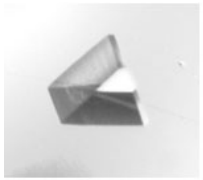
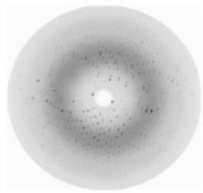
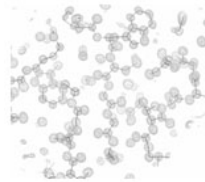
Data Collection Strategies

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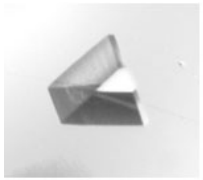
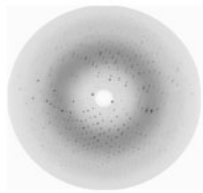
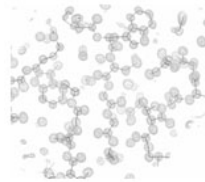
Data Collection Strategies







or

How to Avoid Collecting Suboptimal X-ray Diffraction Data ?

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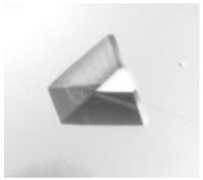
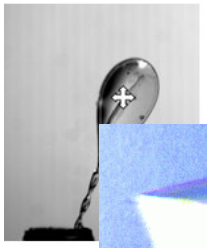
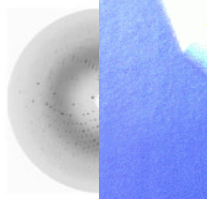
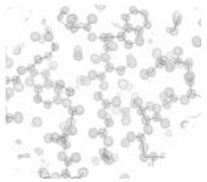
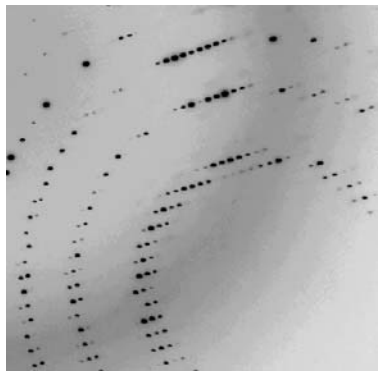
Structure Determination

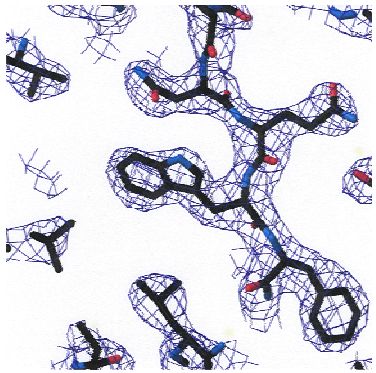






Phases α(hkl)

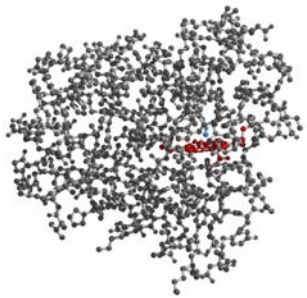
Crystal



h, k, l, |I|, σ(I)

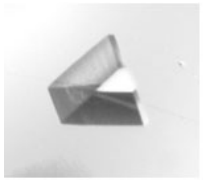


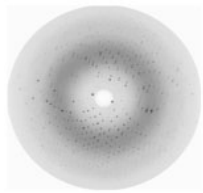
ρ(x,y,z)

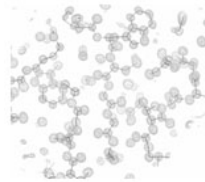


Structure

Diffraction Data Collection





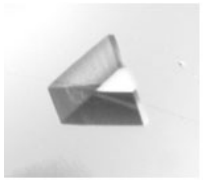


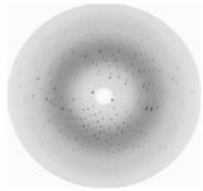
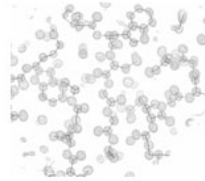
The collection of diffraction data is the last real **experiment** that is conducted before the determination and refinement of the structure.

The factors involved in diffraction data collection are complex and require some thought in order to produce the highest quality data set possible.

The quality of the diffraction data ultimately determines the quality of the resulting structure.

Diffraction Data Collection

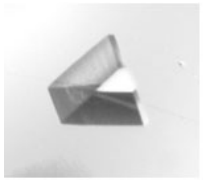


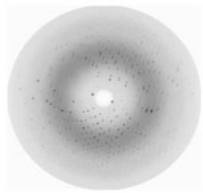
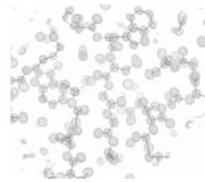



