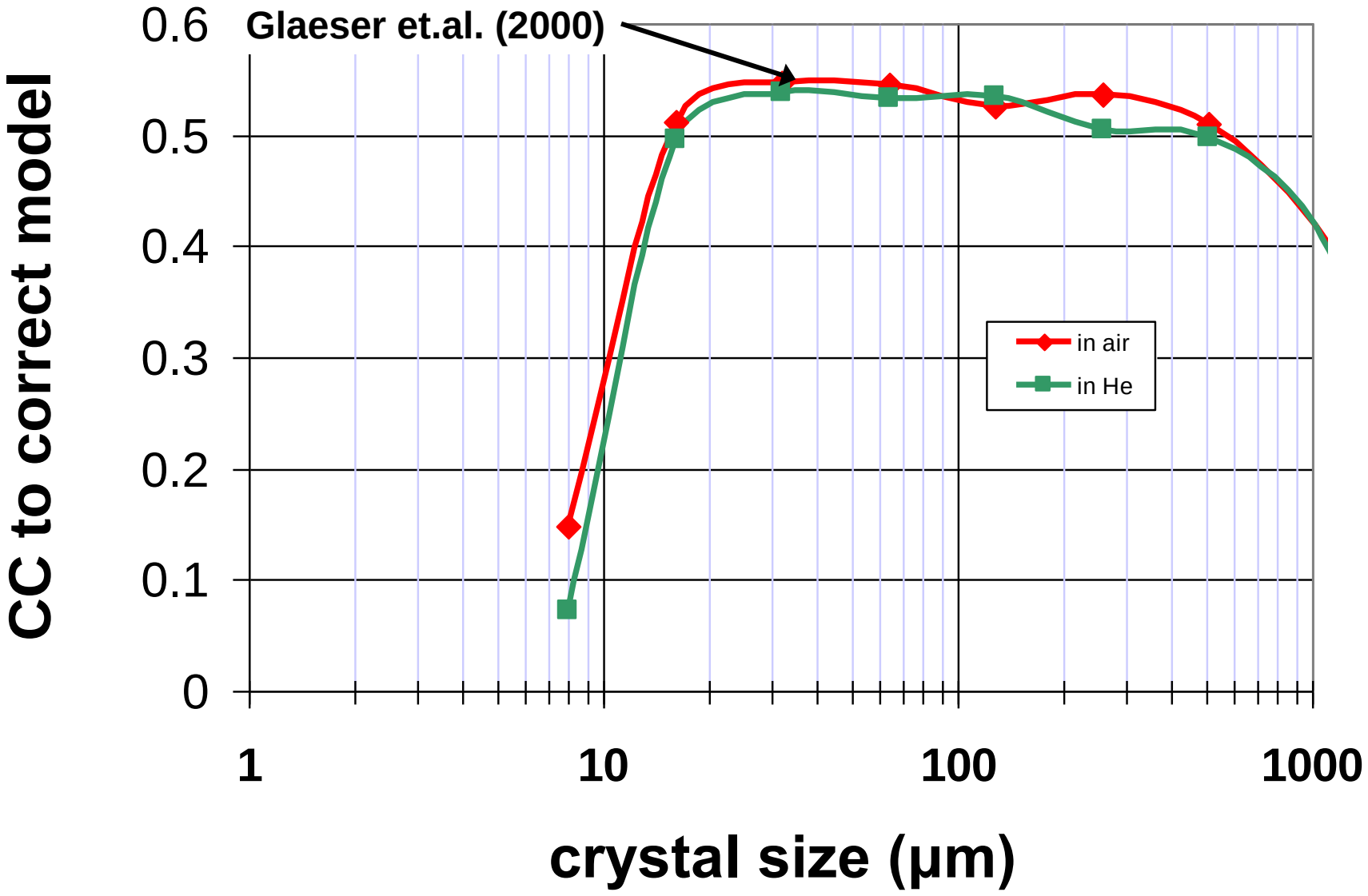
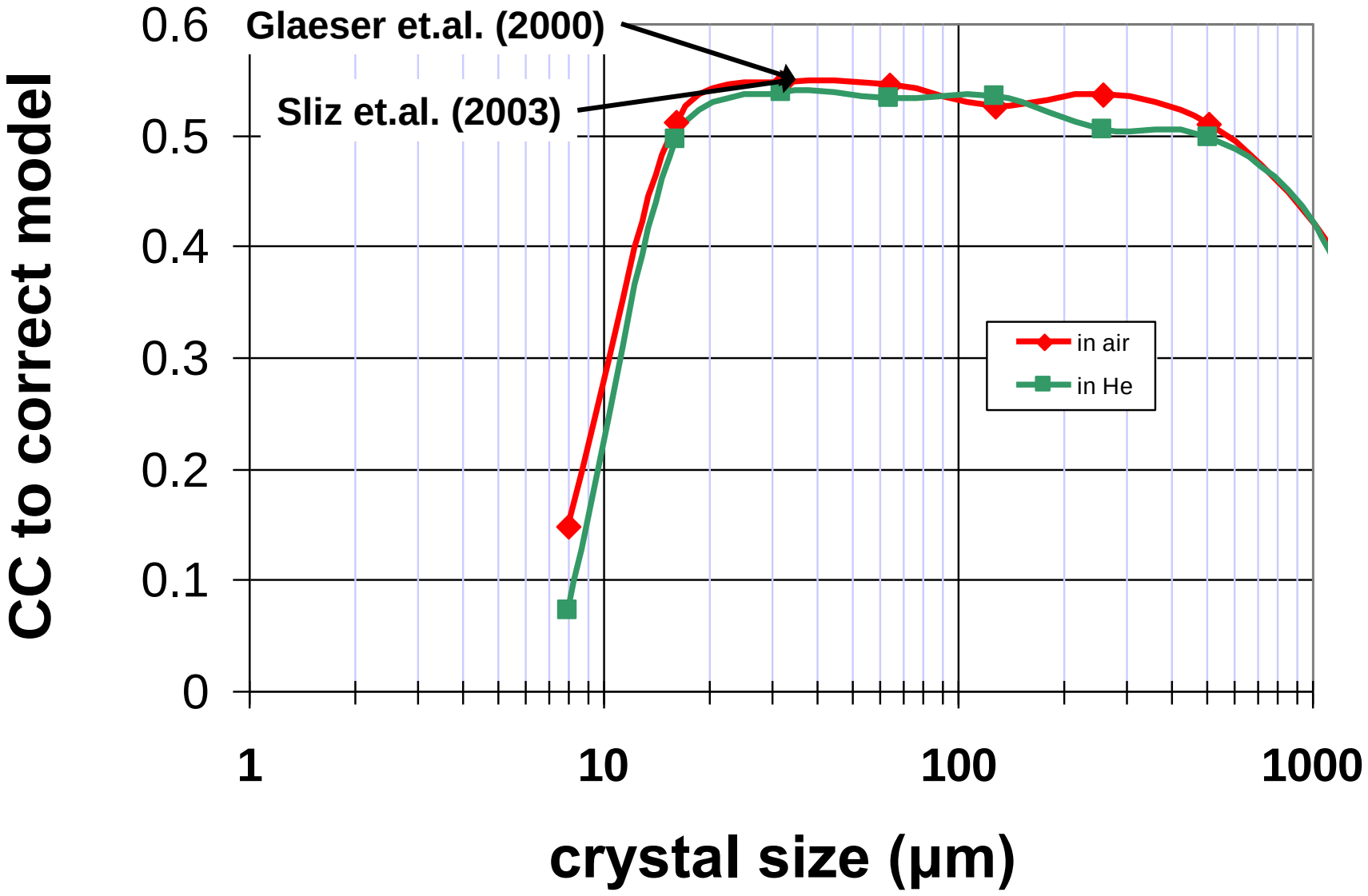
C. G. Darwin (1914)

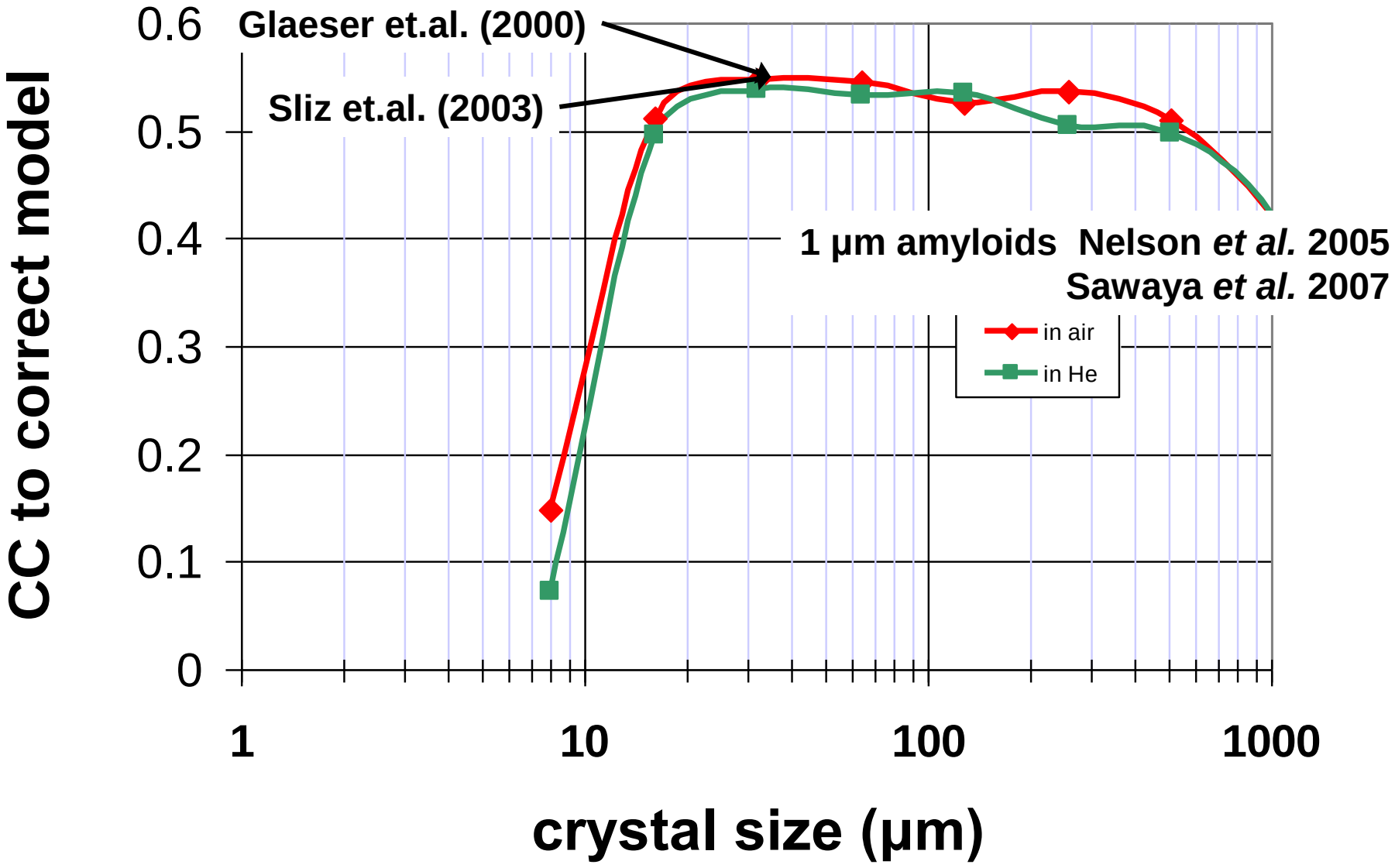
Crystal Size



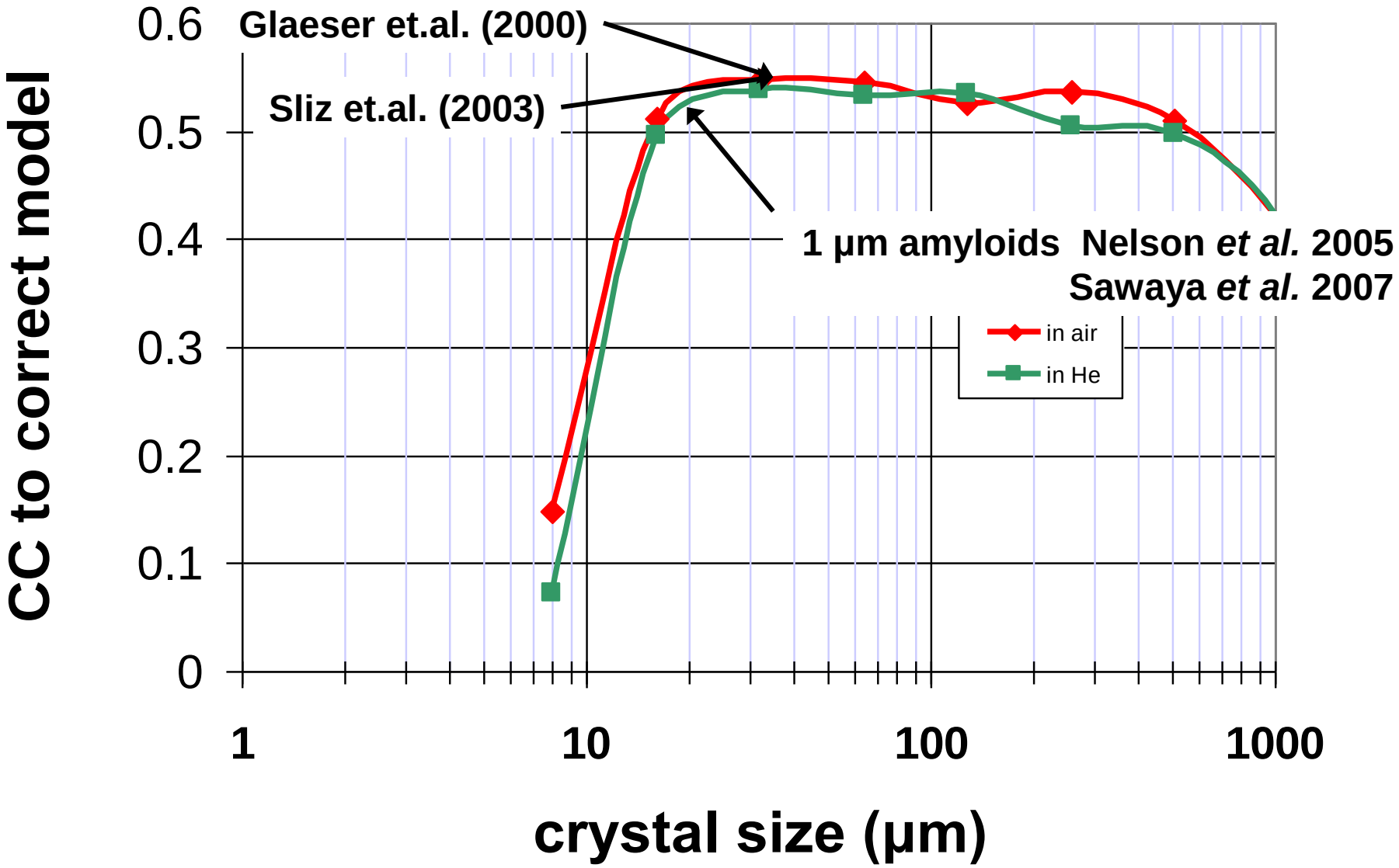
Crystal Size



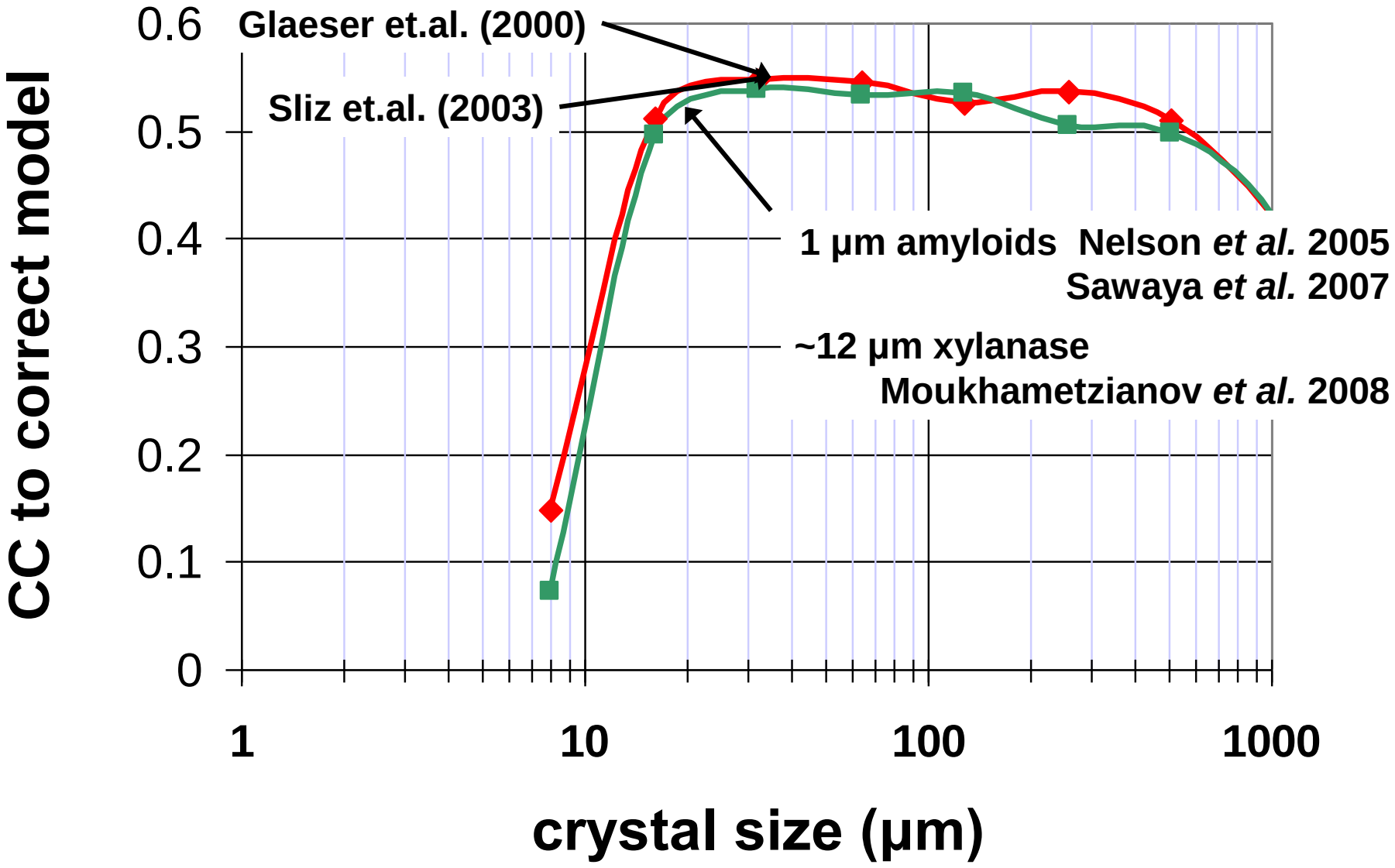
Crystal Size



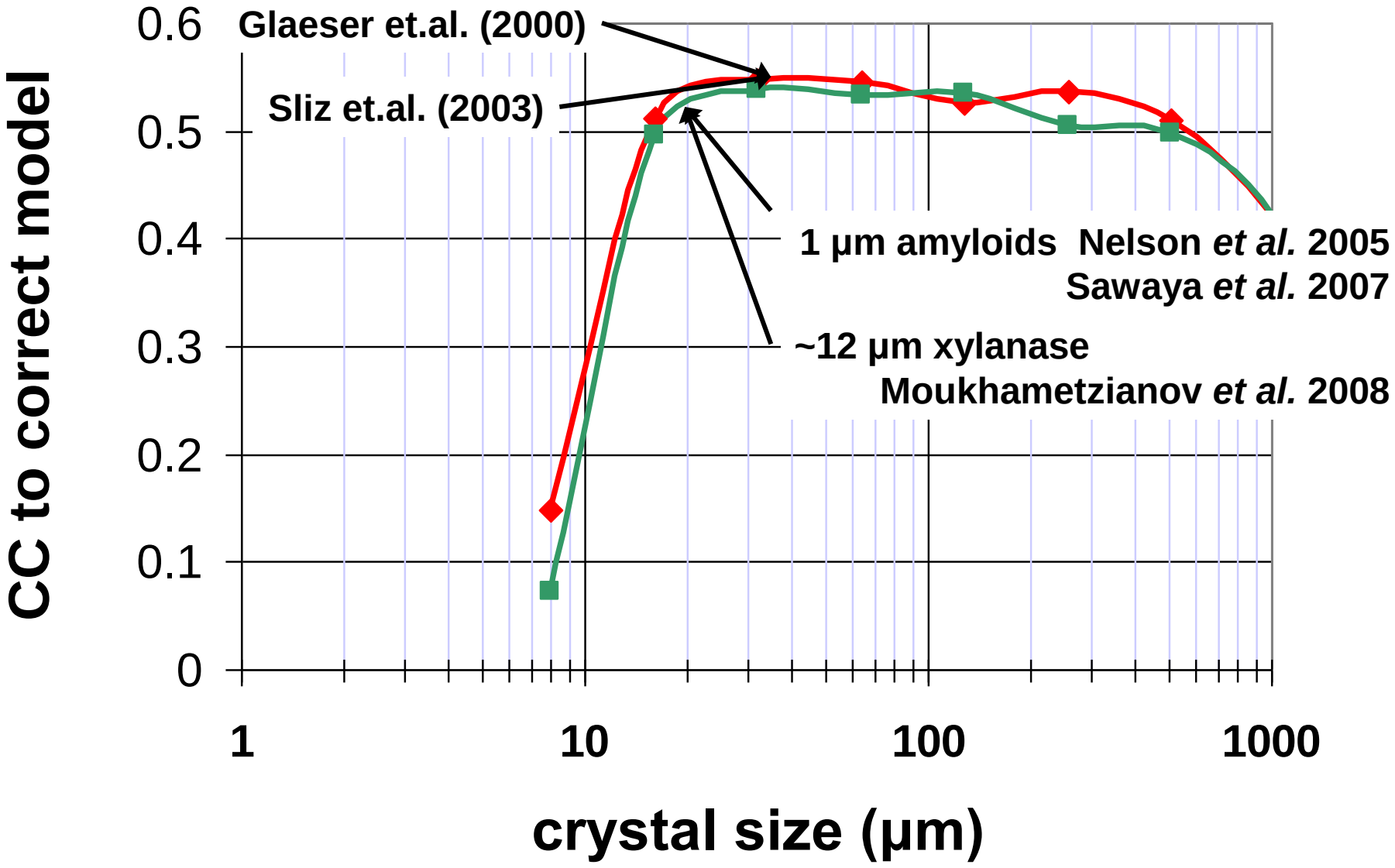
Crystal Size



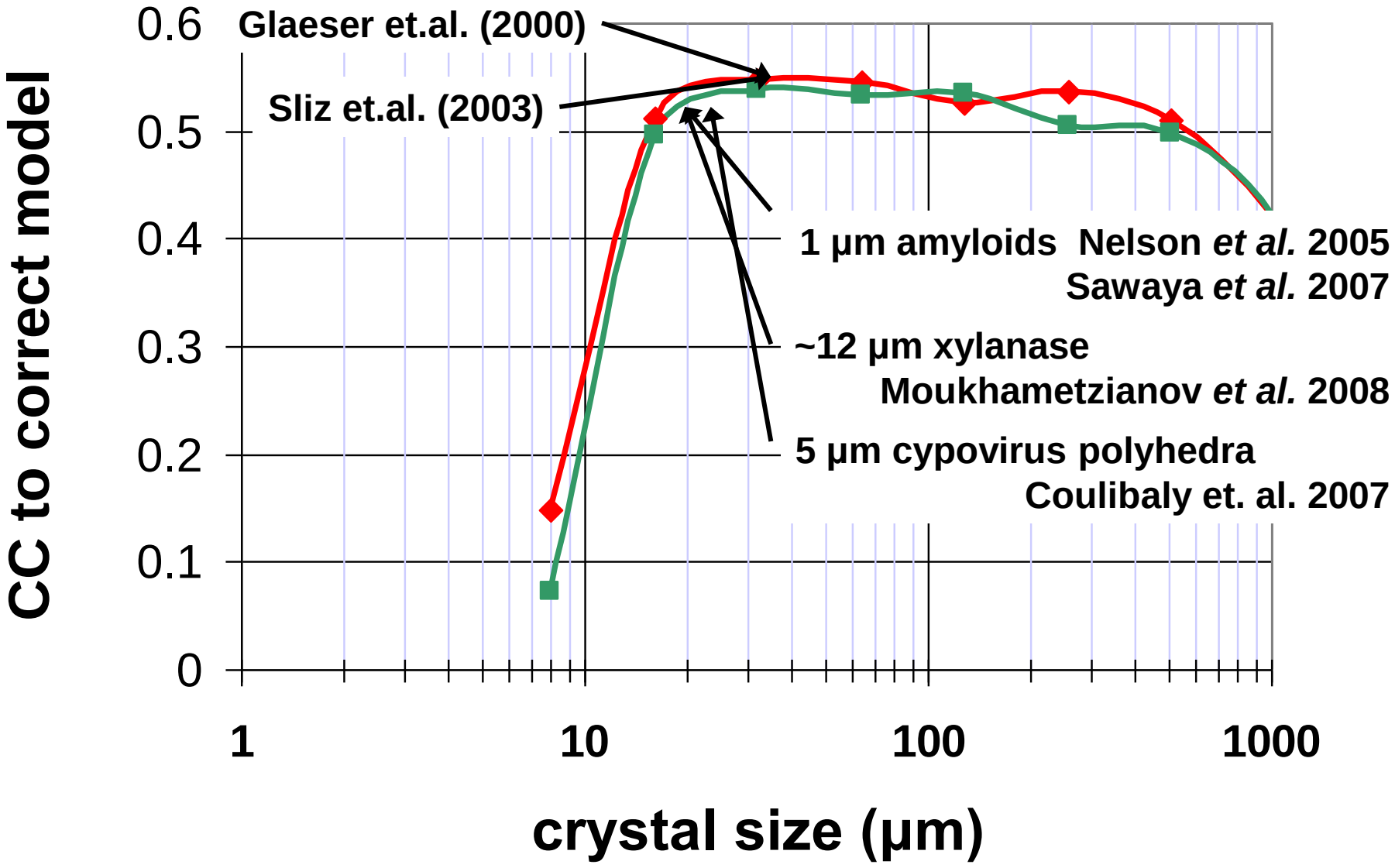
Crystal Size



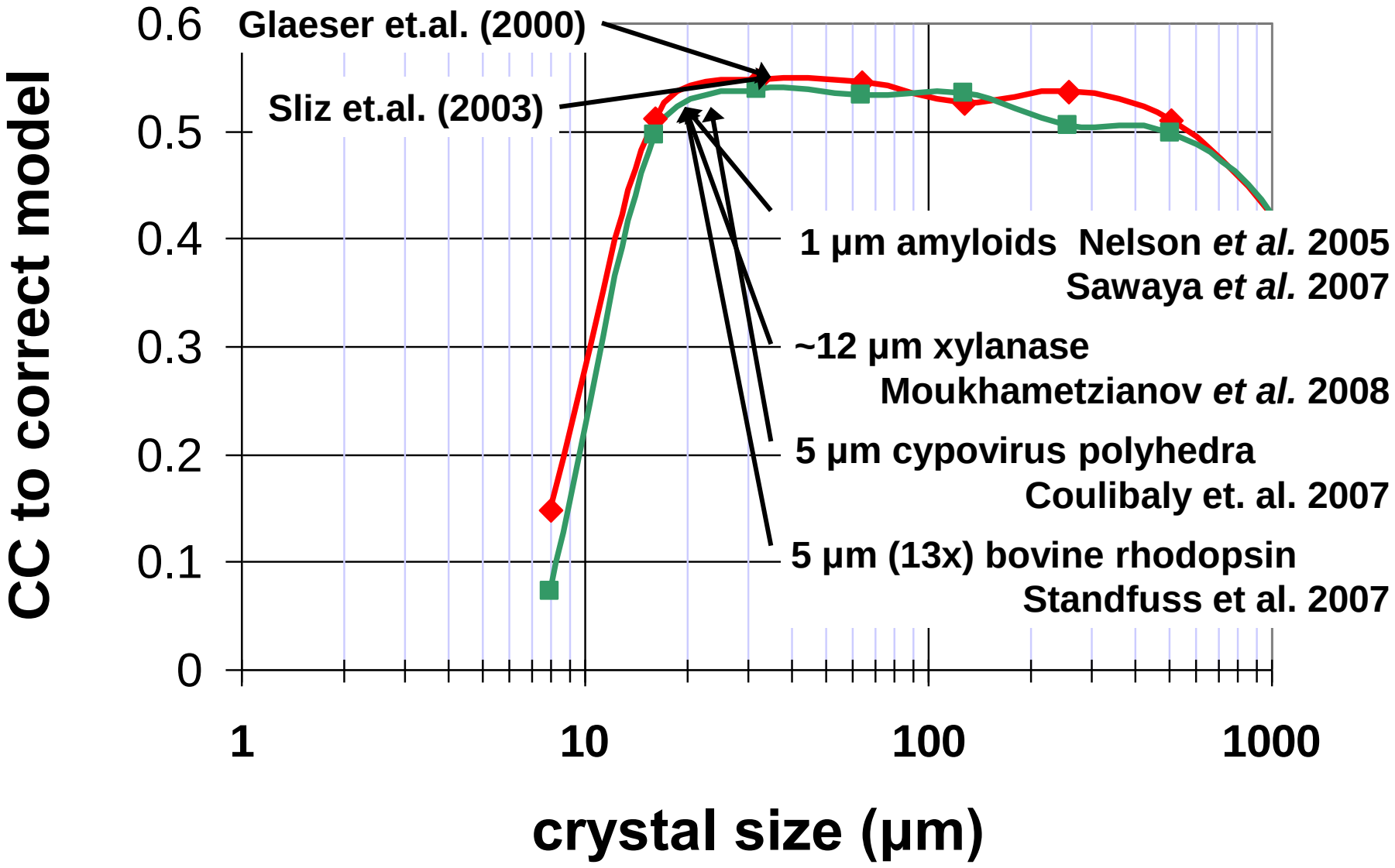
Crystal Size



Crystal Size



Crystal Size



Minimum Crystal Size

$$n_{xtal} = n_0 \frac{MW \; V_M^{\,2}}{\ell_x \ell_y \ell_z \, (d^3 - 1.53) \exp(-0.5\, B/d^2)}$$

n_{xtal} - number of crystals needed

n_0 - empirical constant (~ 3)

MW - molecular weight (kDa)

V_M - Matthews number (~2.5 Å^3/Da)

ℓ - crystal size (microns)

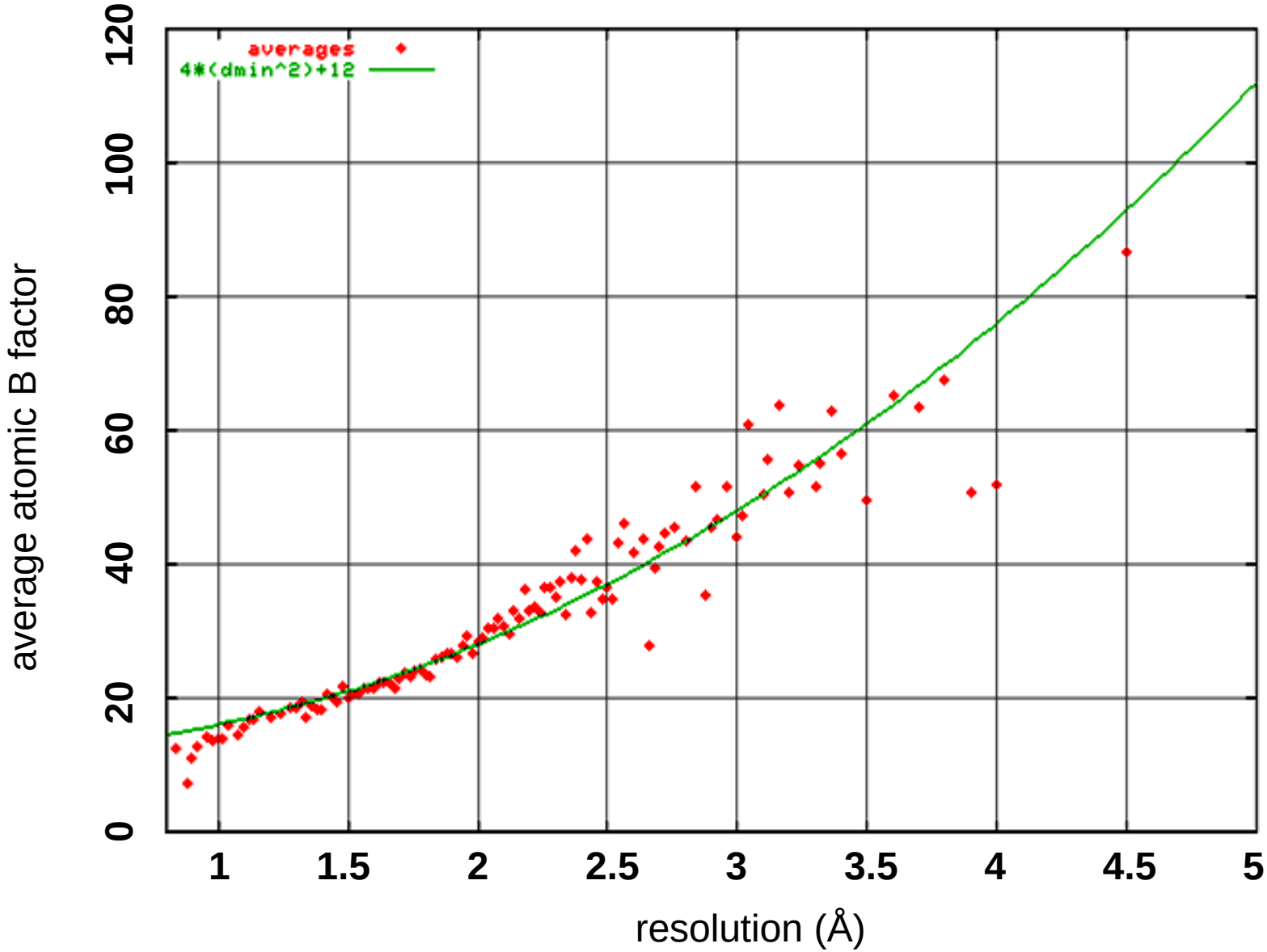
d - d-spacing of interest (Å)

B - Wilson B factor (Å^2)

$$B \approx 4\, d^2 + 12$$

Holton J. M. (2009) *J. Synchrotron Rad.* **16** 133-42

$B \approx 4\ d^2 + 12$



Minimum Crystal Size

http://bl831.als.lbl.gov/~jamesh/xtalsize.html

$$n_{xtal} = n_0 \frac{MW \; V_M^2}{\ell_x \ell_y \ell_z \, (d^3 - 1.53) \exp(-0.5 \, B/d^2)}$$

n_{xtal} - number of crystals needed

n_0 - empirical constant (~ 3)

MW - molecular weight (kDa)

V_M - Matthews number (~2.5 Å^3/Da)

ℓ - crystal size (microns)

d - d-spacing of interest (Å)

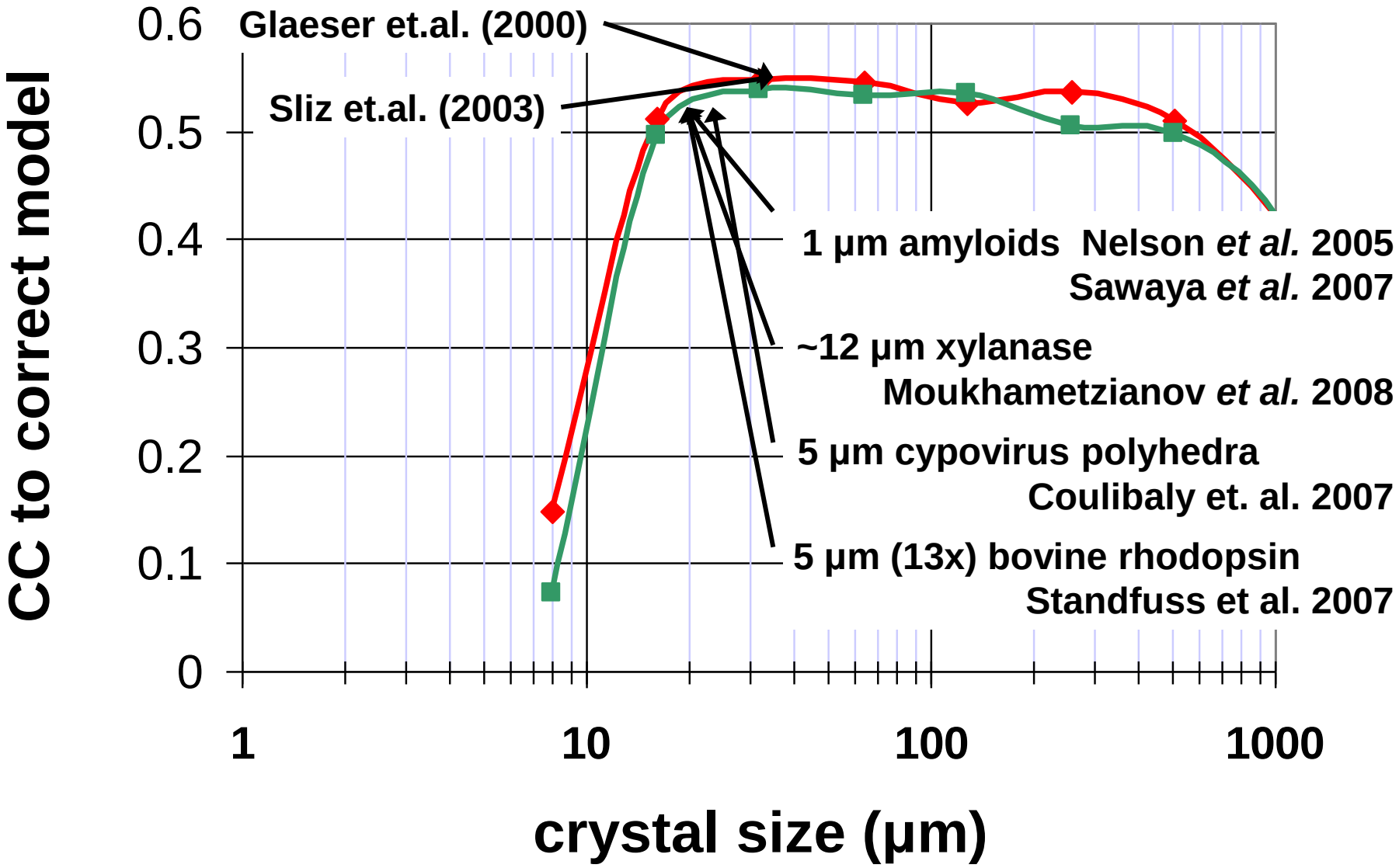
B - Wilson B factor (Å^2)

$$B \approx 4 \, d^2 + 12$$

Holton J. M. (2009) *J. Synchrotron Rad.* **16** 133-42

Crystal Size

http://bl831.als.lbl.gov/~jamesh/xtalsize.html



Crystal Size

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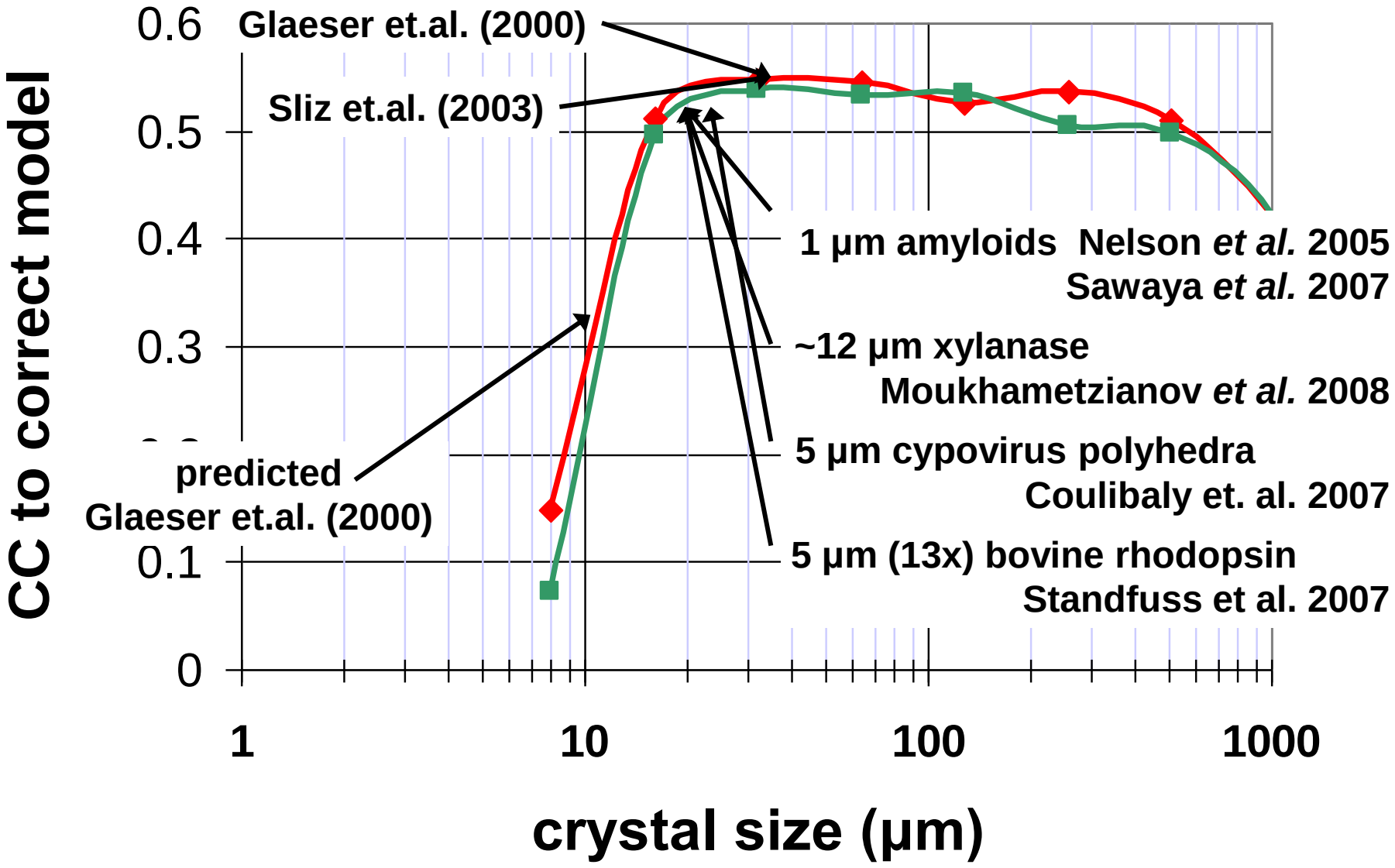
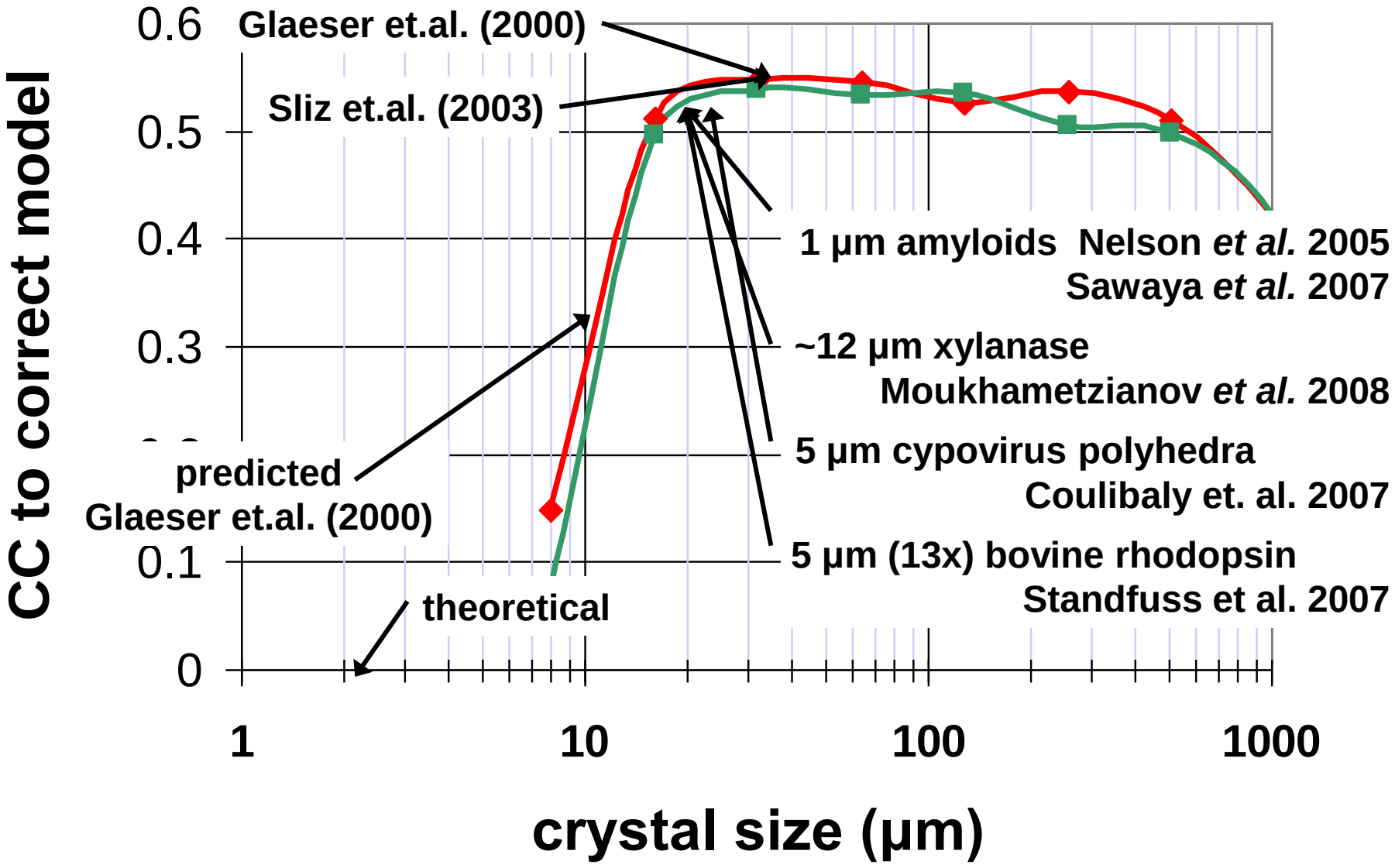


Crystal Size

http://bl831.als.lbl.gov/~jamesh/xtalsize.html



Theoretical limit for lysozyme:

$$< I_{max} > (s) \cong \frac{8 \cdot 10^{29}\, r_e^{\,2}\, \rho R^4 \lambda^4}{9\pi\, hc\, H\, s\, n_{ASU}\, M_r V_M^{\,2}} \left(\frac{1.05 \cdot \pi}{4\, s\, \lambda} - \frac{1}{2} \right) \cdot \frac{T_{sphere}(2\theta, \mu, R)}{1 - T_{sphere}(0, \mu_{en}, R)} \cdot \frac{< f_a(s) >^2 \exp(-2Bs^2)}{< M_a >}$$

Where:

$<I_{max}>$ (s)	- average damage-limited spot intensity (photons) at "s"
s	- sin(θ)/λ or 0.5/d if d is the d-spacing of interest ($Å^{-1}$)
θ	- Bragg angle
r_e	- classical electron radius (2.818 x 10^{-15} m)
10^{29}	- conversion from m^4 to $Å^4$, g/cm^3 to kg/m^3 and MGy to Gy
ρ	- density of crystal (~1.2 g/cm^3)
R	- radius of the spherical crystal (m)
λ	- x-ray wavelength (Å)
h	- Plank's constant (6.626 x 10^{-34} J·s)
c	- speed of light (299792458 m/s)
H	- Howells's coefficient (11 x 10^{-3} Å/MGy)
n_{ASU}	- number of proteins in the asymmetric unit
M_r	- molecular weight of the protein (Daltons or g/mol)
VM	- Matthews's coefficient (~2.4 $Å^3$/Dalton)
$<f_a(s)>^2$	- number-averaged squared protein atom structure factor (electron units^2)
$<M_a>$	- number-averaged atomic weight of a protein atom (~7.1 Daltons)
B	- average (Wilson) temperature factor ($Å^2$)
μ	- attenuation coefficient of sphere material (m^{-1})
μ_{en}	- mass energy-absorption coefficient of sphere material (m^{-1})

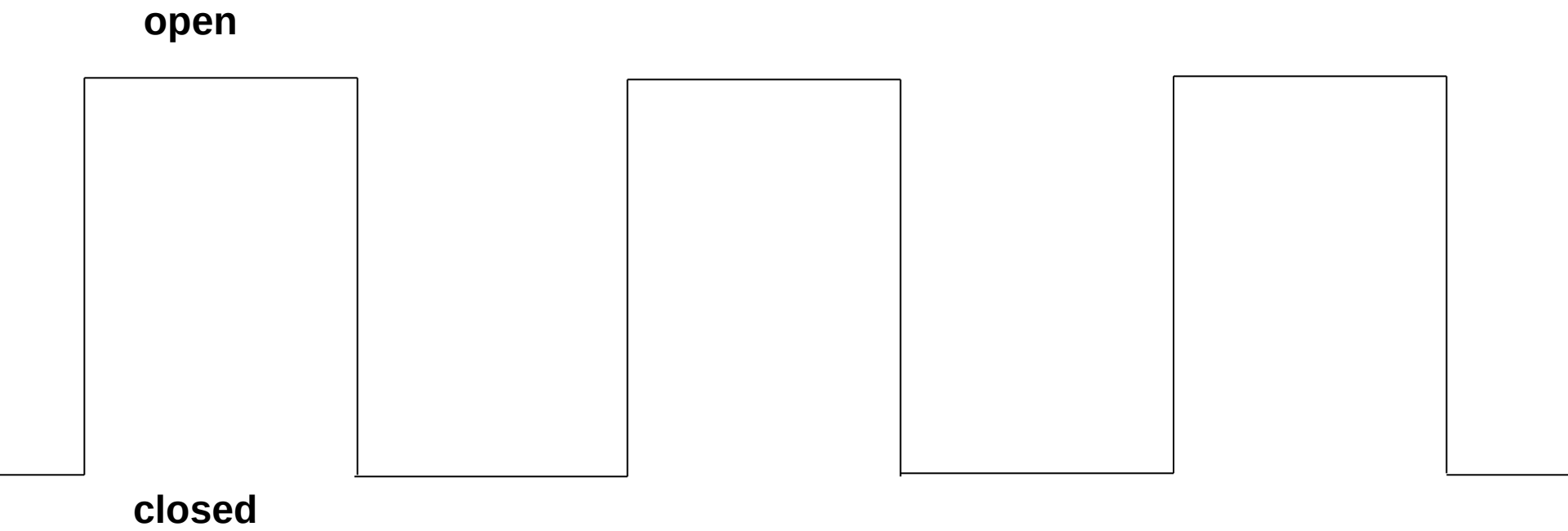
Theoretical limit for lysozyme:

$$1.0 \frac{\text{photon}}{\text{spot } \mu\text{m}^3}$$

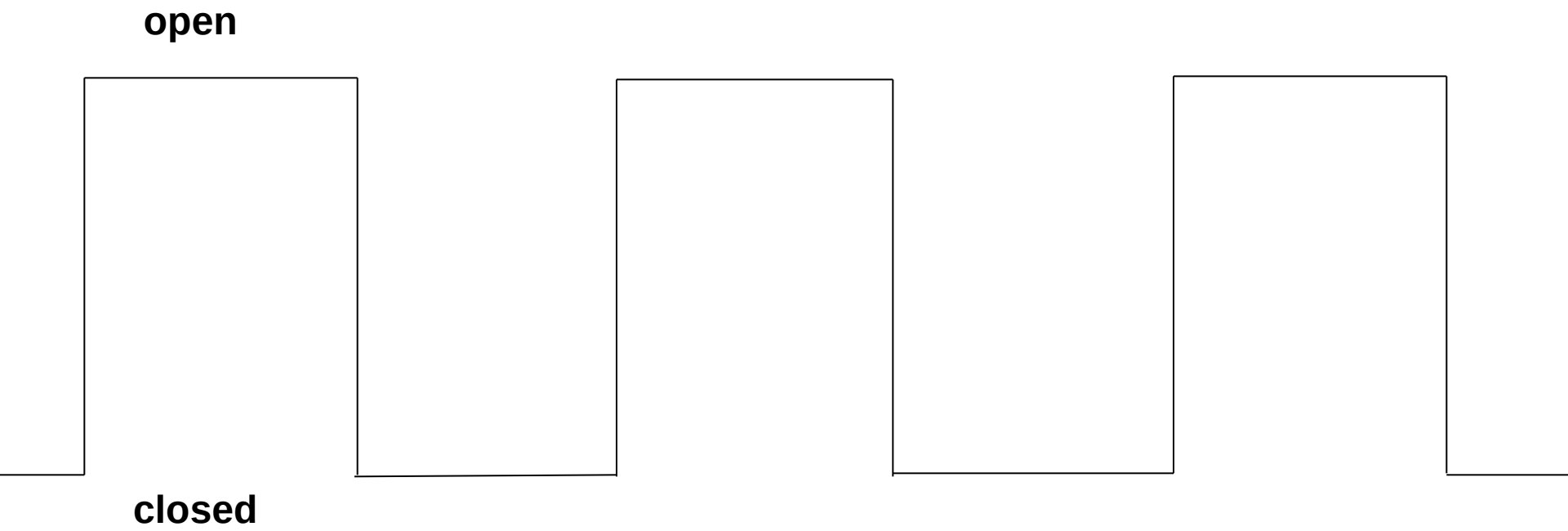
at ~2.4 Å

What if we had a “better” beamline?

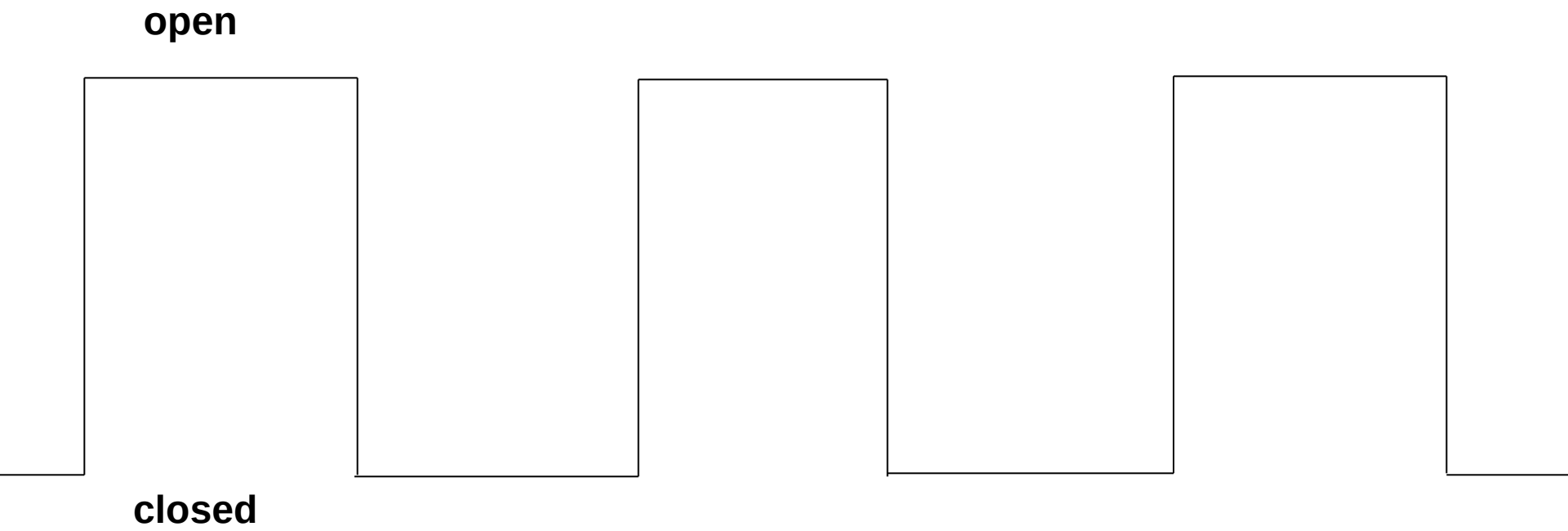
Shutter Jitter



Shutter Jitter



Shutter Jitter



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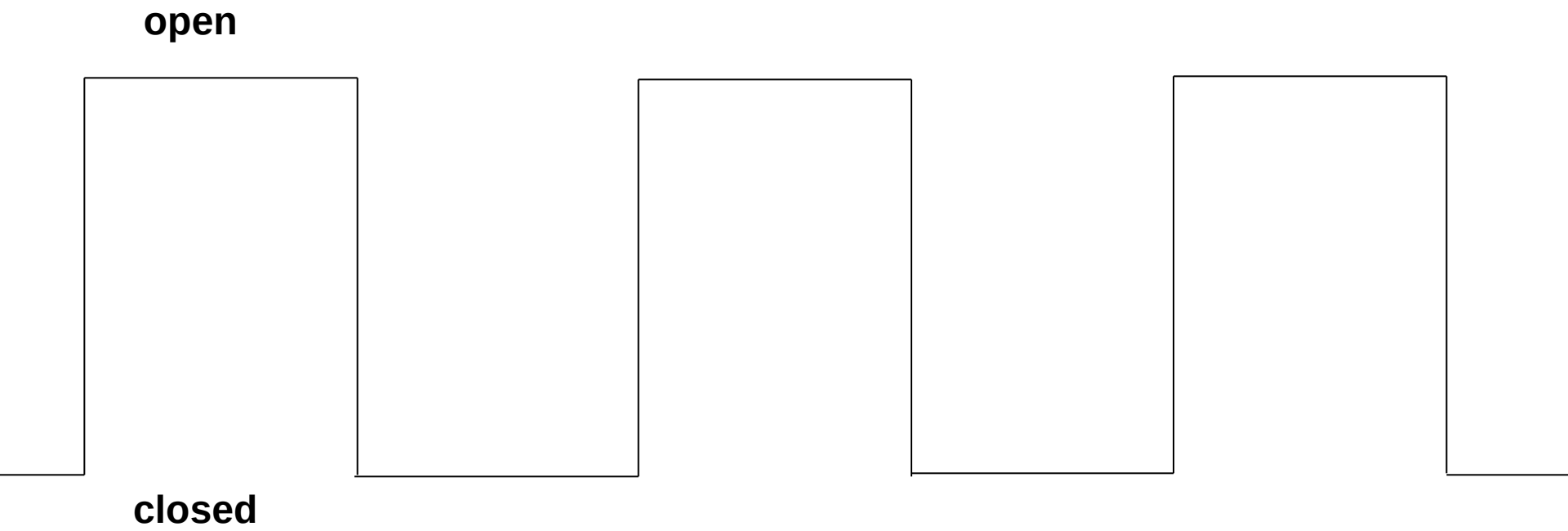

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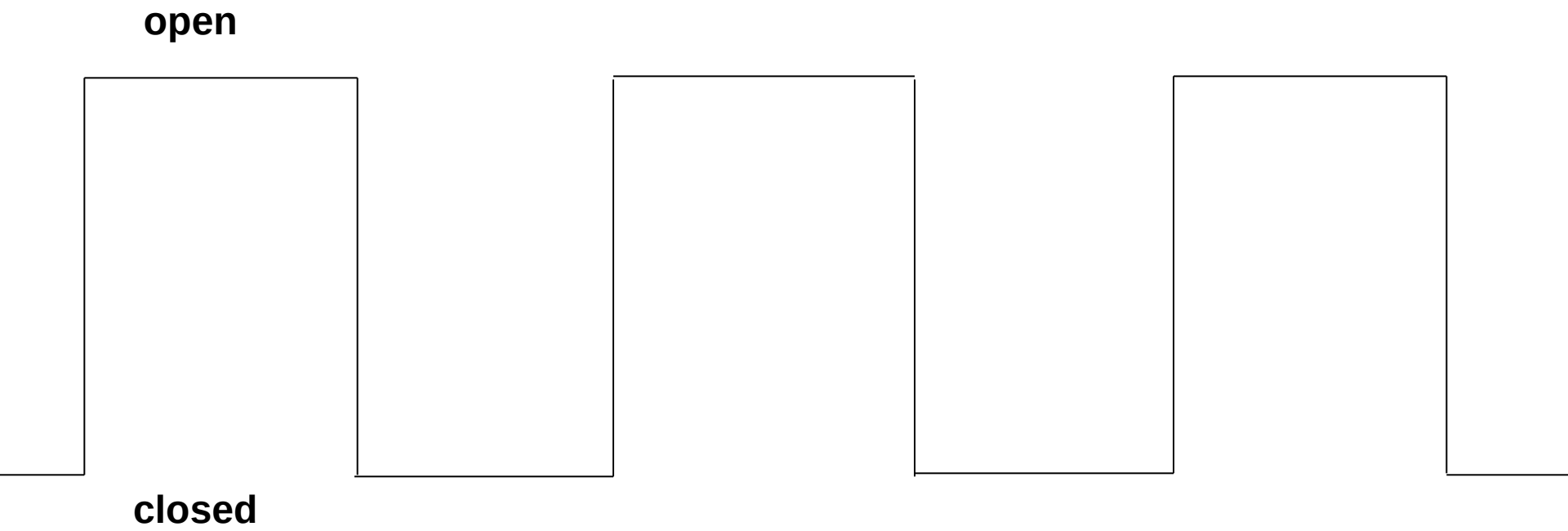

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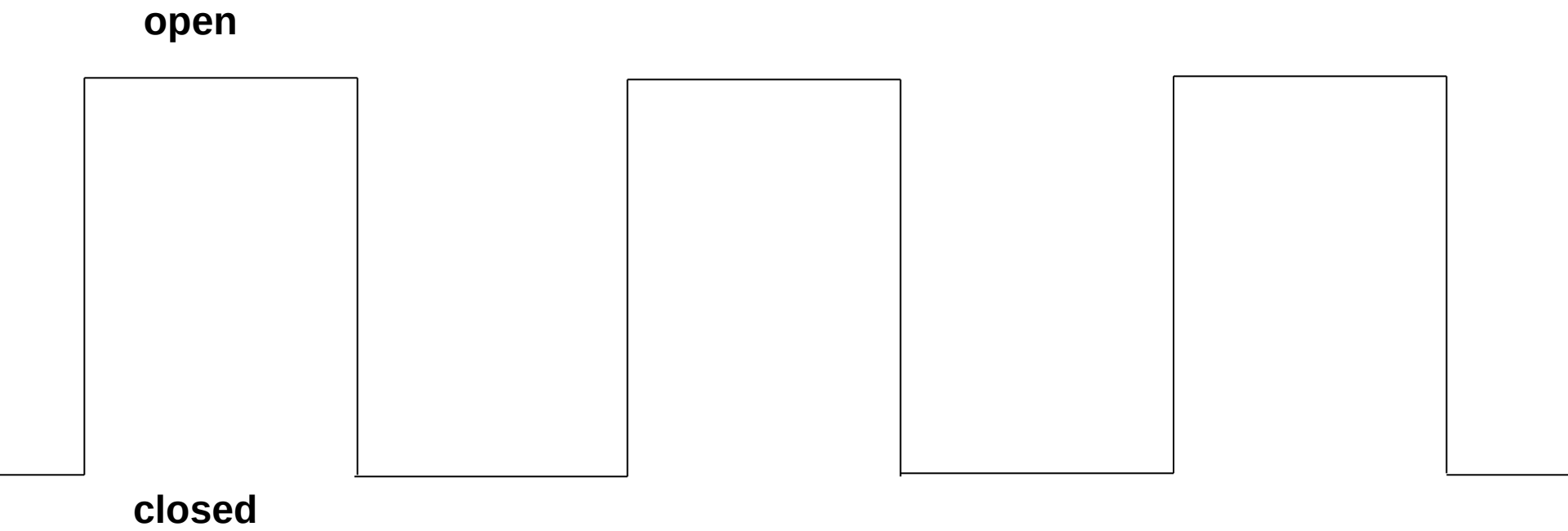

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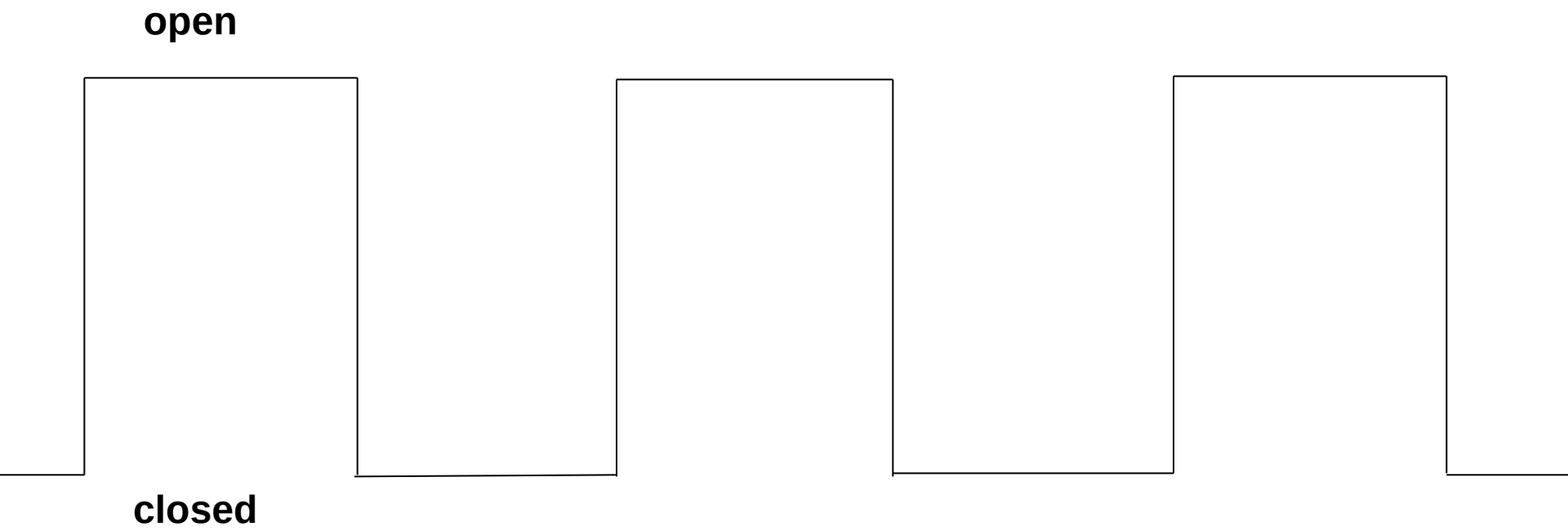

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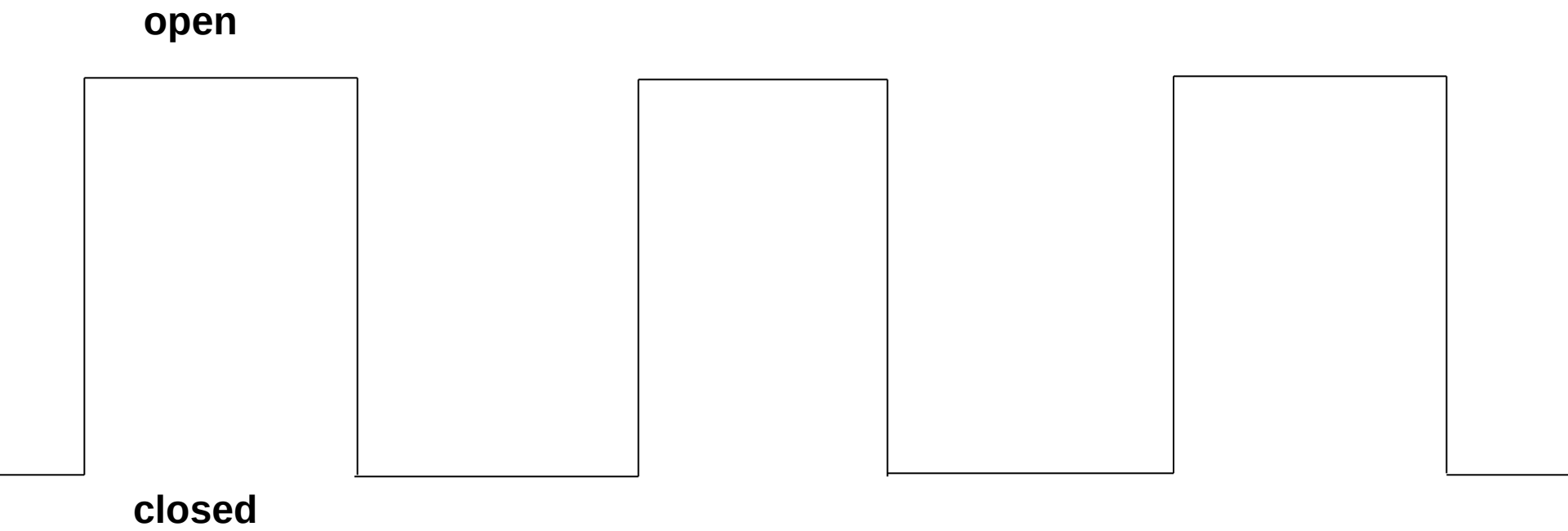

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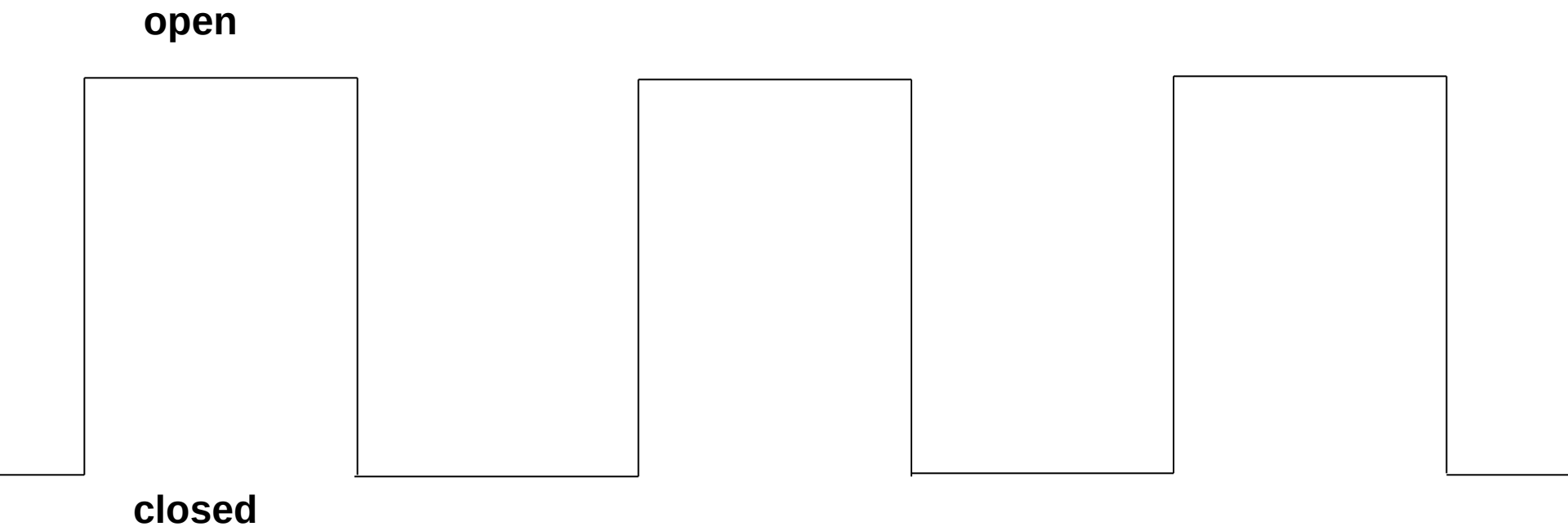

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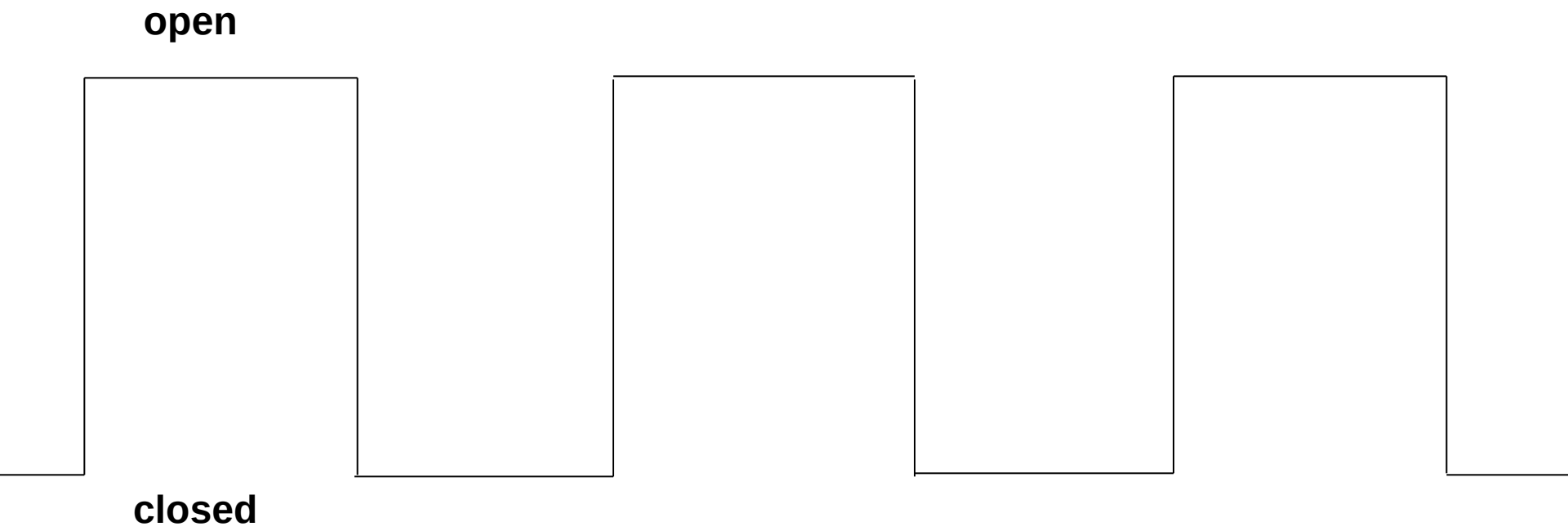

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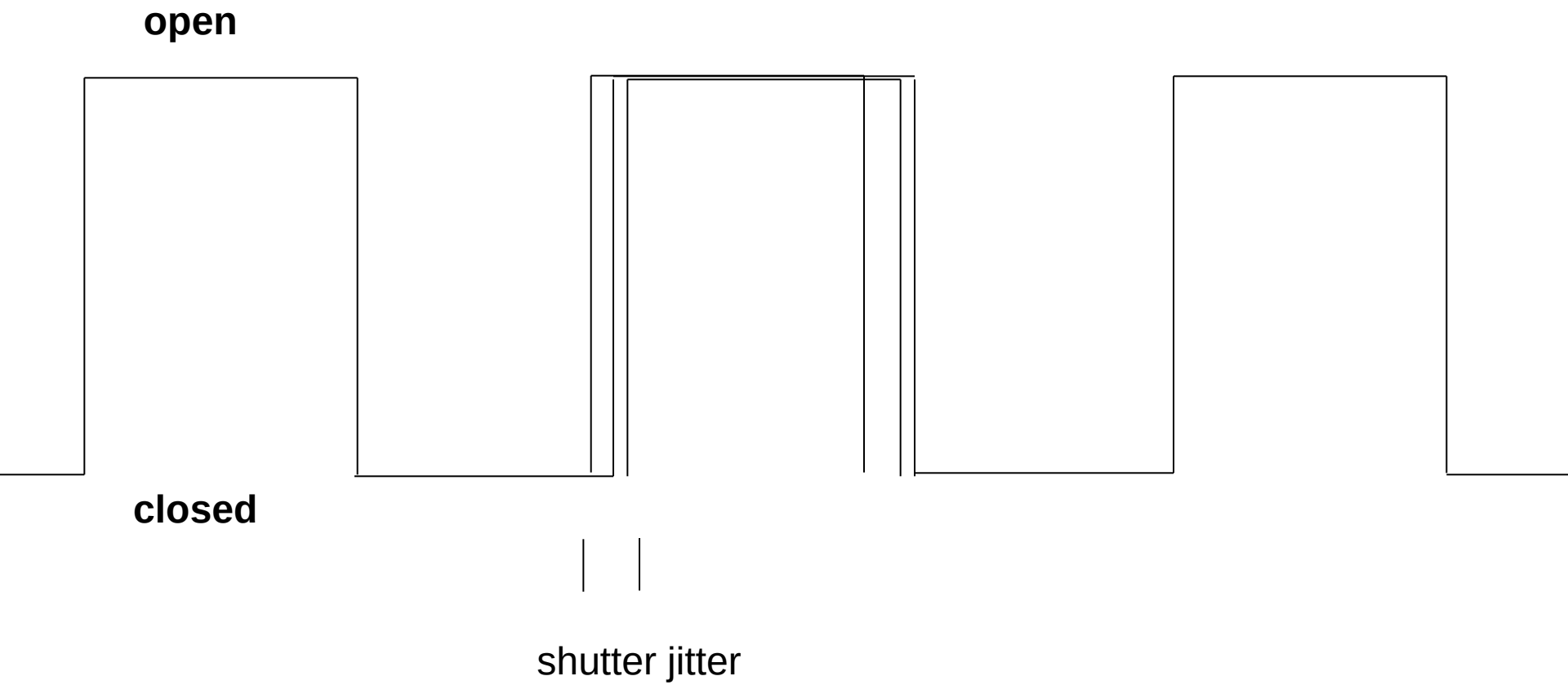

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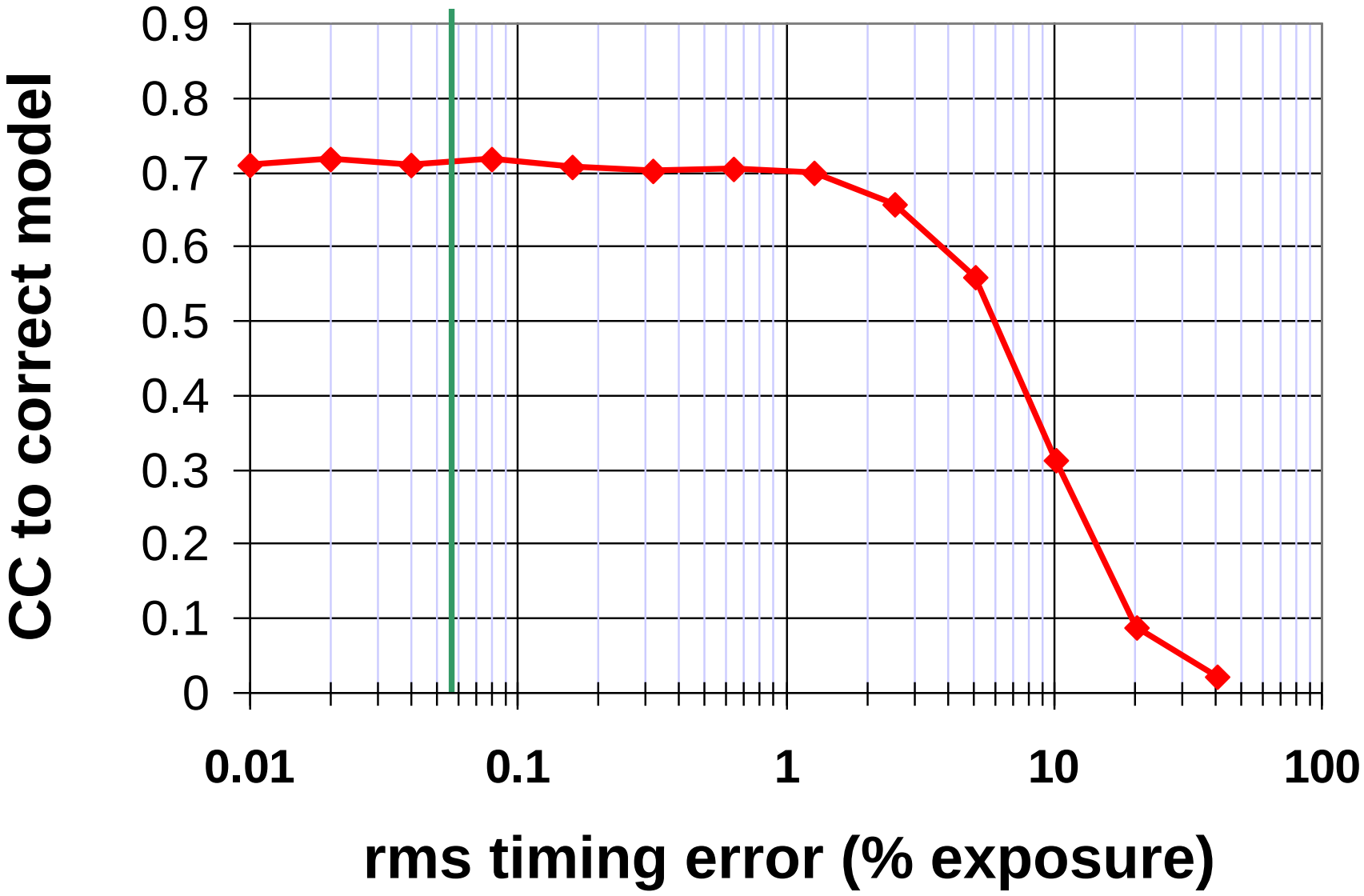


What about crystal vibration?

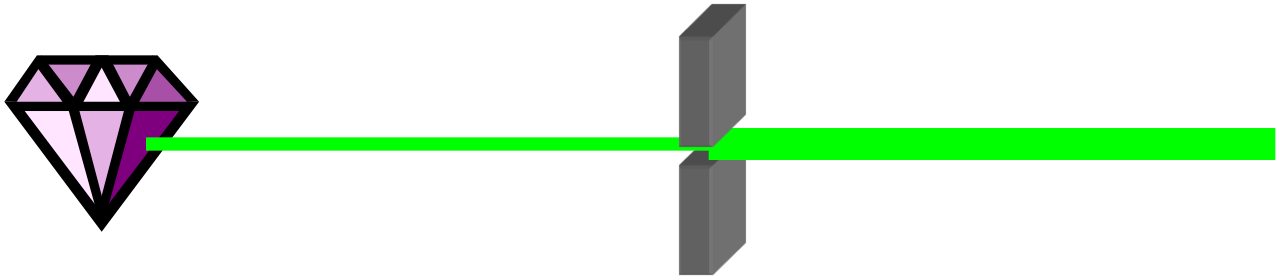
Beam Flicker

1/f noise or “flicker noise”

Beam Flicker

1/f noise or “flicker noise”

comes from everything



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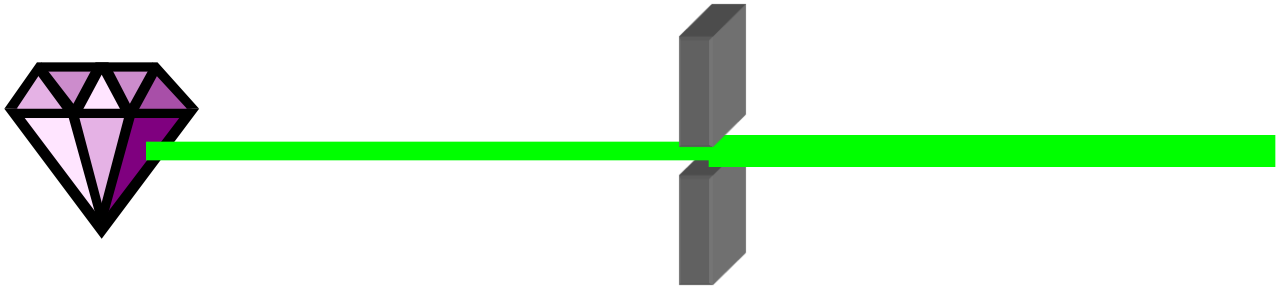

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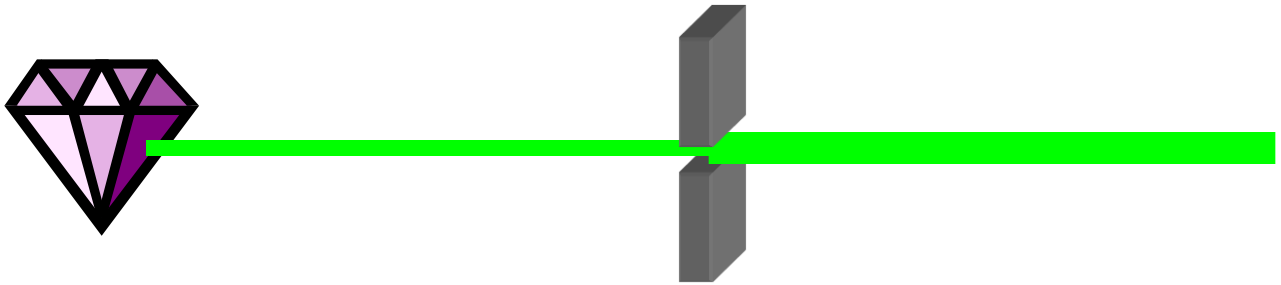

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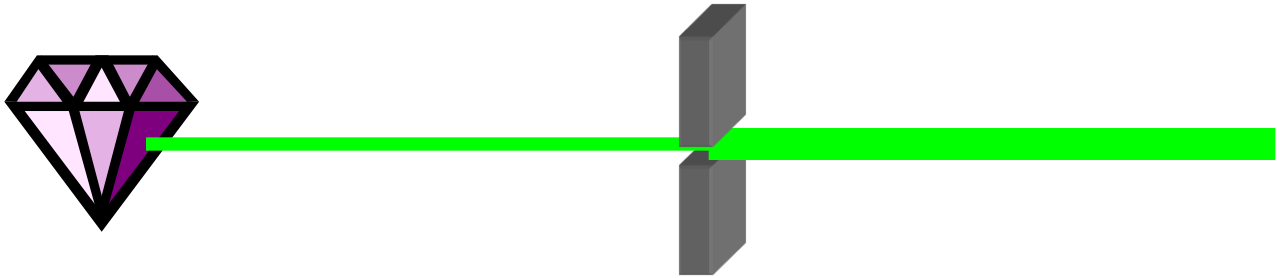

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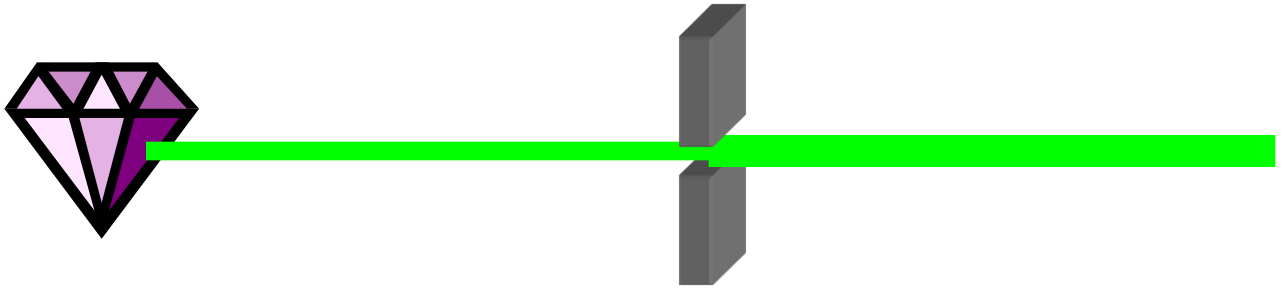

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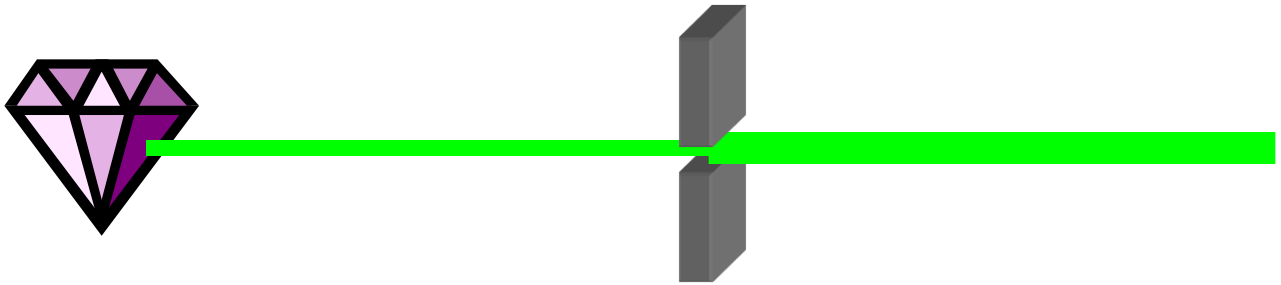

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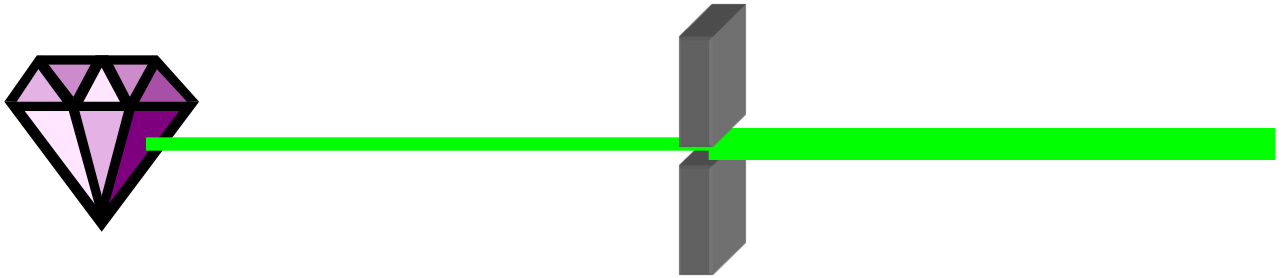

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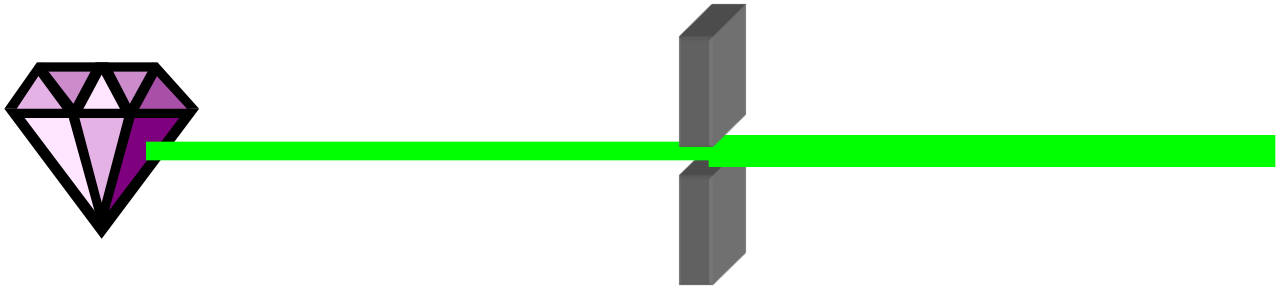

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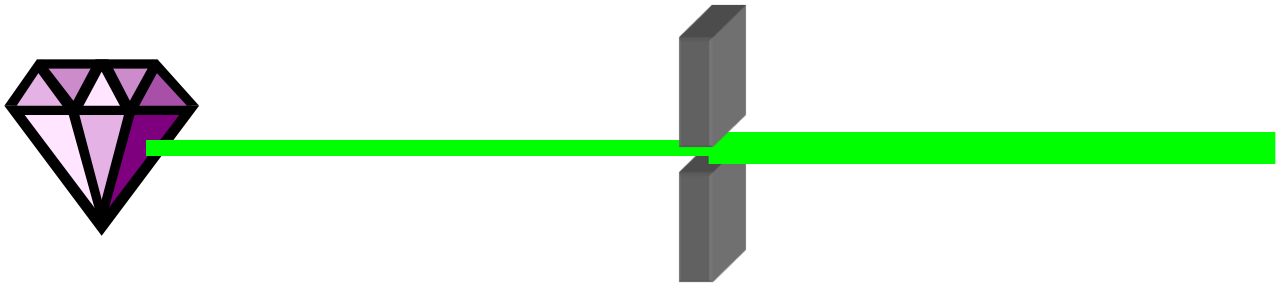

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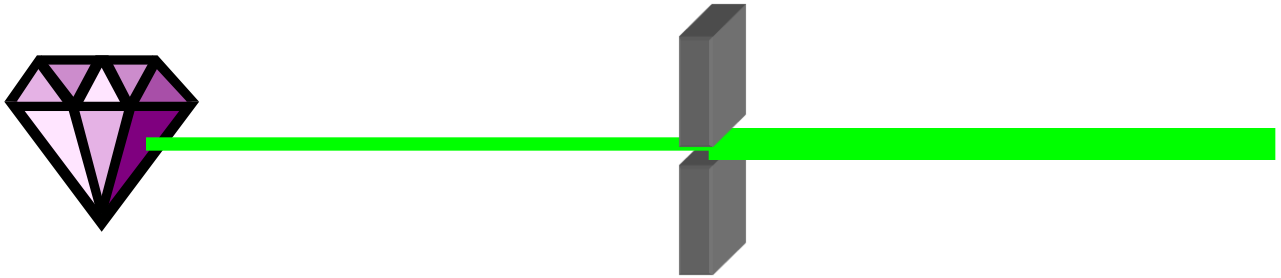

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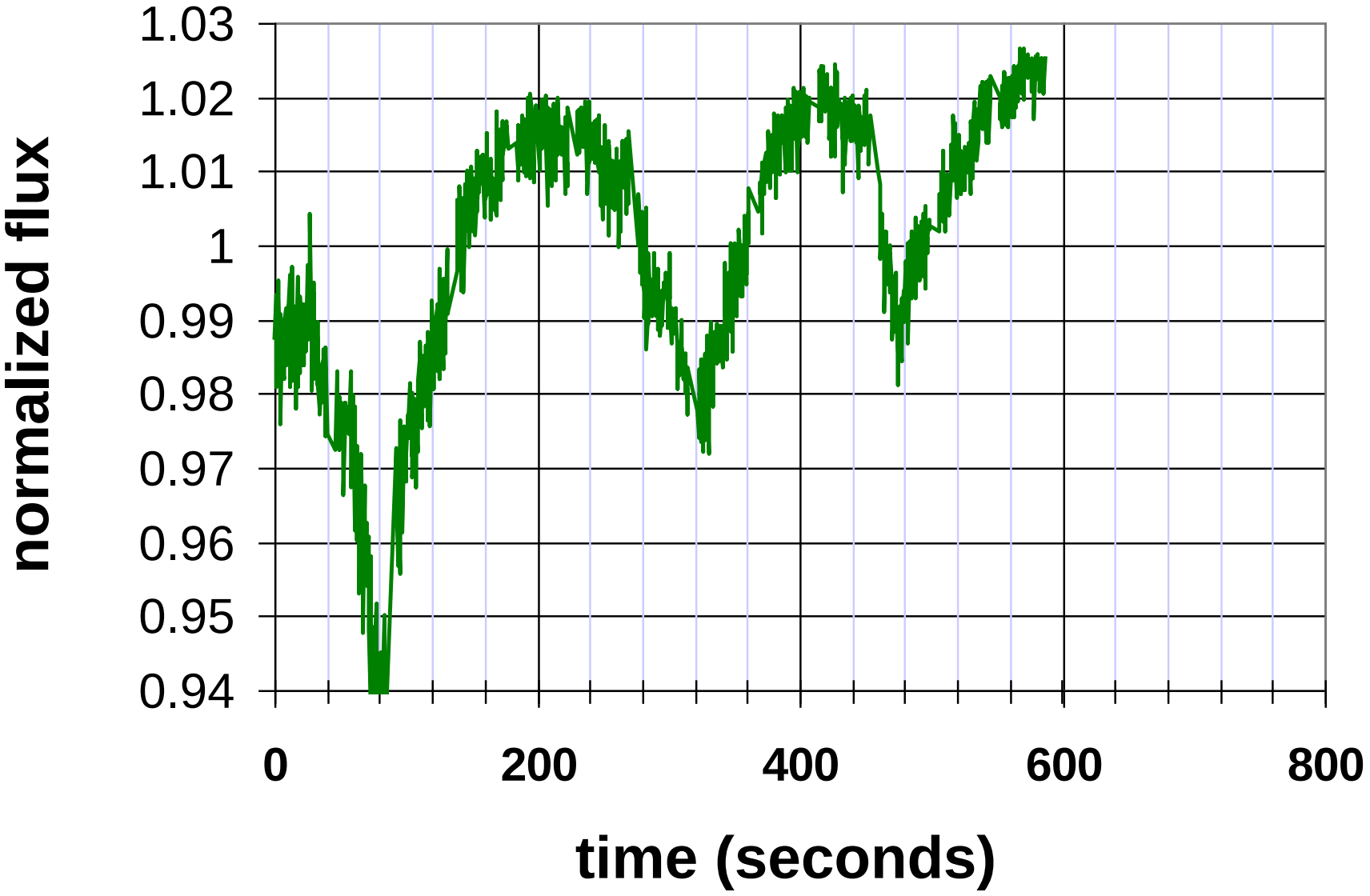

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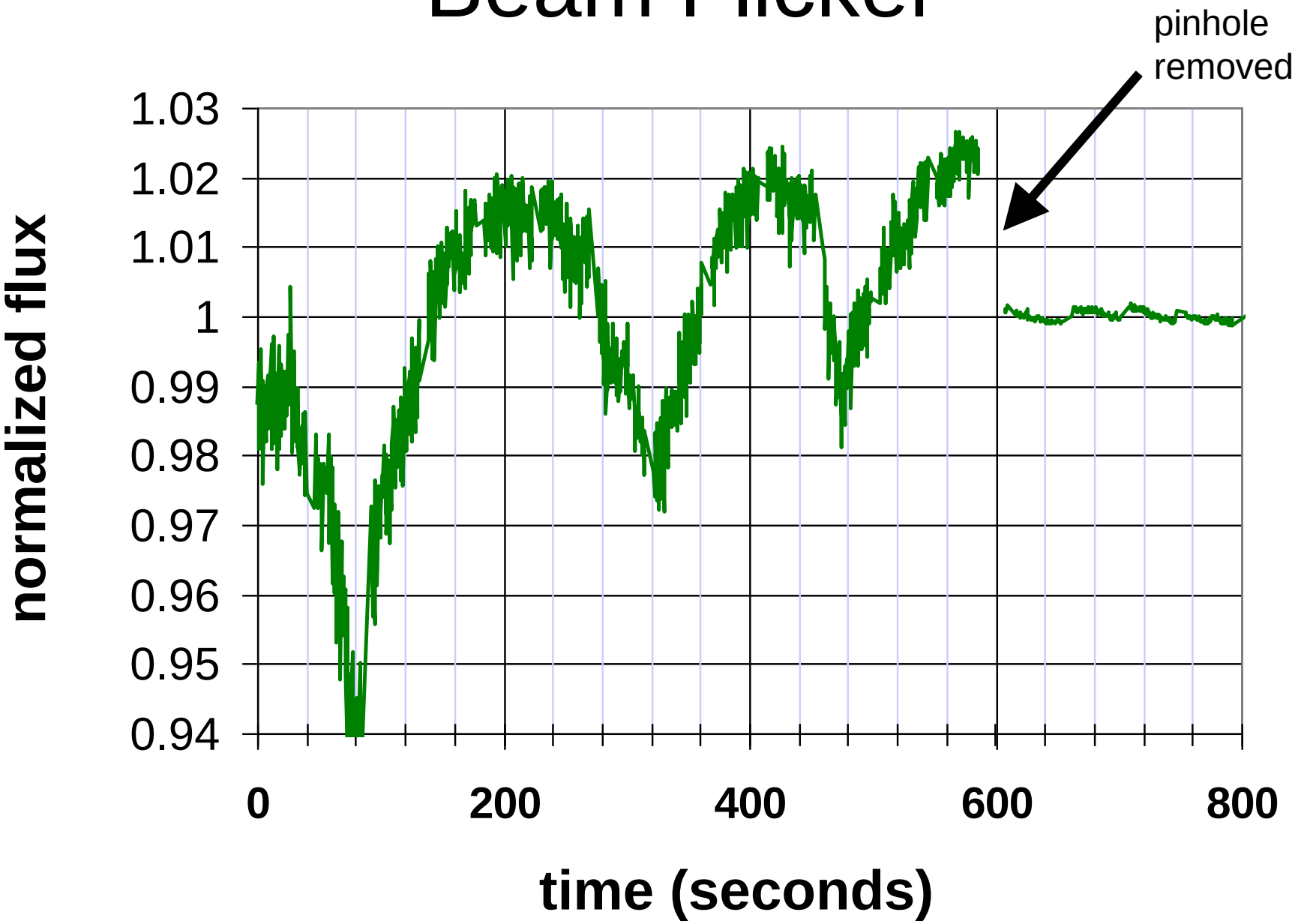
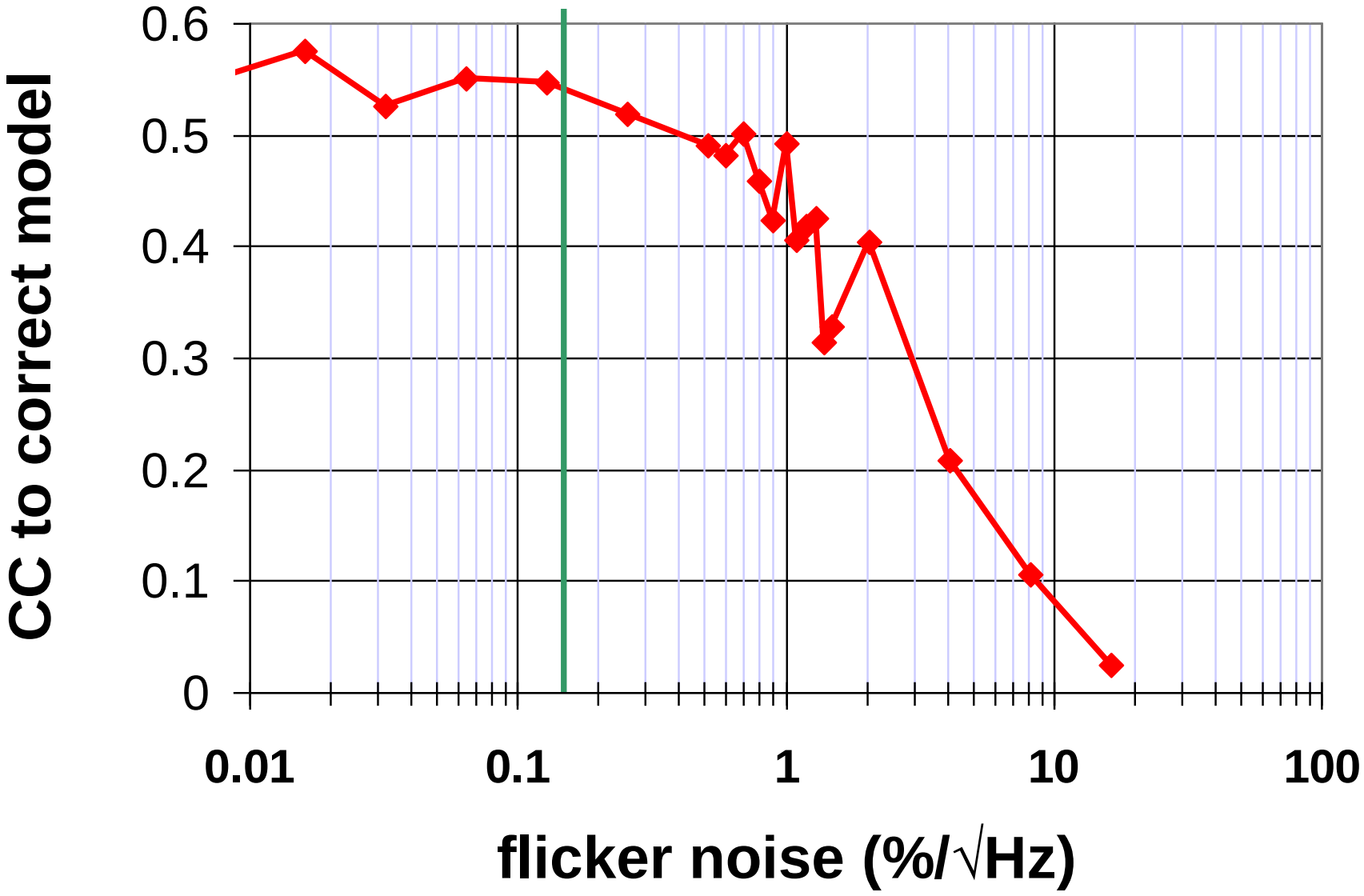


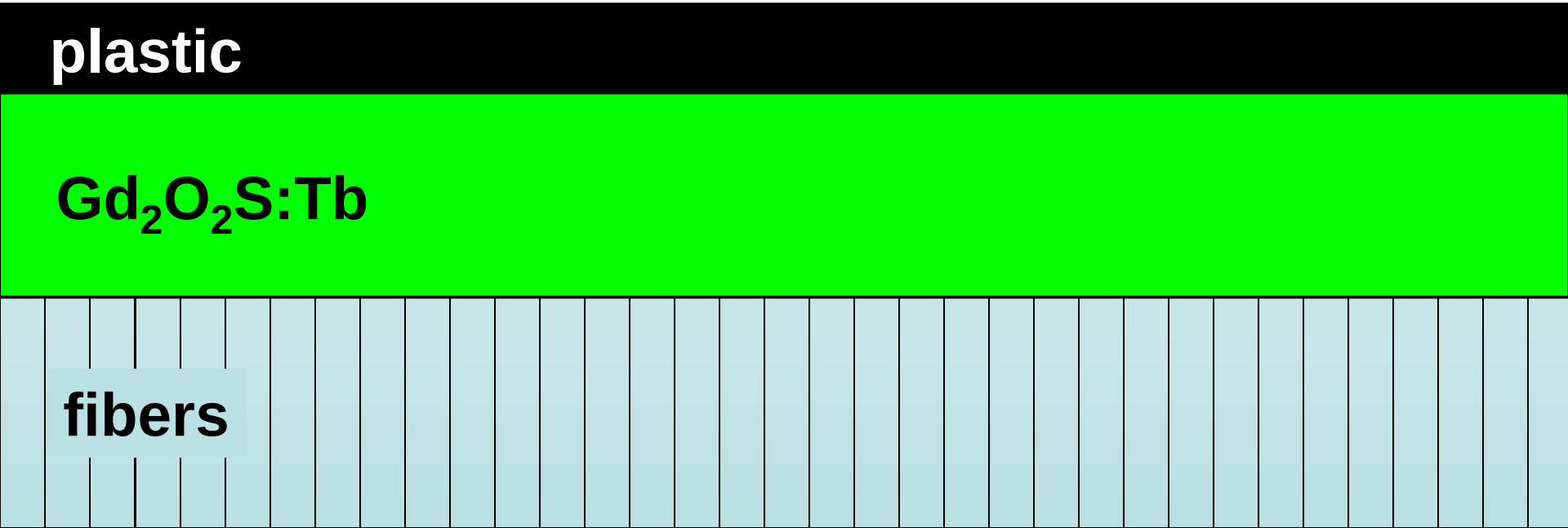
Beam Flicker



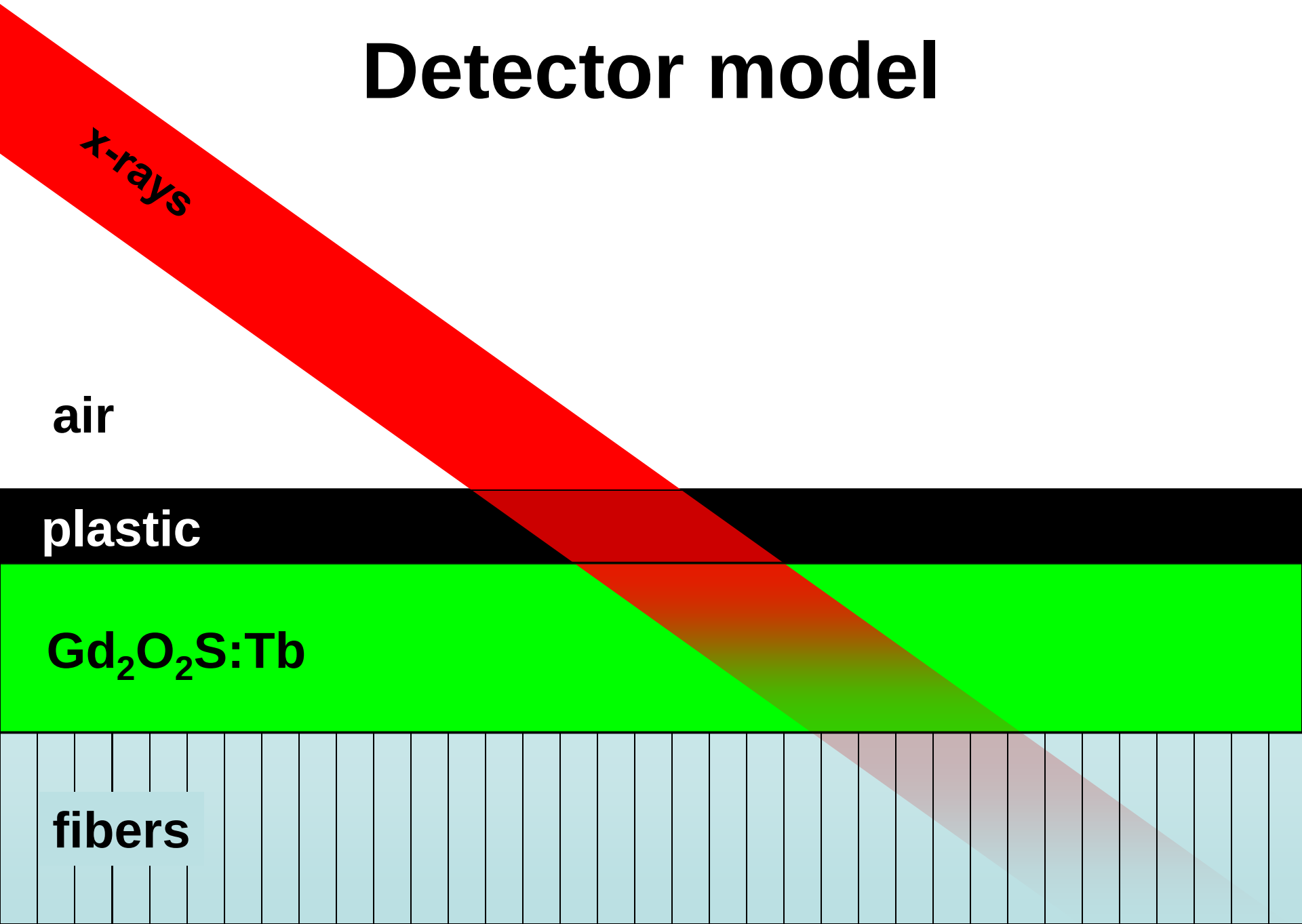
What about a better detector?

What if we had a perfect detector?

Detector model



Detector model



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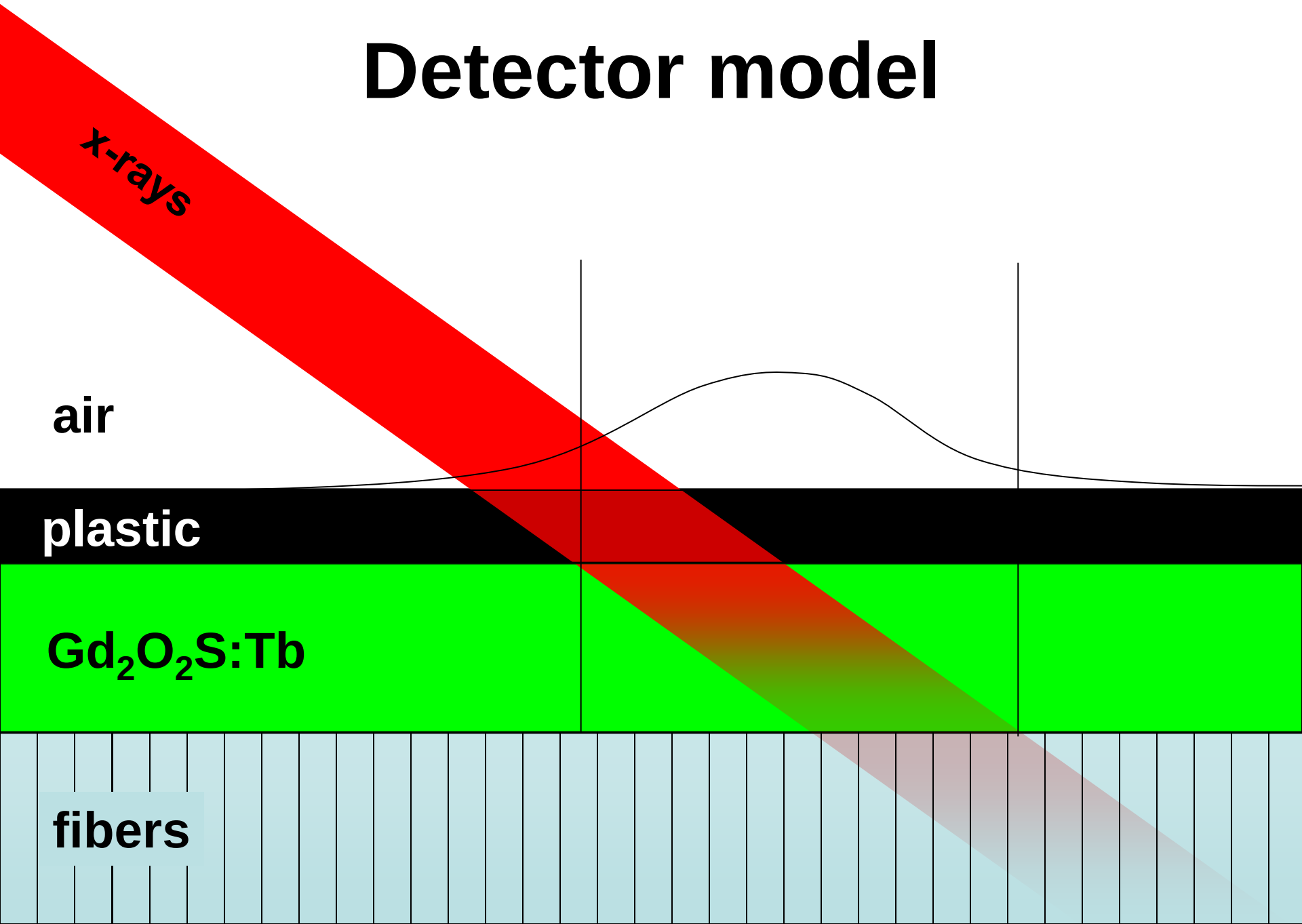
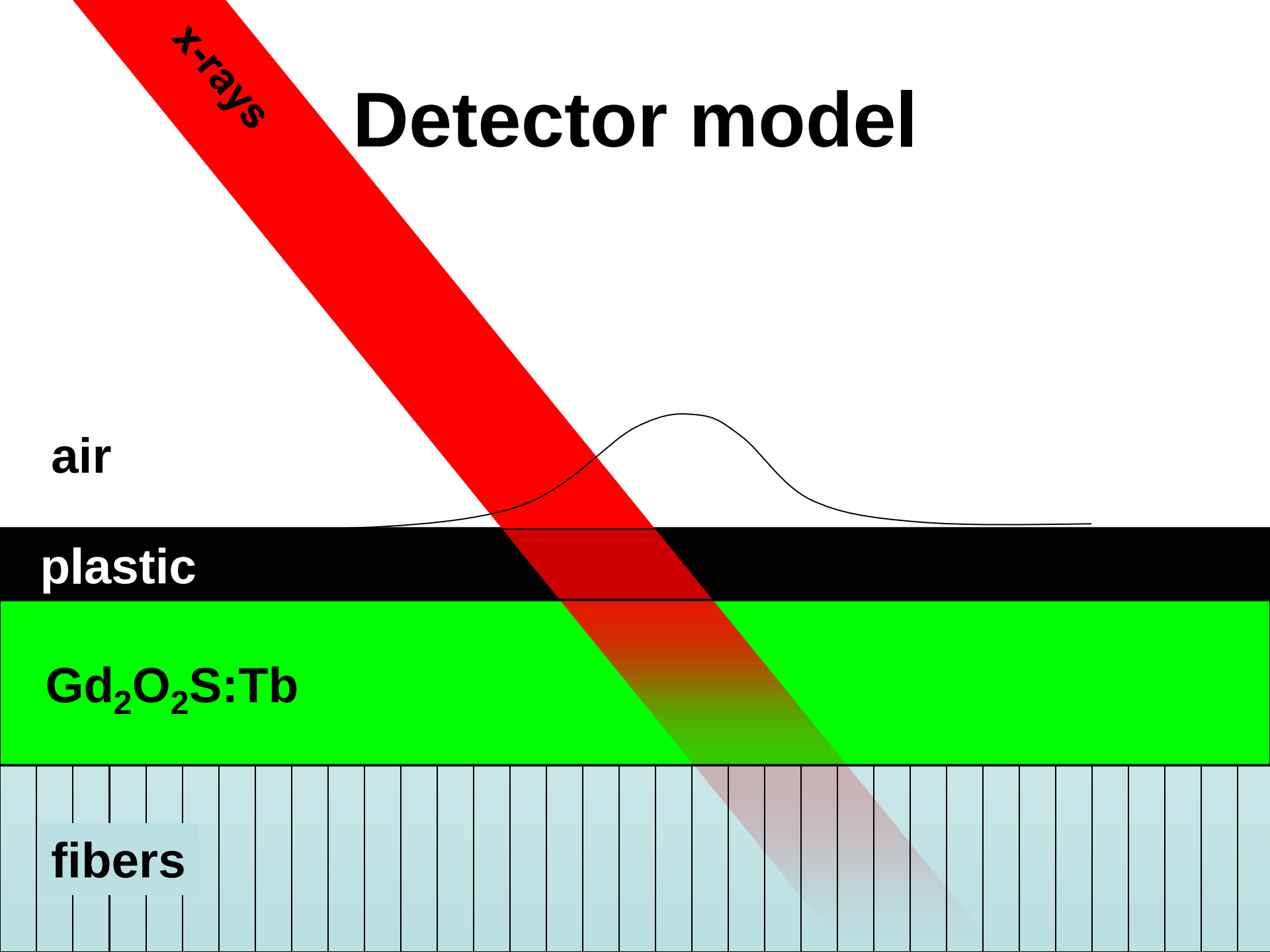


Detector model



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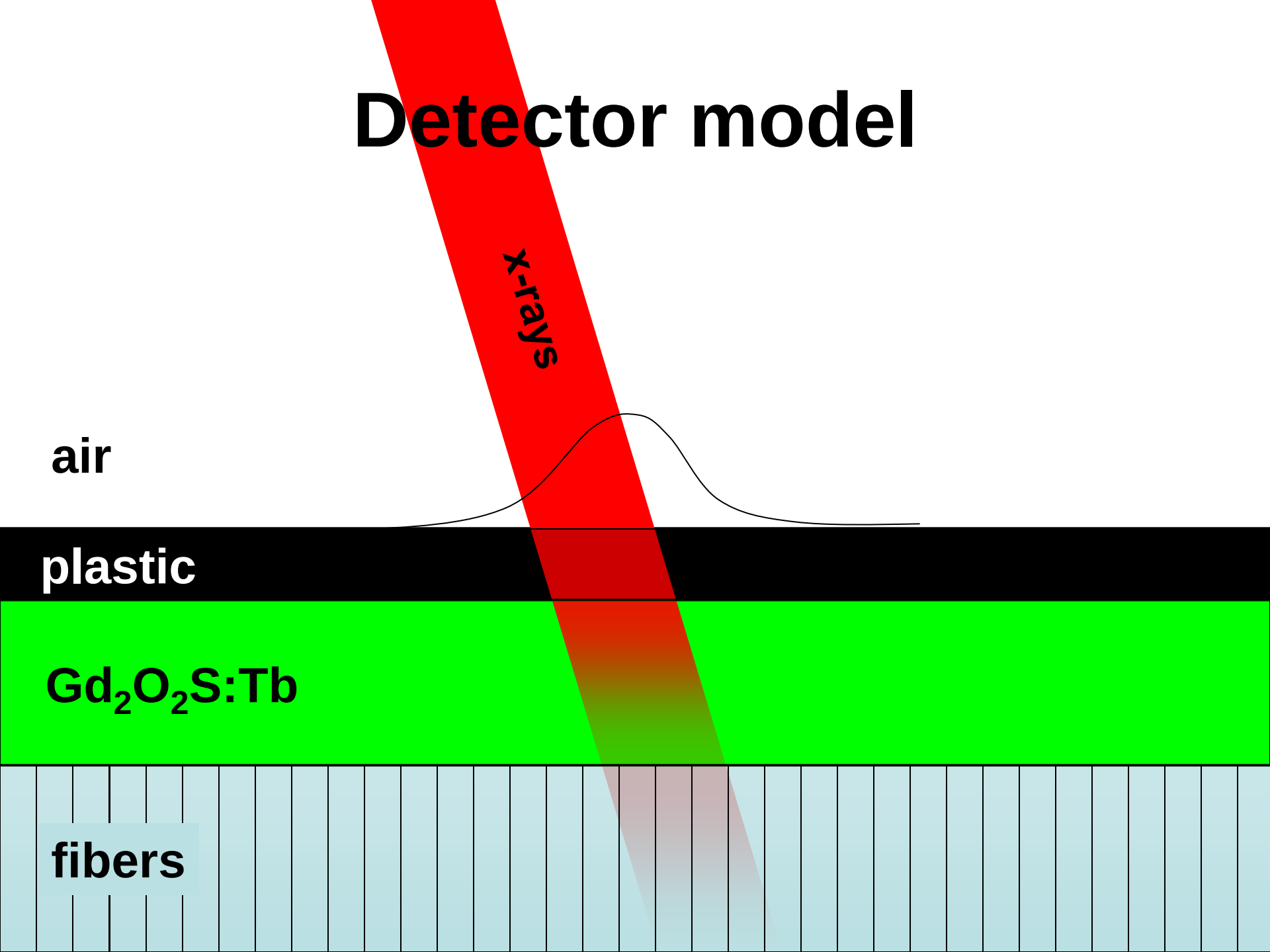

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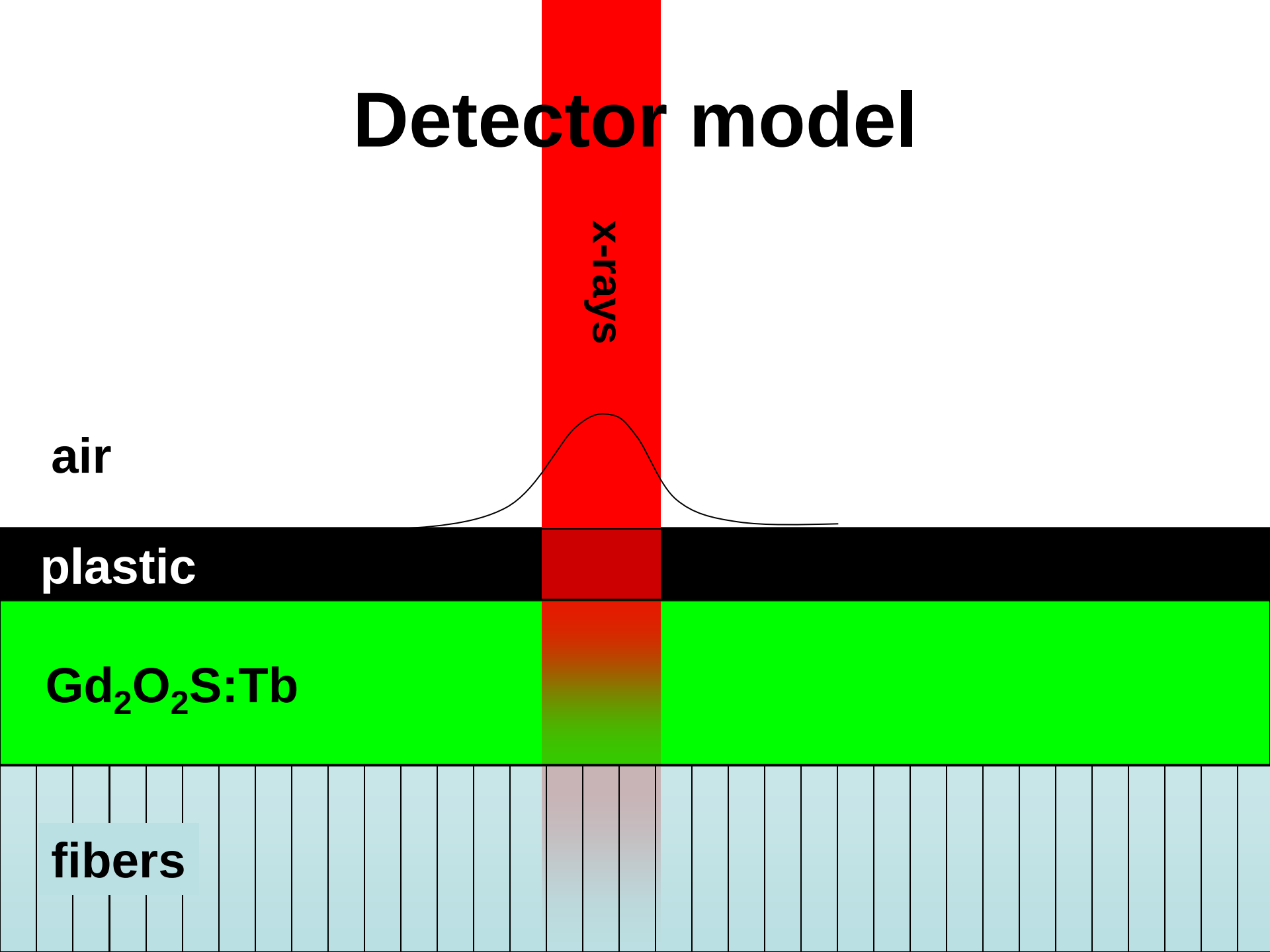

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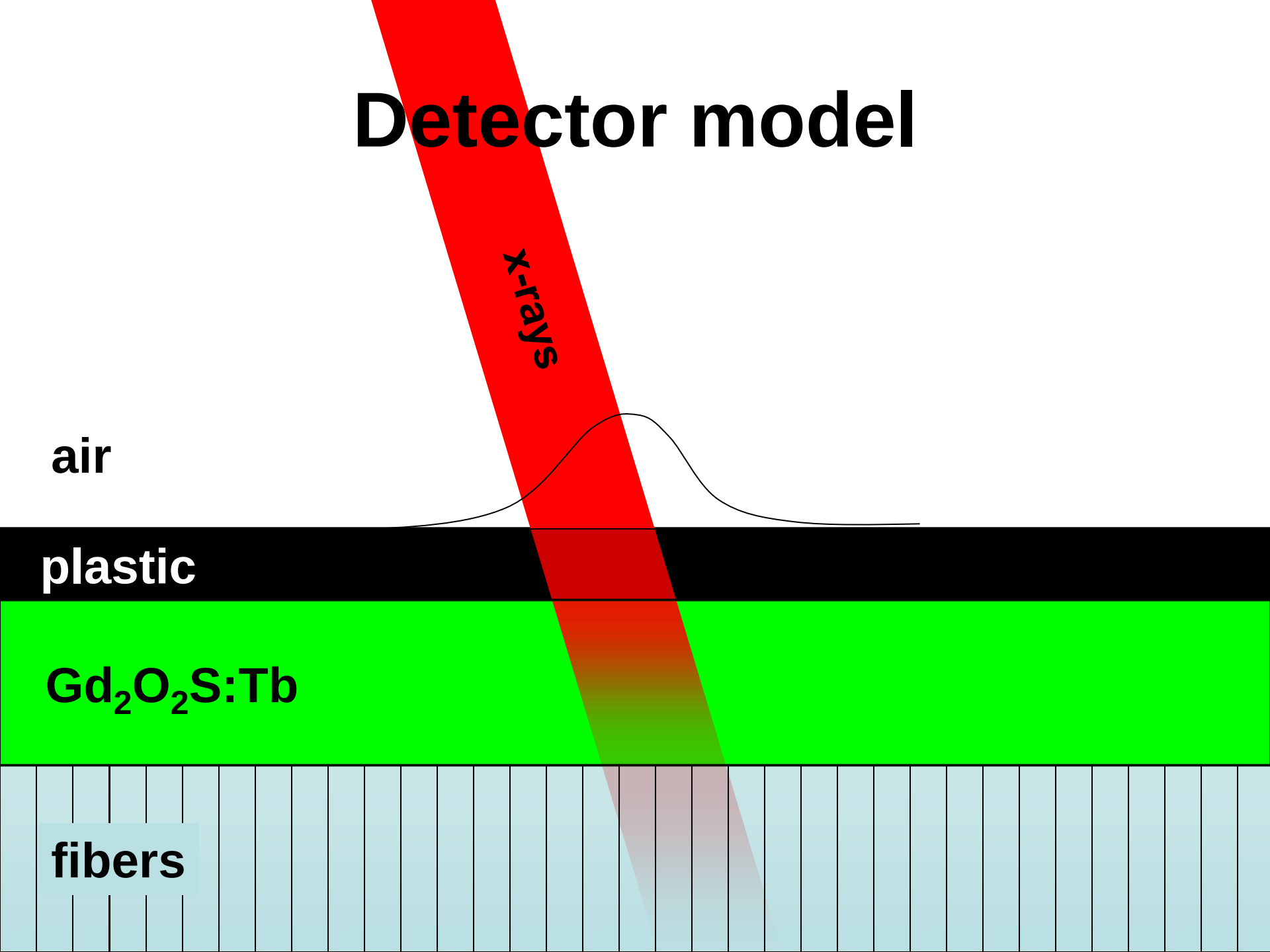

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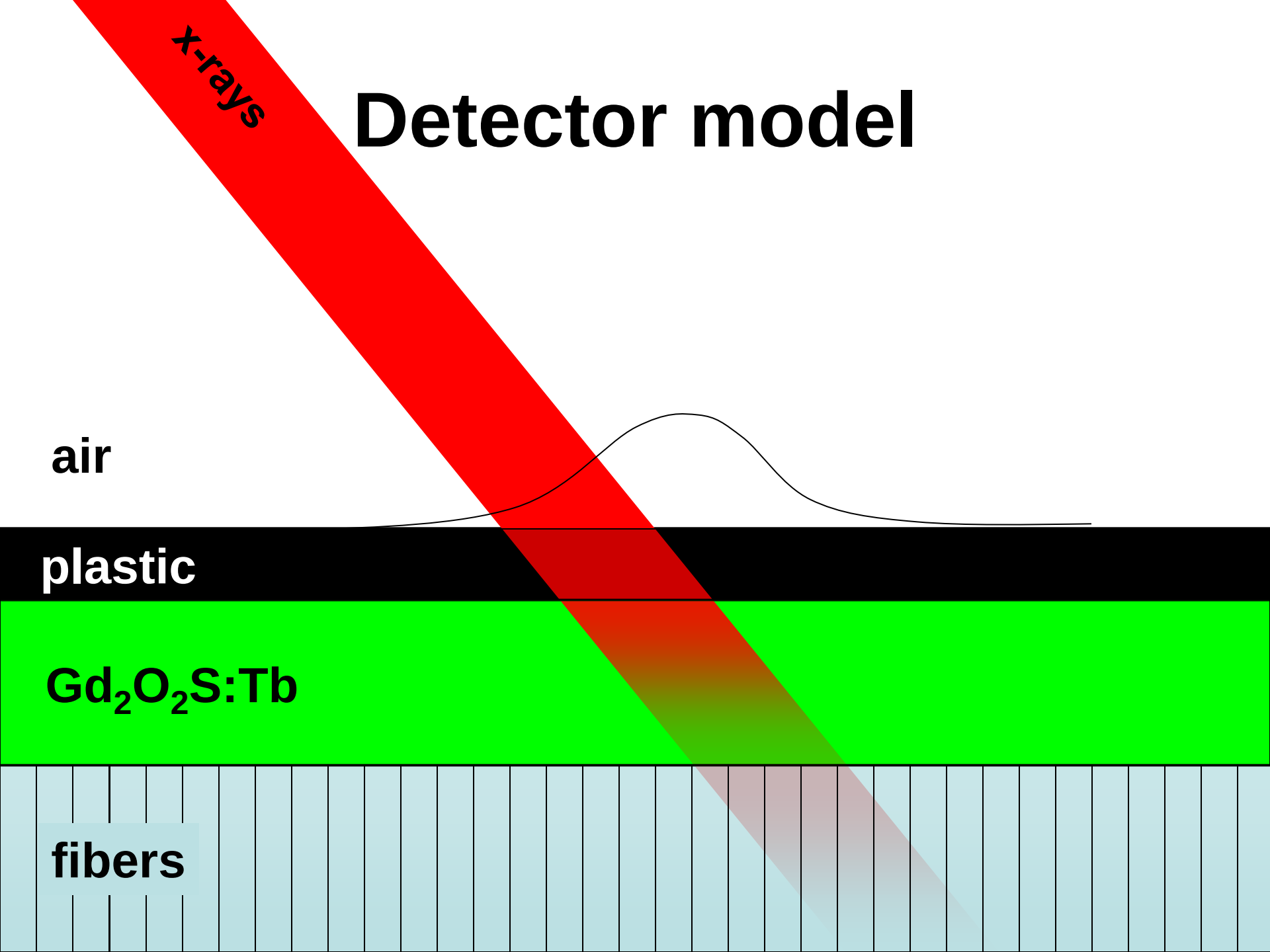

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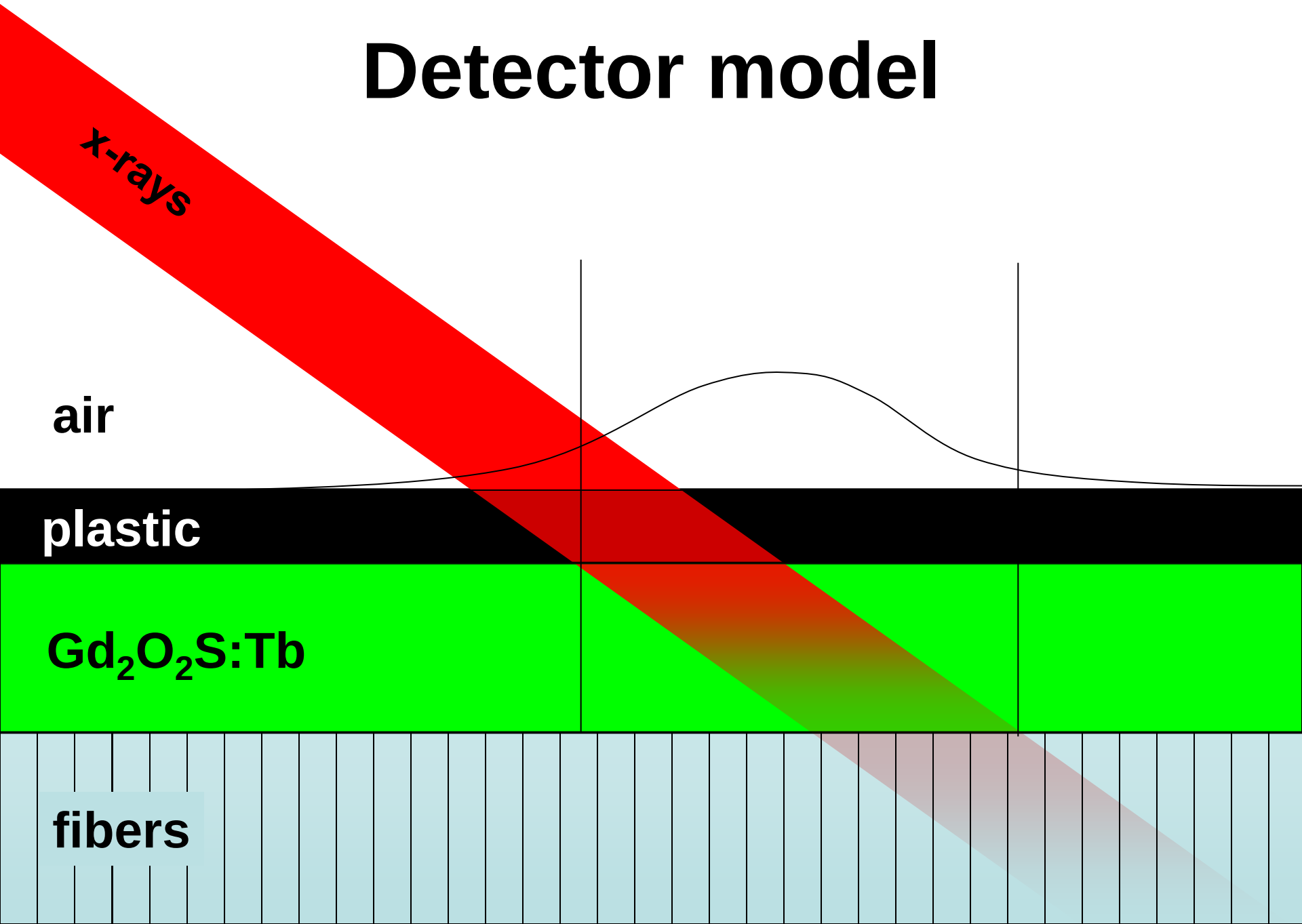
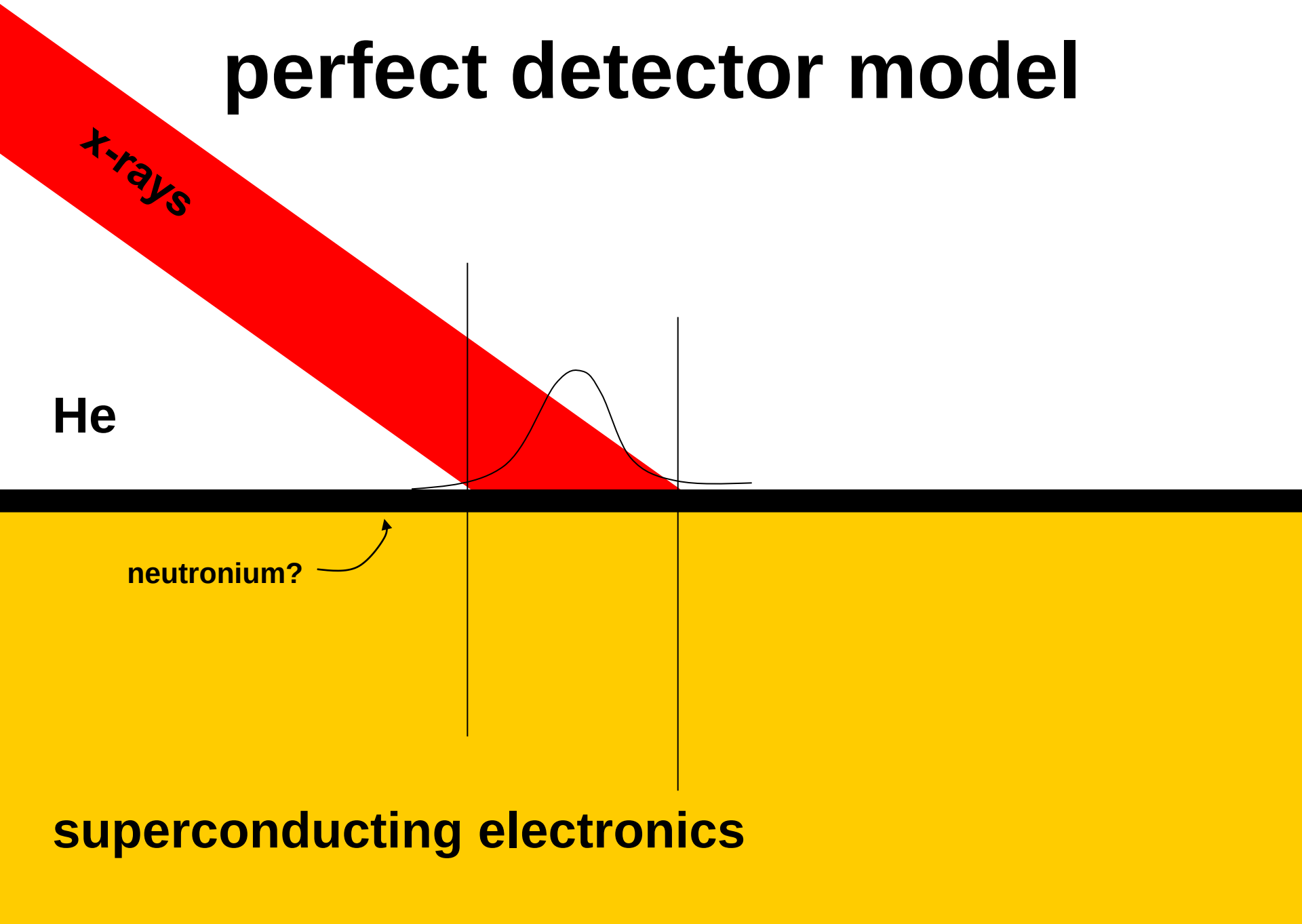
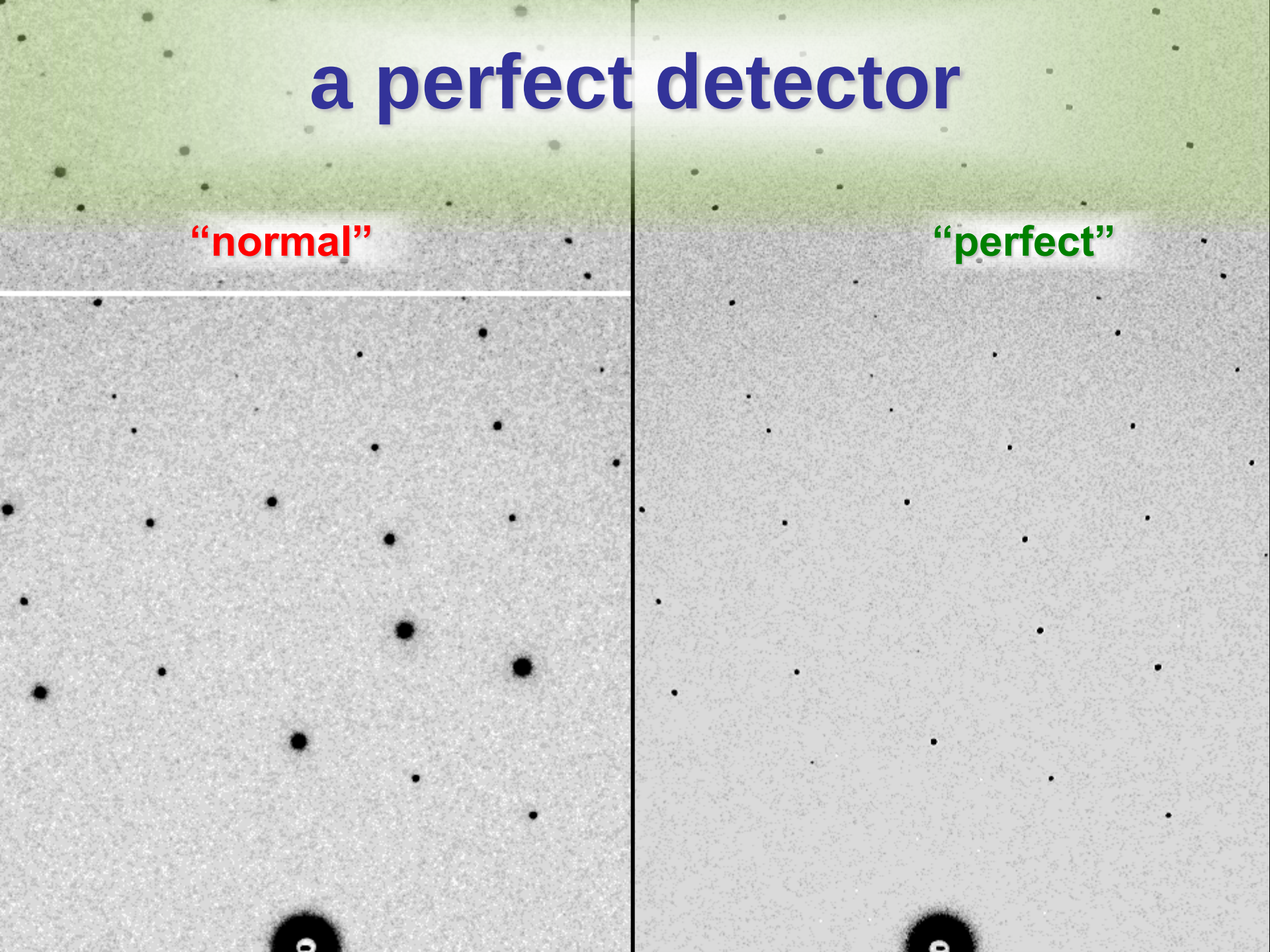


perfect detector model



a perfect detector



normal	statistic	perfect
4.0%	R_{merge}	3.9%
24.3	I/sd	28.1
3.7	I/sd (1.4 Å)	7.3
1.37 3 0.02	SDCORR	0.98 11 0.05
38.01	PADFPH	35.16
4.104	mlphare f”	3.973
0.224	FOM	0.272
0.579	FOMDM	0.563
0.7113	CC(1H87)	0.7051
15.72	R_{cryst}	16.64
18.30	R_{free}	19.38

can we collect

shorter exposures
with
higher redundancy?

same total dose with high and low redundancy

dataset	1	2-11	12
exposure	1.0s	0.1s	1.0s
frames	100	100 x 10	100
R_{merge}			
R_{anom}			
I/sd			
I/sd (2.0 Å)			
redundancy			
PADFPH			
FOM			
FOMDM			
CC(1H87)			

same total dose with high and low redundancy

dataset	1	2-11	12
exposure	1.0s	0.1s	1.0s
frames	100	100 x 10	100
R_{merge}	5.6%	11.2%	4.7%
R_{anom}	4.8%	4.7%	4.7%
I/sd	29.5	43.4	33.3
I/sd (2.0 Å)	23.3	29.6	25.8
redundancy	7.6	75.7	7.6
PADFPH	36.69	37.11	37.93
FOM	0.342	0.343	0.366
FOMDM	0.698	0.711	0.726
CC(1H87)	0.418	0.492	0.468

same total dose with high and low redundancy

dataset	1	2-11	12
exposure	1.0s	0.1s	1.0s
frames	100	100 x 10	100
R_{merge}	5.6%	11.2%	4.7%
R_{anom}	4.8%	4.7%	4.7%
I/sd	29.5	43.4	33.3
I/sd (2.0 Å)	23.3	29.6	25.8
redundancy	7.6	75.7	7.6
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dataset	1	2-11	12
exposure	1.0s	0.1s	1.0s
frames	100	100 x 10	100
R_{merge}	5.6%	11.2%	4.7%
R_{anom}	4.8%	4.7%	4.7%
I/sd	29.5	43.4	33.3
I/sd (2.0 Å)	23.3	29.6	25.8
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PADFPH	36.69	37.11	37.93
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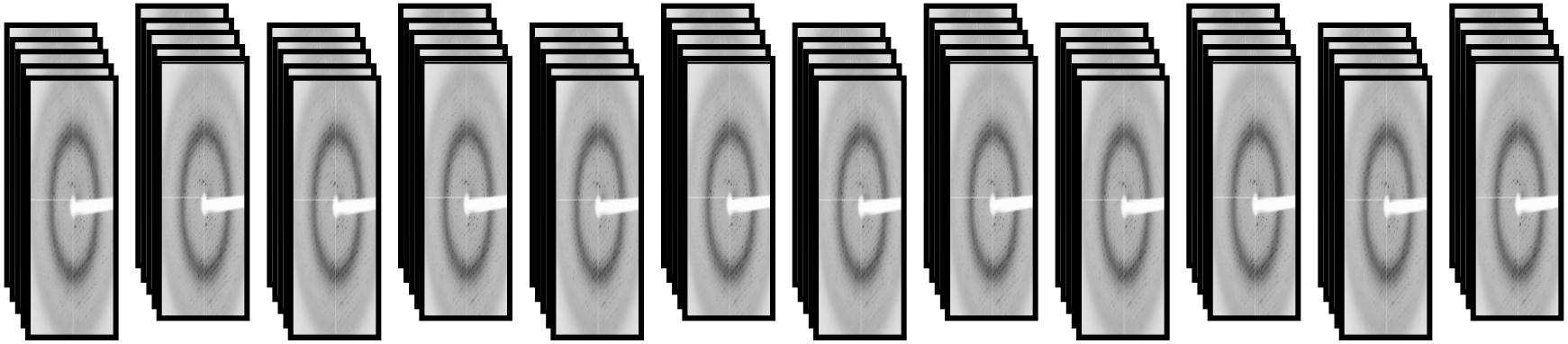
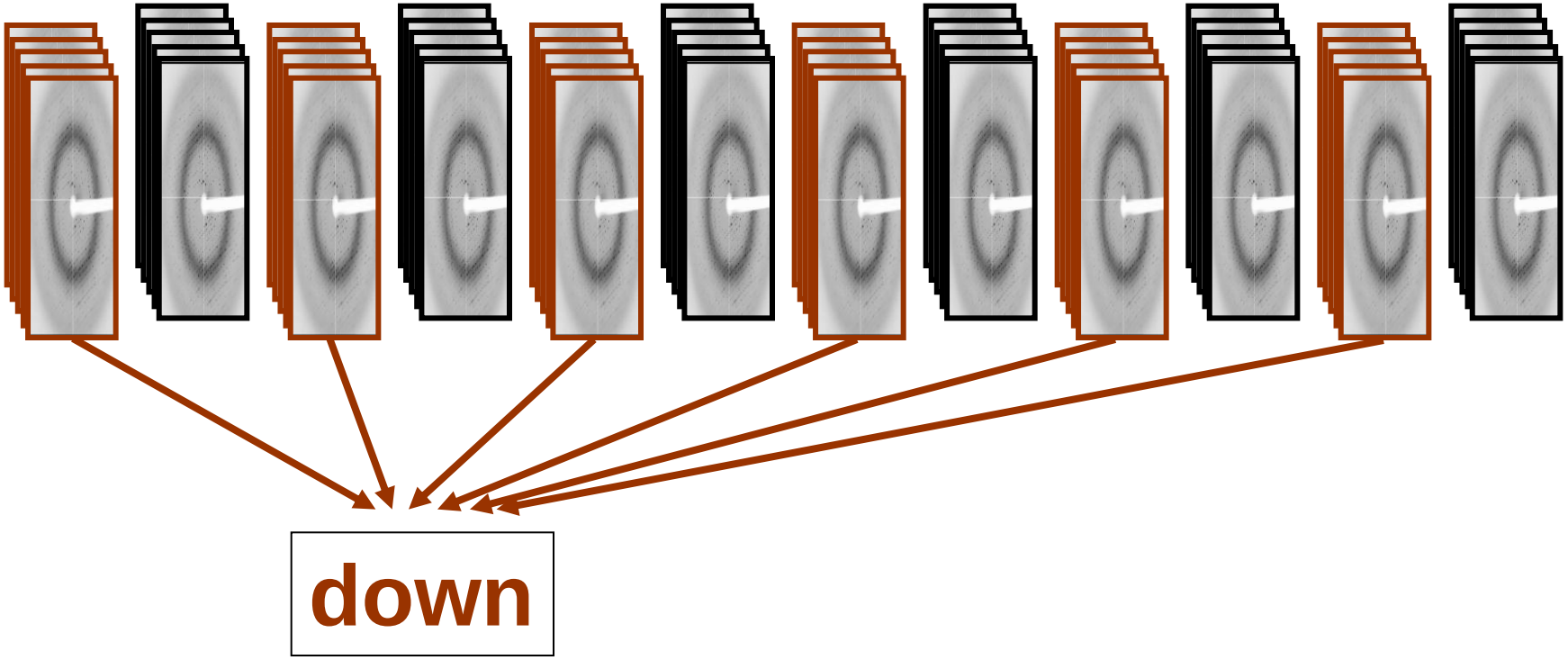
Spatial Noise



Spatial Noise



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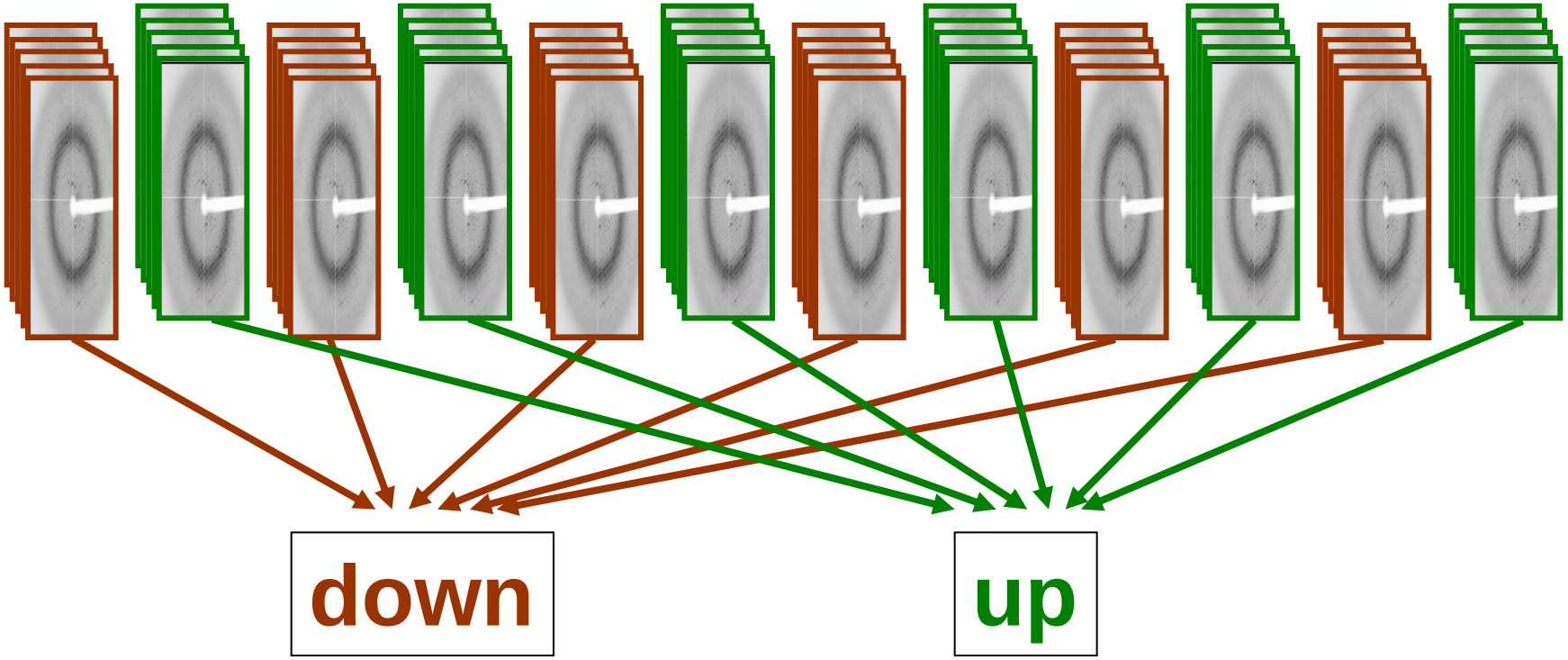
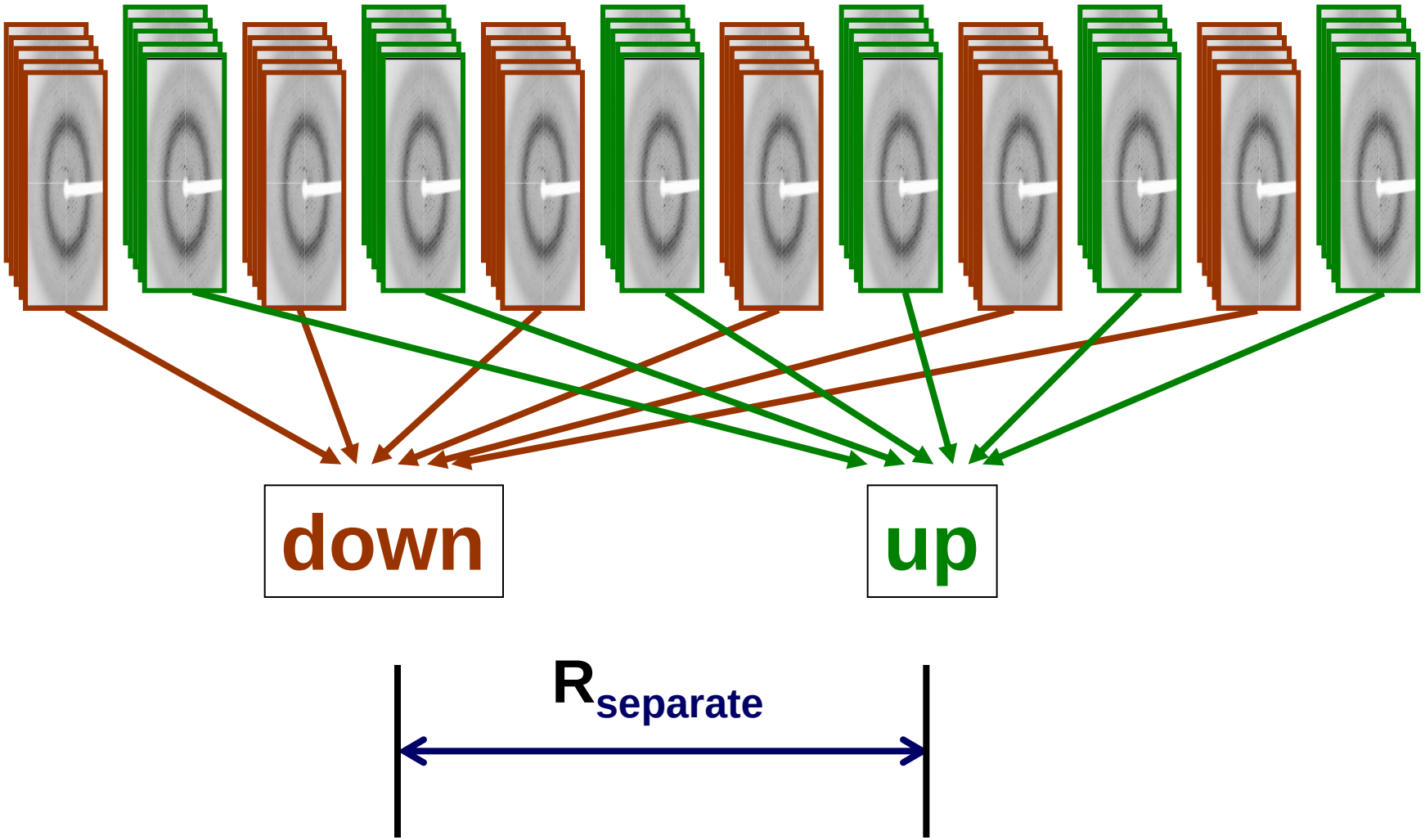
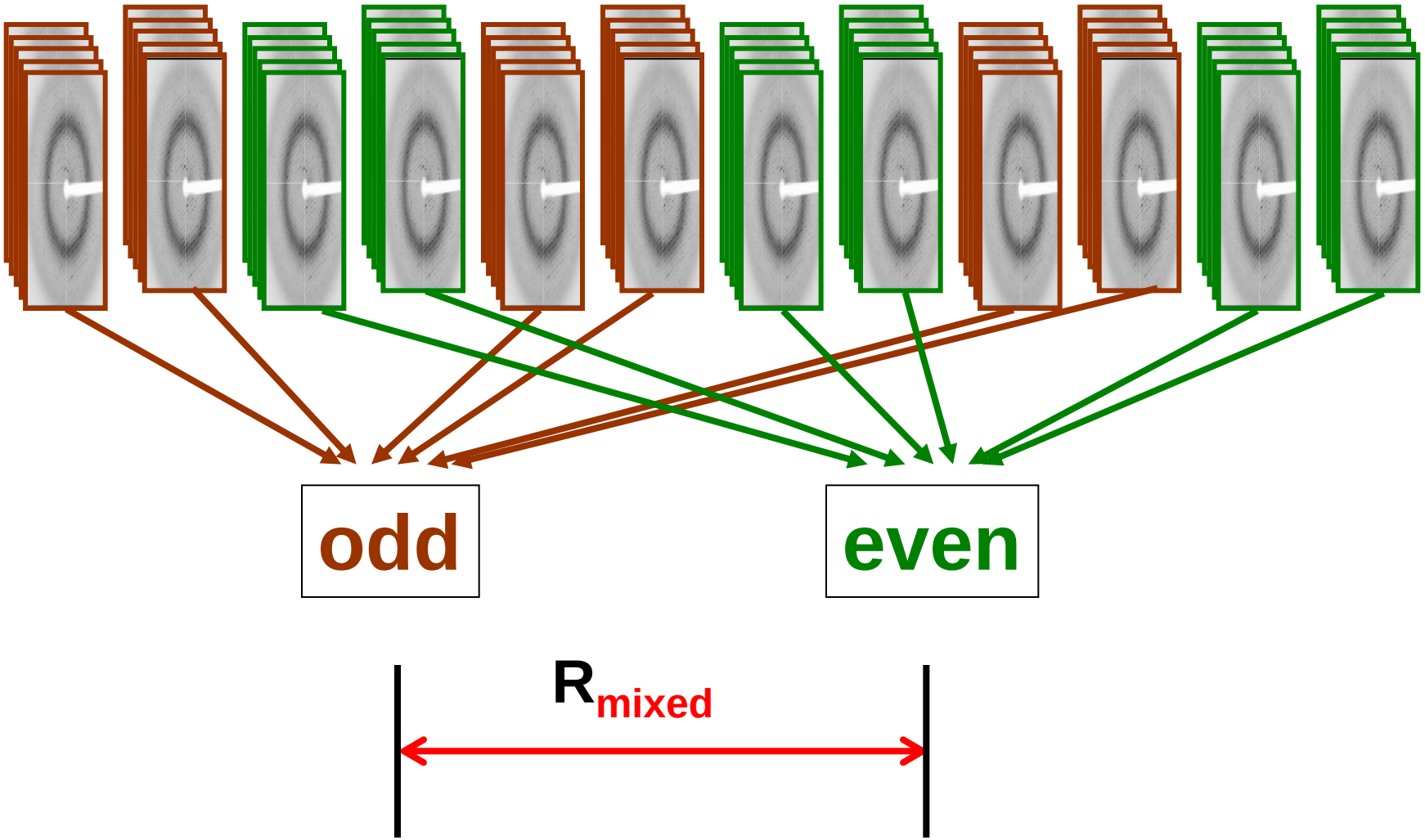


Spatial Noise



Spatial Noise



Spatial Noise

separate: 2.5%

Spatial Noise

separate: 2.5%

mixed: 0.9%

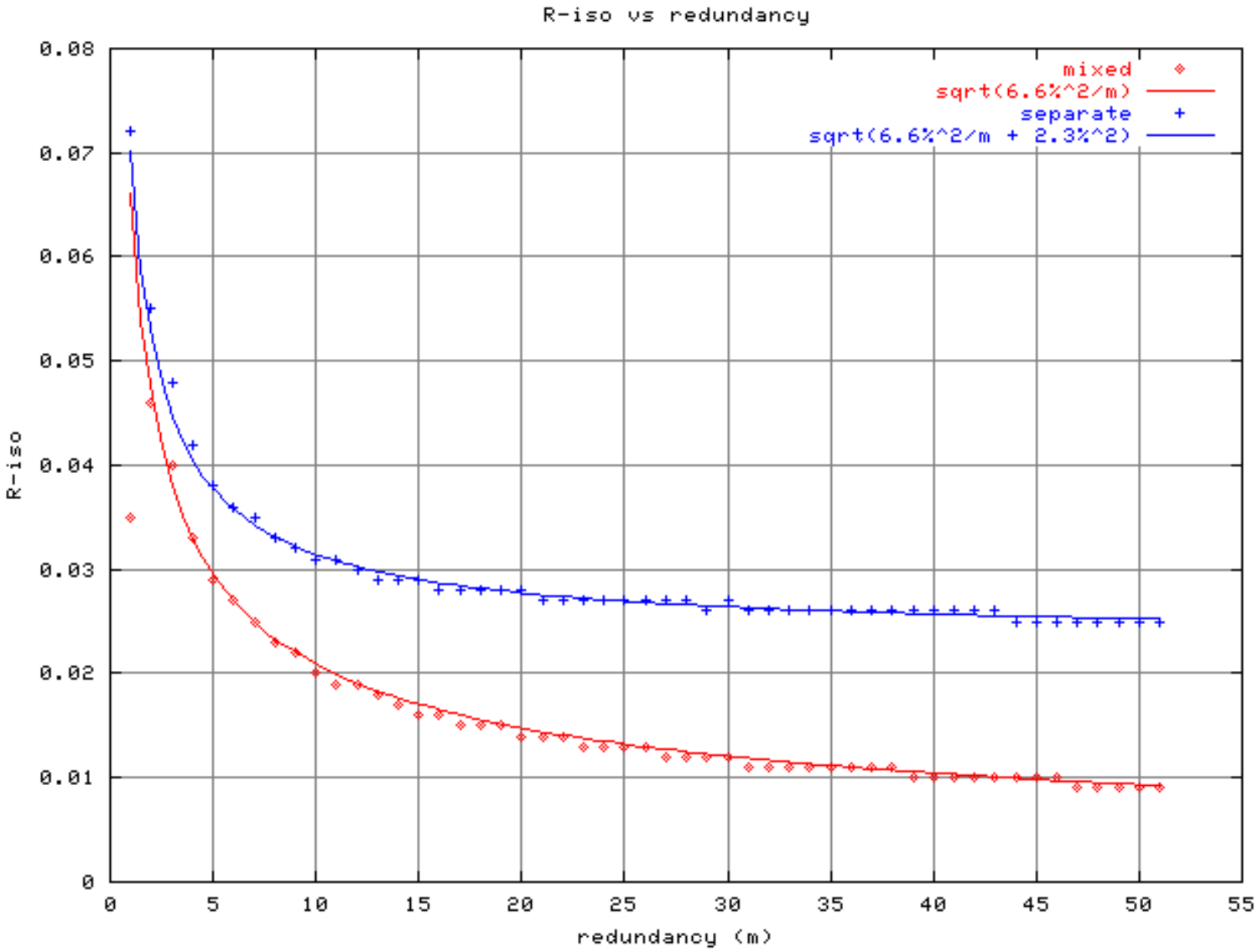
Spatial Noise

separate: 2.5%

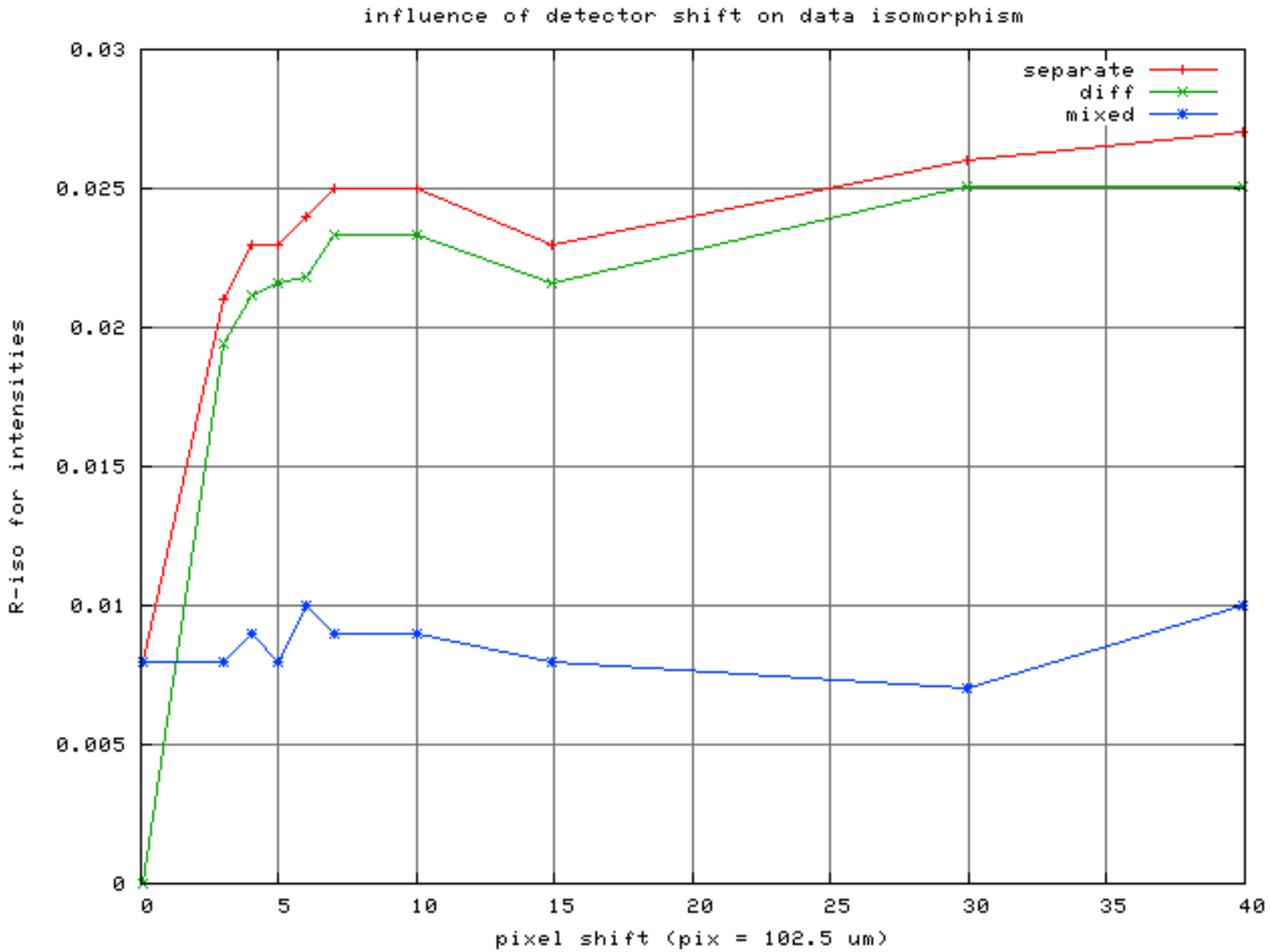
mixed: 0.9%

$2.5\%^2 - 0.9\%^2 = 2.3\%^2$

Spatial Noise

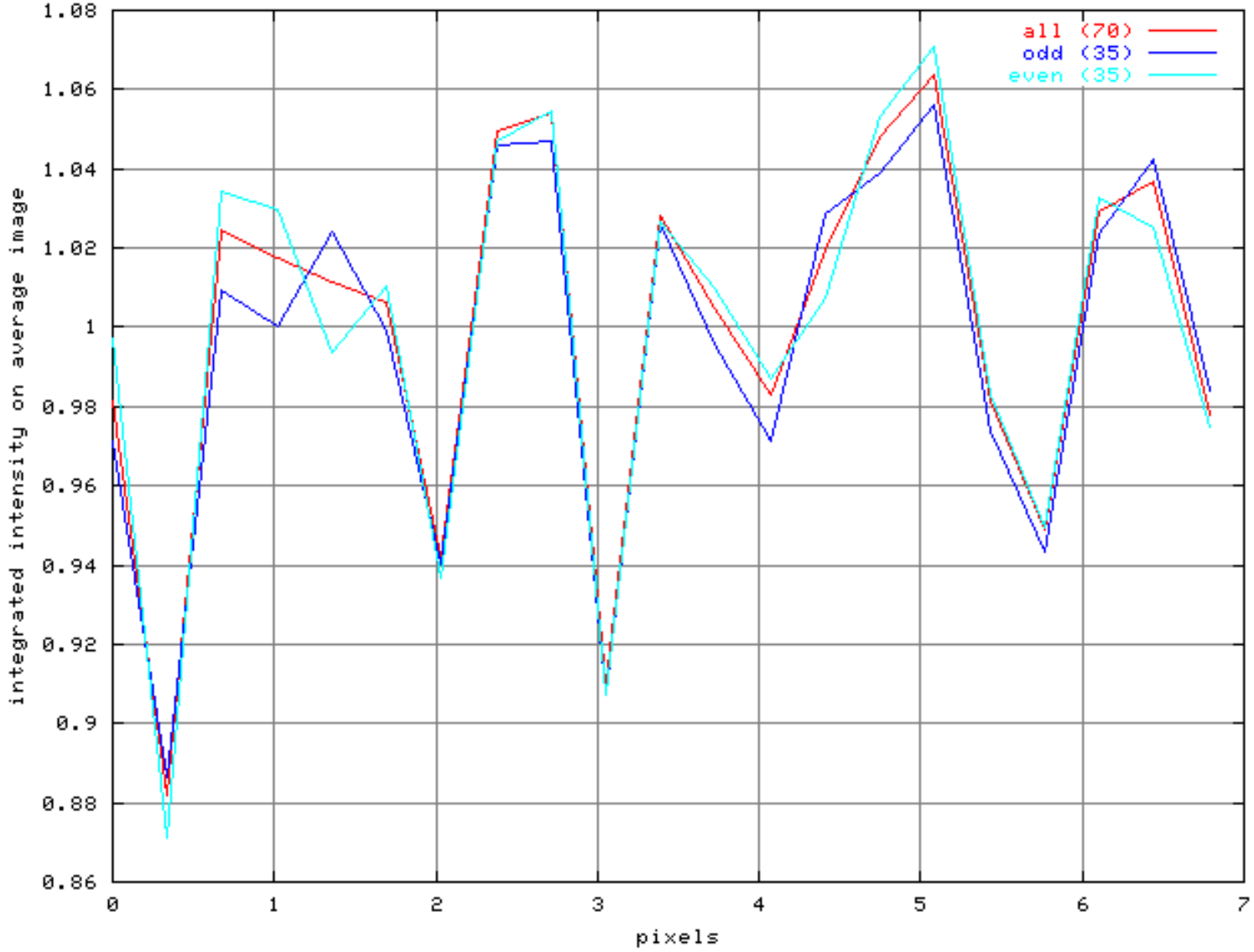


Spatial Noise



Spatial Noise

Spatial Noise



Summary

98% screening

short exposures FIRST

“dose slicing”

10 µm lysozyme

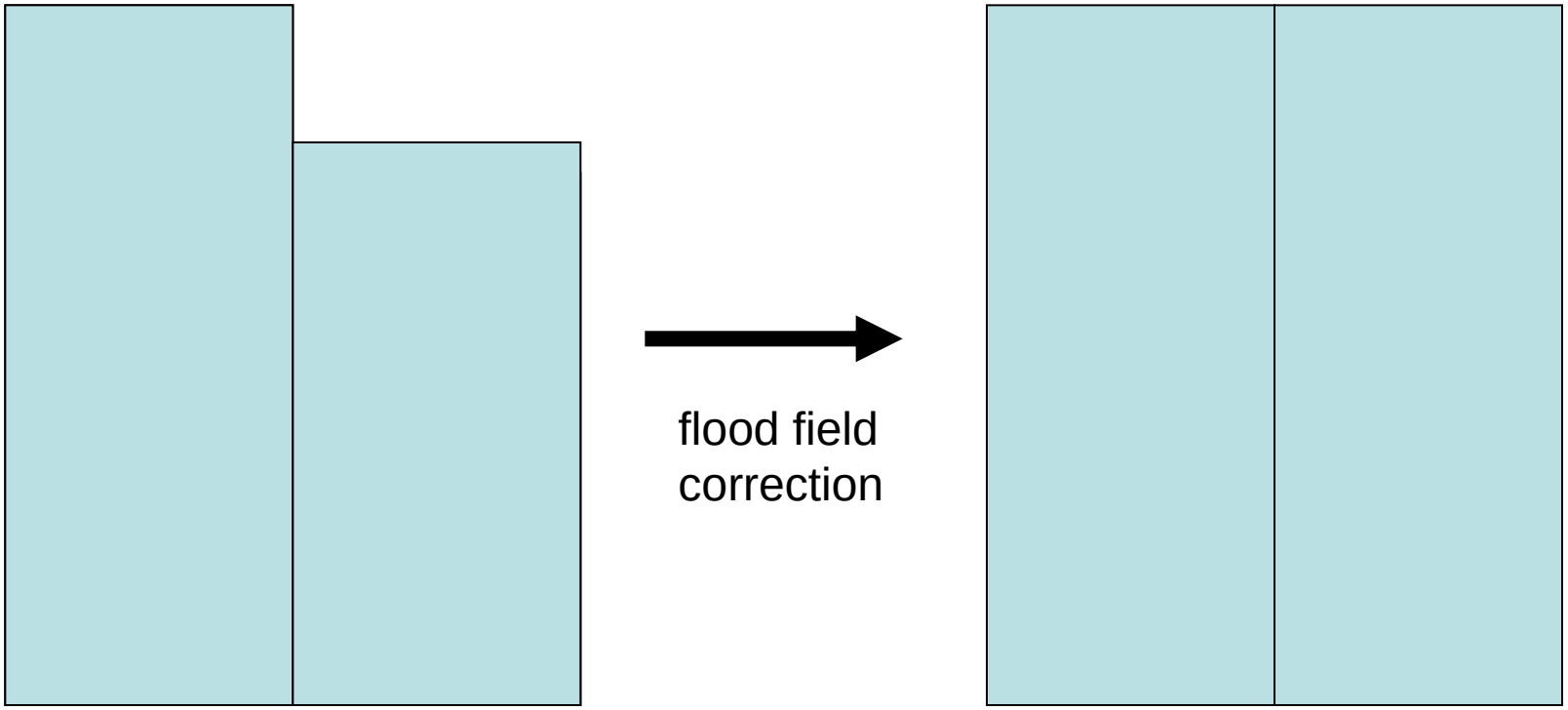
site damage is unpredictable

Development Snapshot

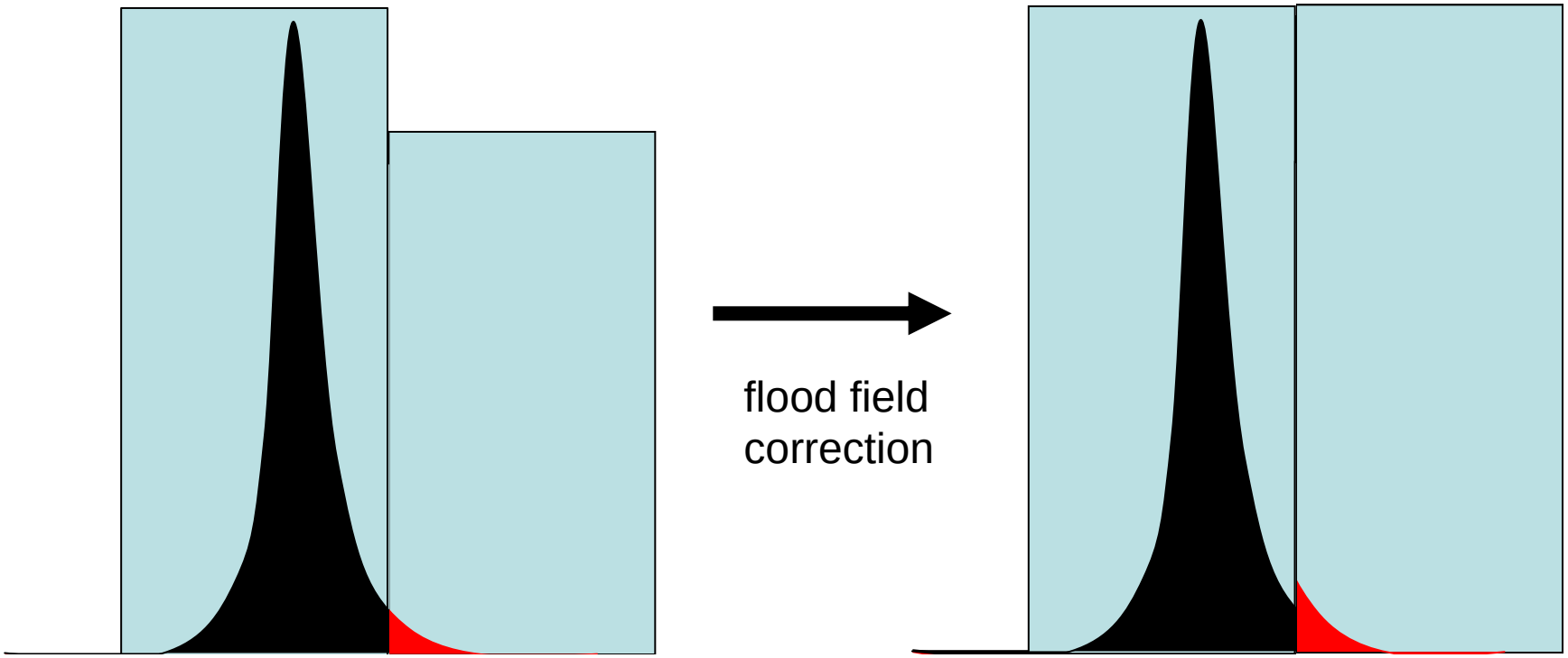
http://bl831.als.lbl.gov/~jamesh/mlfsom/development_snapshot.tar.gz

http://bl831.als.lbl.gov/~jamesh/powerpoint/BNL_2009.ppt

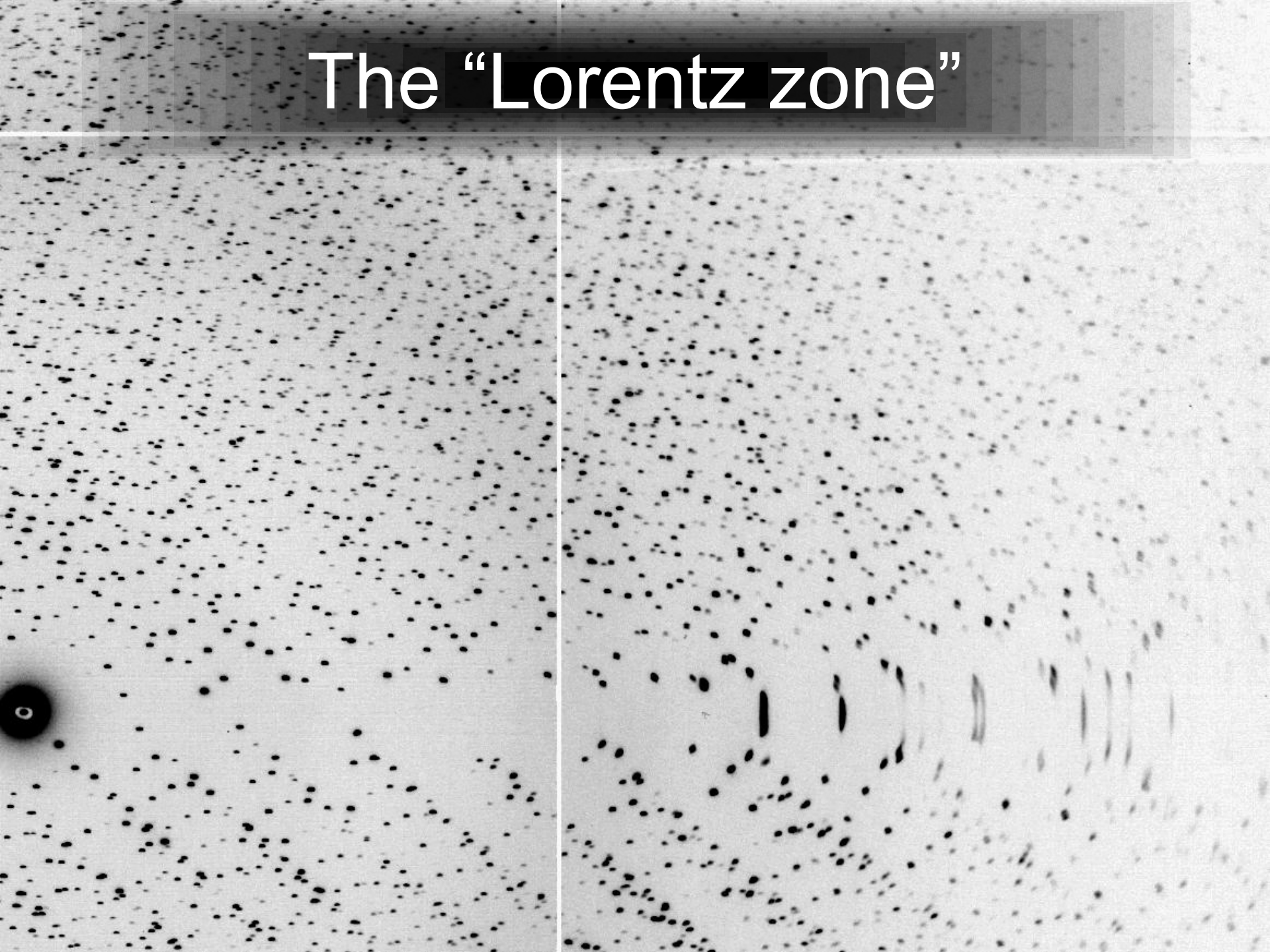
Spatial Noise



Spatial Noise

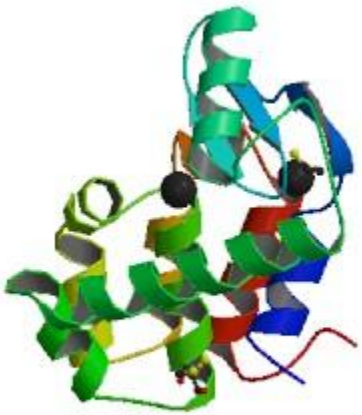


The “Lorentz zone”



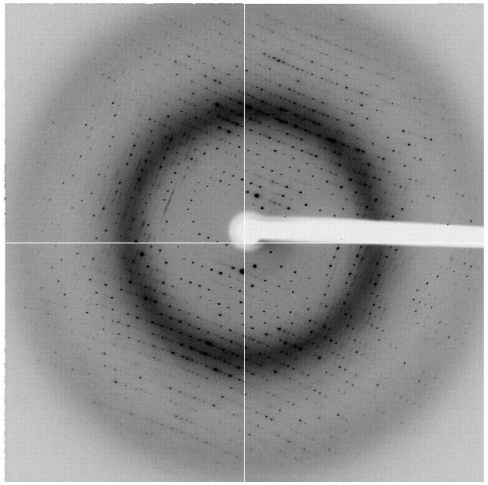
The R-factor Gap

multi-conformer PDB file



1H87

MLFSOM



Elves

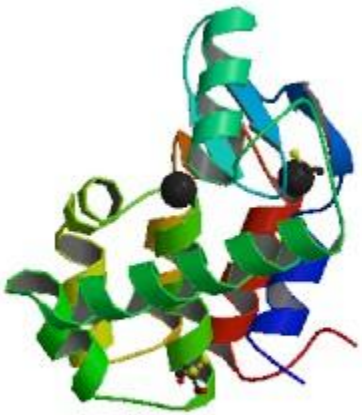
R_{merge} = 6%

R_{cryst} = 17%

R_{free} = 20%

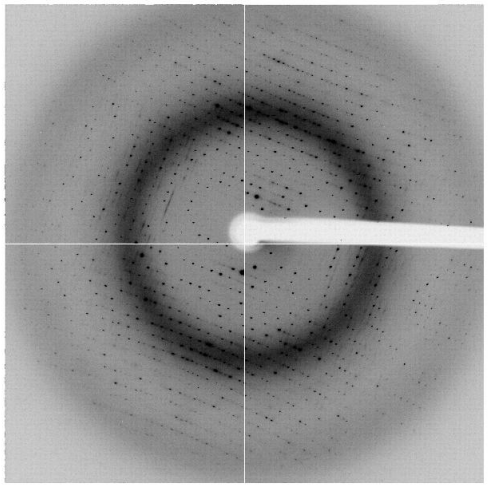
The R-factor Gap

single-conformer PDB file



1H87; conf “A”

MLFSOM



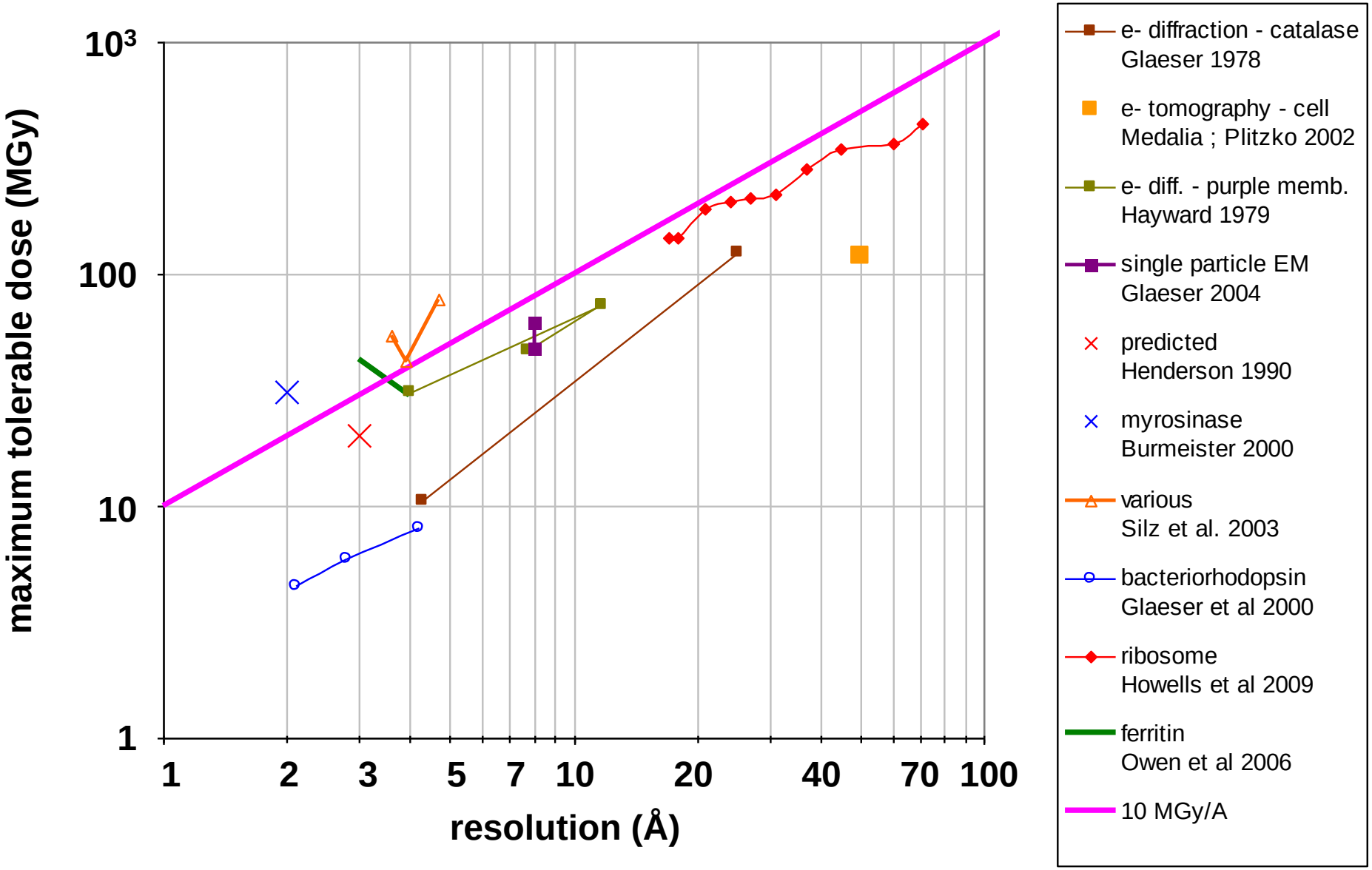
Elves

R_{merge} = 6%

R_{cryst} = 7%

R_{free} = 8%

Howells *et al.* (2009)
J. Electron. Spectrosc. Relat. Phenom. **170** 4-12



Radiation Damage Model

global (lattice) damage

$$|F_{used}| = |F_{undam}| \exp\left(-\ln(2) \frac{dose}{d \cdot H}\right)$$

F_{used}	- structure factor used for spot
F_{undam}	- structure factor of undamaged crystal
dose	- absorbed dose (MGy)
H	- 10 MGy/Å
d	- resolution of spot (Å)

Radiation Damage Model

global (lattice) damage

$$\mathbf{F = F_0 \exp(- A \cdot s)}$$

F	- structure factor used for spot
$\mathbf{F_0}$	- structure factor of undamaged crystal
A	- something Debye said was zero
s	- 0.5/**d**
d	- resolution of spot (Å)

Radiation Damage Model

global (lattice) damage

$$\mathbf{F = F_0 \exp(- A \cdot s)}$$

F	- structure factor used for spot
$\mathbf{F_0}$	- structure factor of undamaged crystal
A	- something Debye said was zero
s	- 0.5/**d**
d	- resolution of spot (Å)

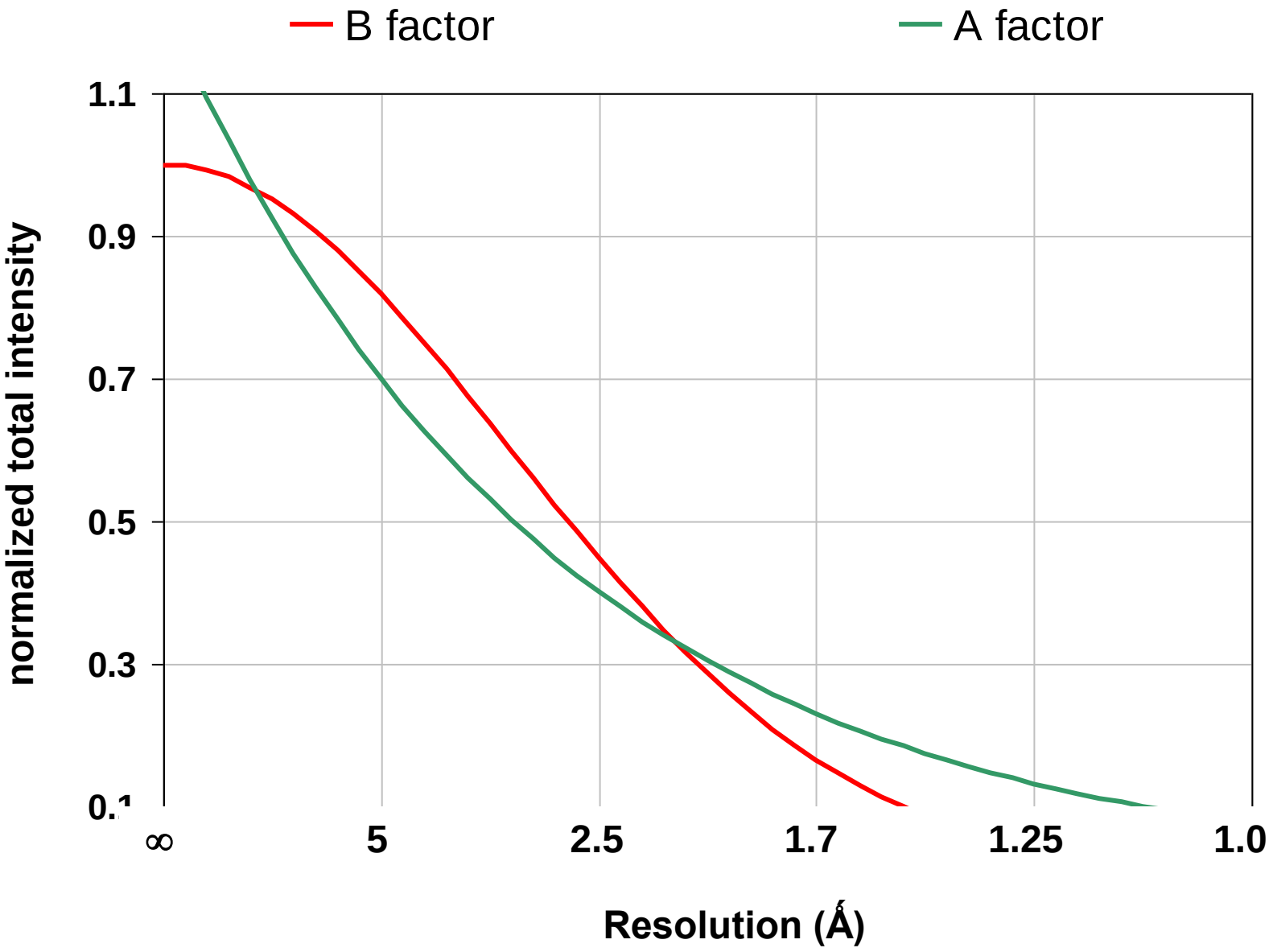
Radiation Damage Model

global (lattice) damage

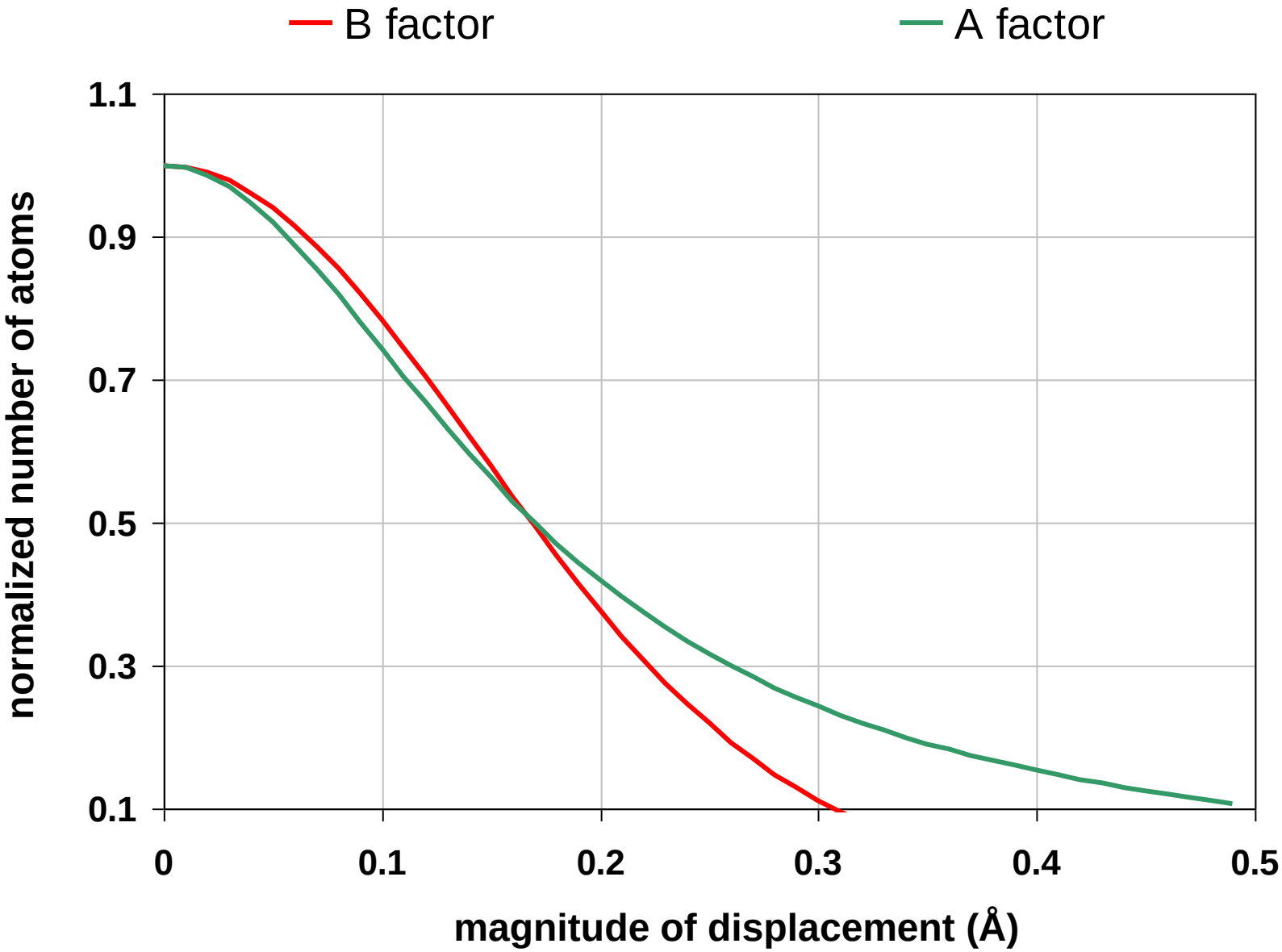
$$\mathbf{F = F_0 \exp(- A \cdot s - B \cdot s^2 - C \cdot s^3 - \ldots)}$$

A	- something Debye said was zero
B	- canonical Debye-Waller factor
C	- something else Debye said was zero
s	- 0.5/**d**
d	- resolution of spot (Å)

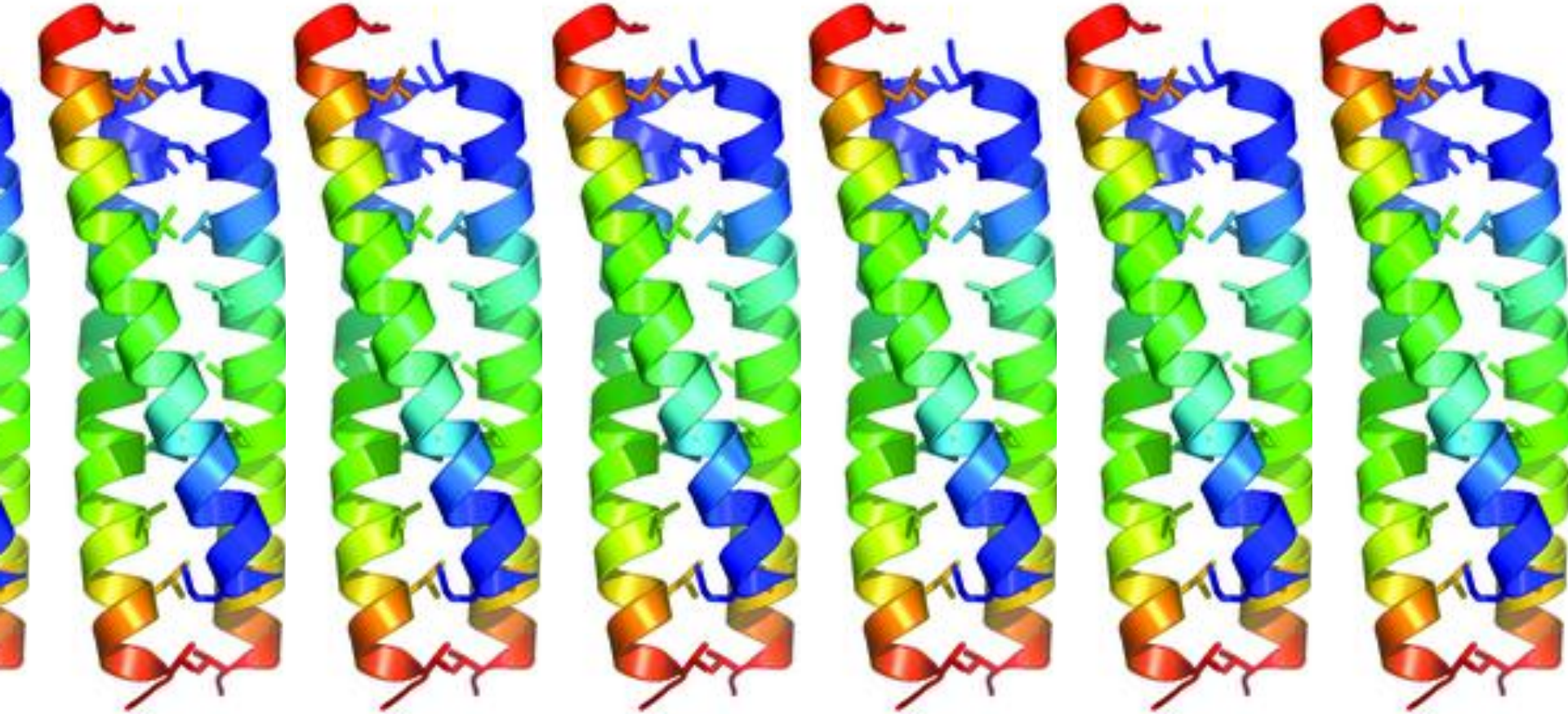
Radiation Damage Model



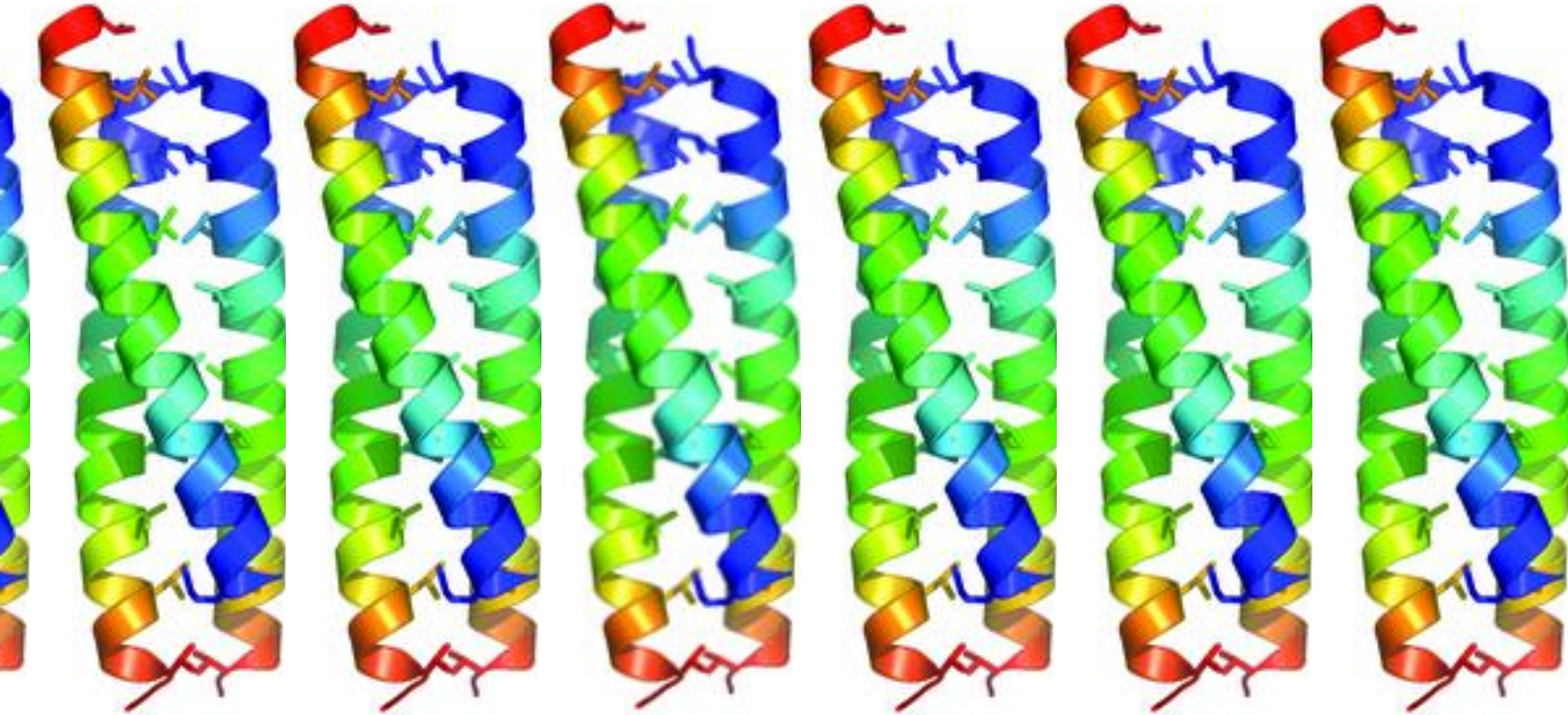
Radiation Damage Model



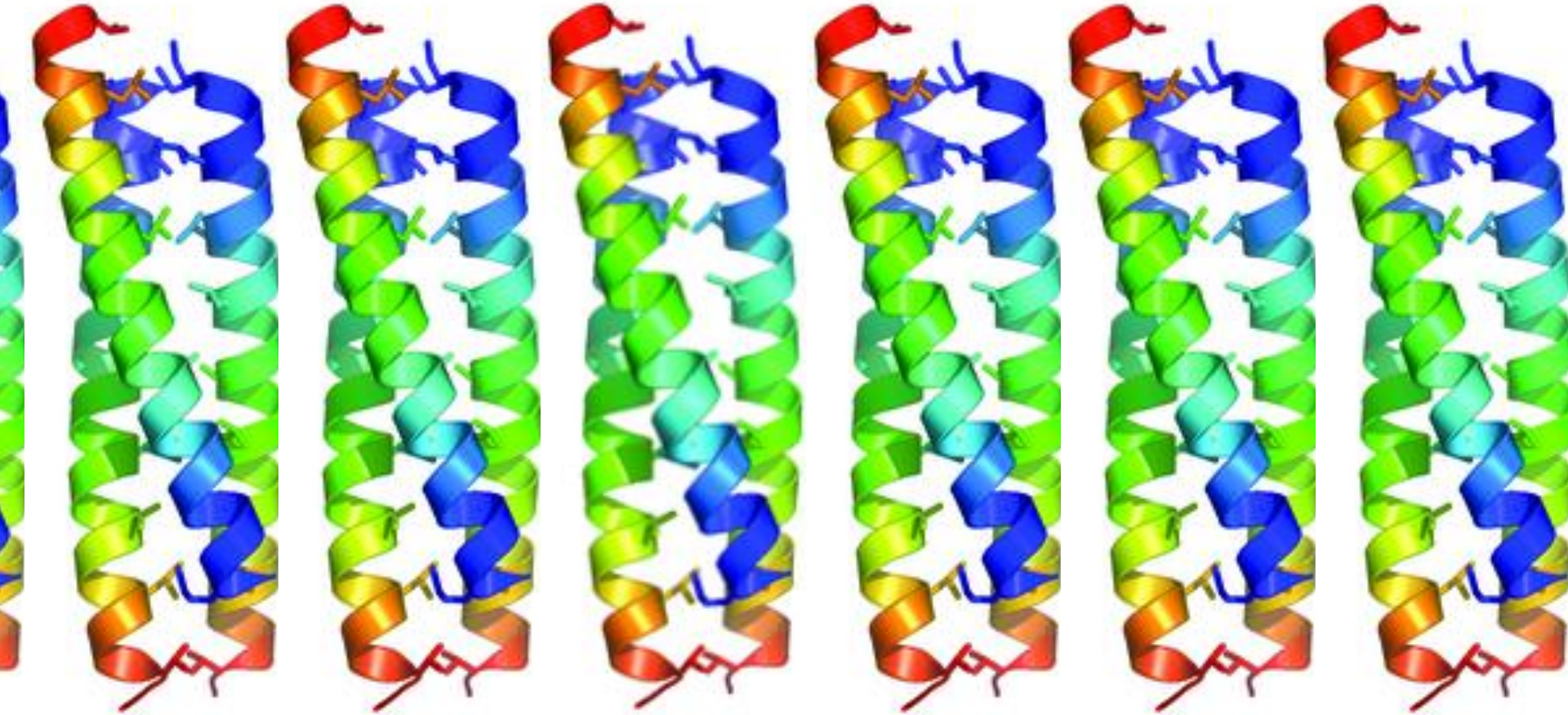
Radiation Damage Model



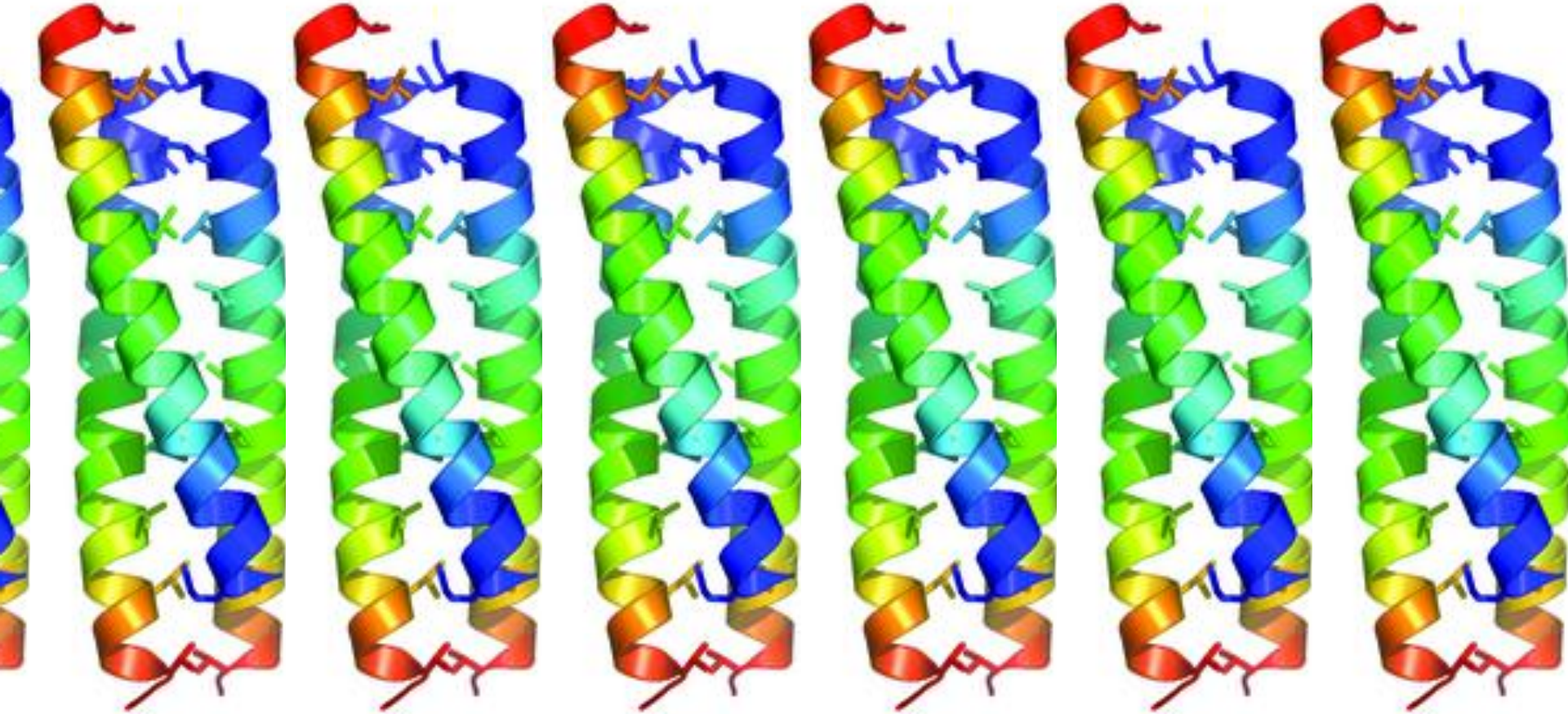
Radiation Damage Model



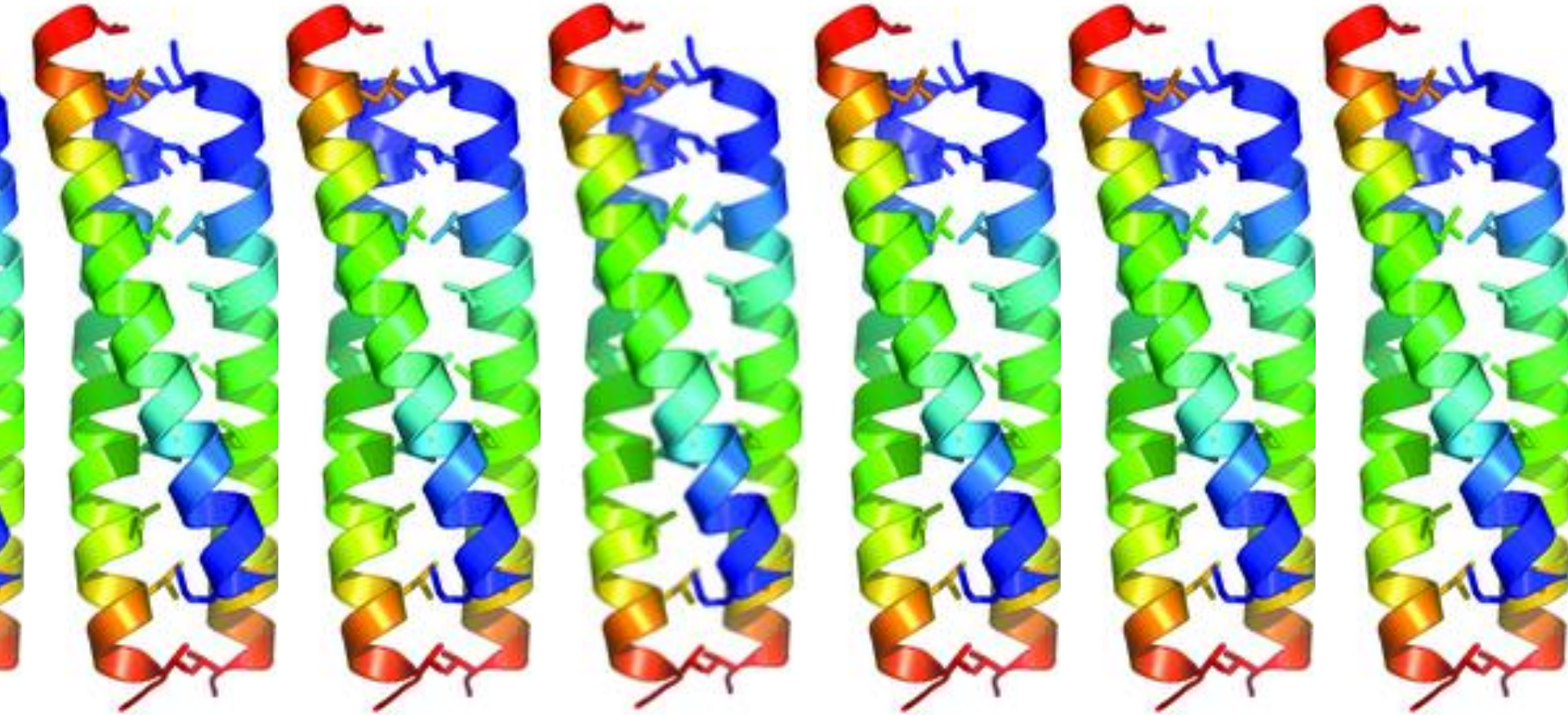
Radiation Damage Model



Radiation Damage Model

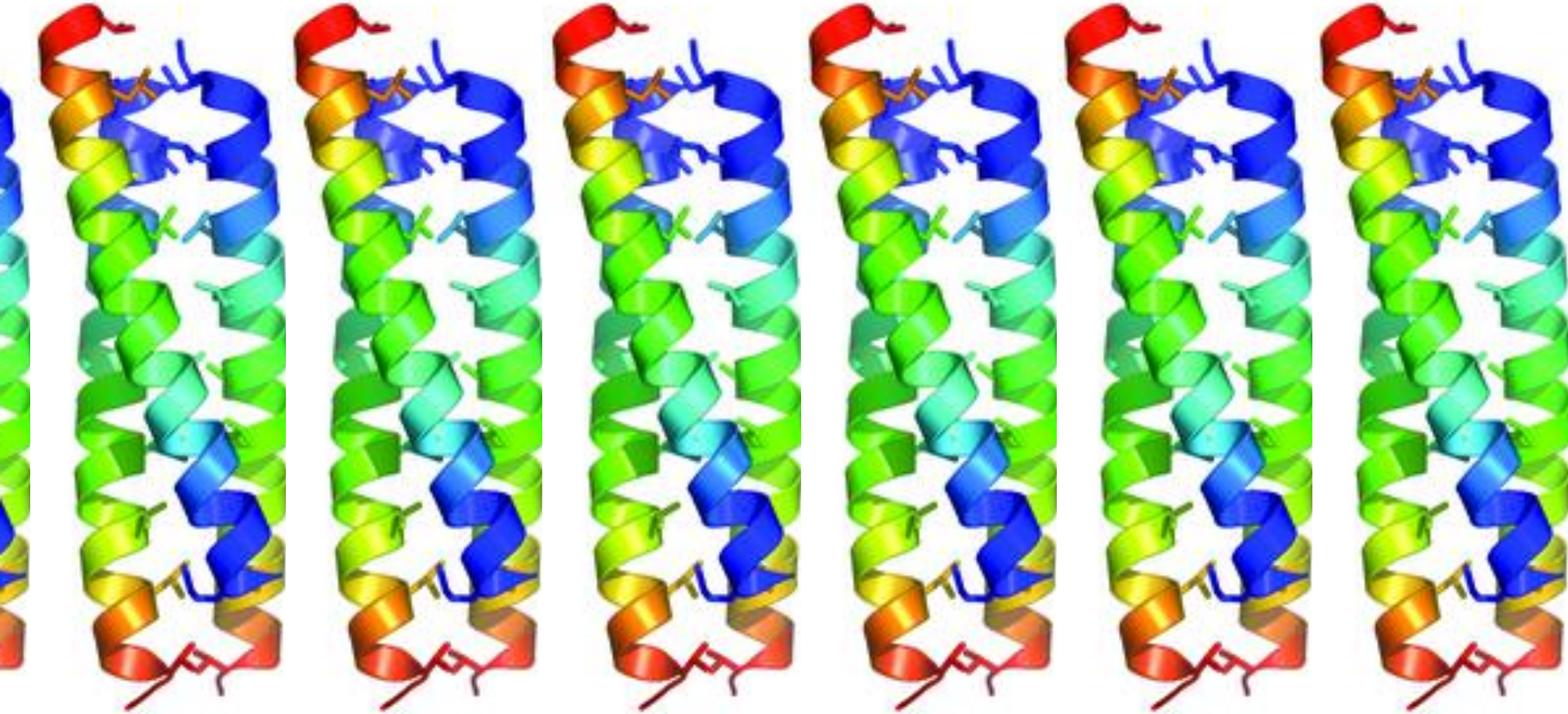


Radiation Damage Model



Kanzaki 1957

Radiation Damage Model



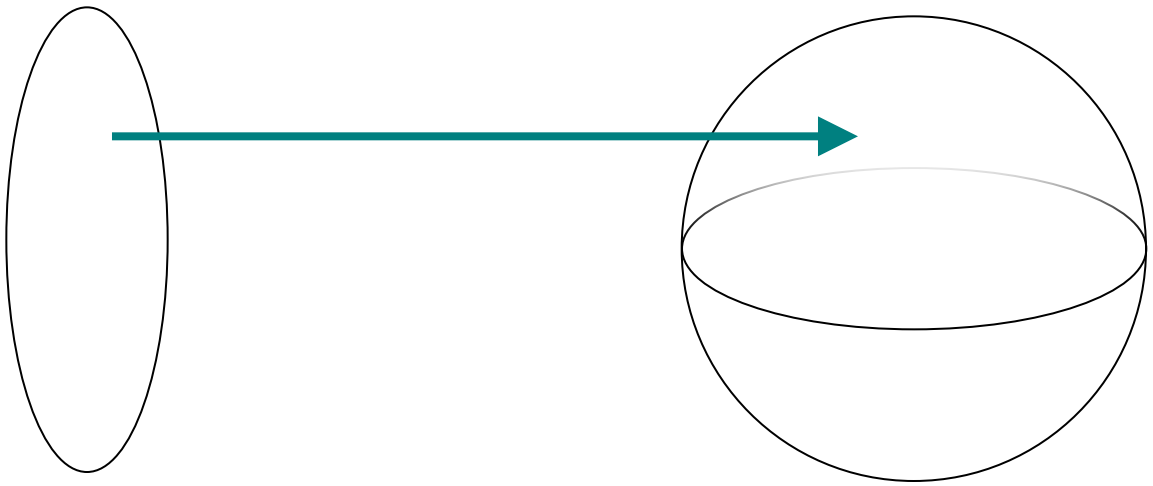
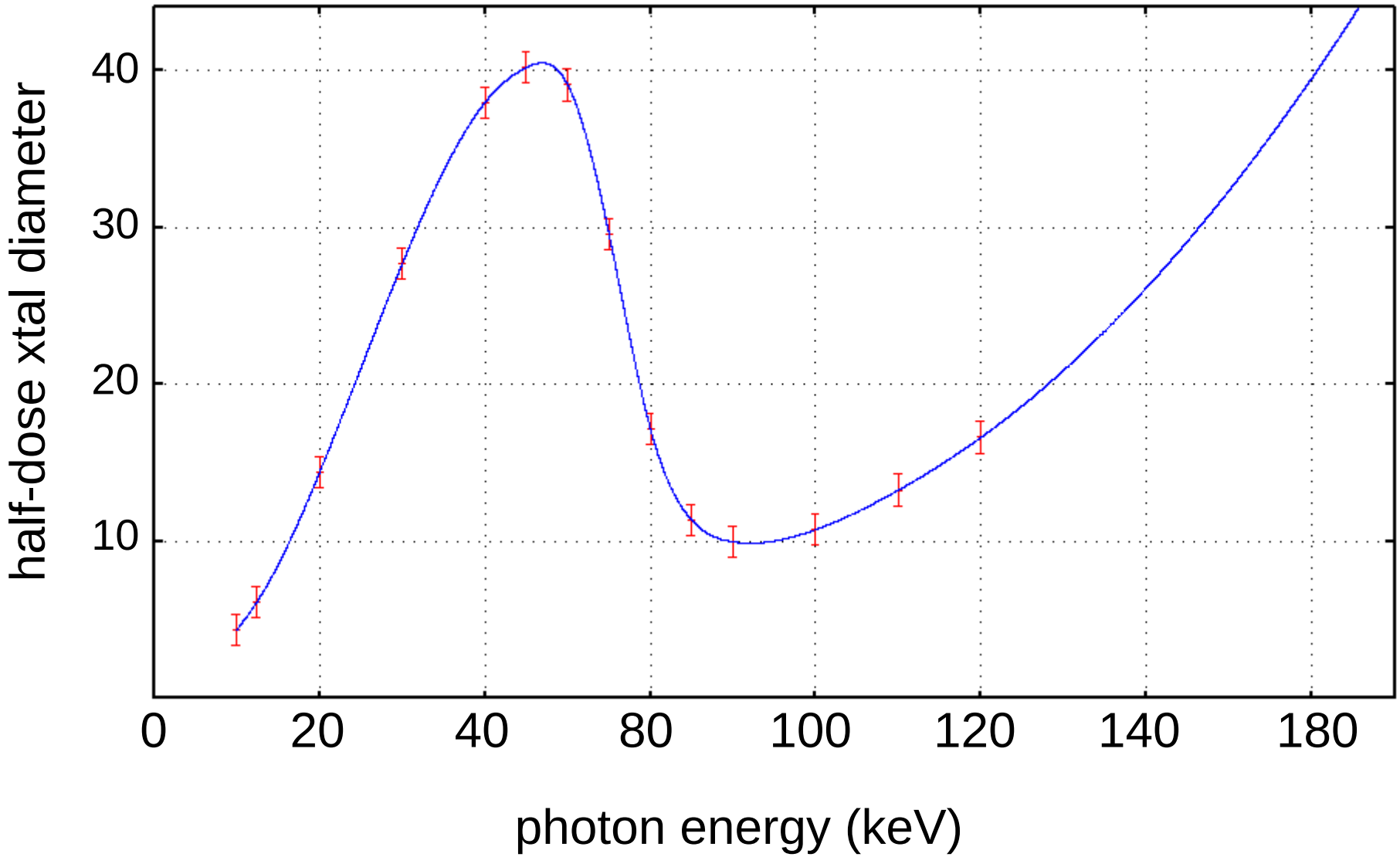
Kanzaki 1957

Radiation Damage prediction

$$\frac{\text{data}}{\text{damage}} \approx k + \left(\frac{2\ \text{ps}}{\text{exposure}} \right)^3$$

particle transport simulation using MCNP

(other codes exist: EGSnrc)



Nave-Hill effect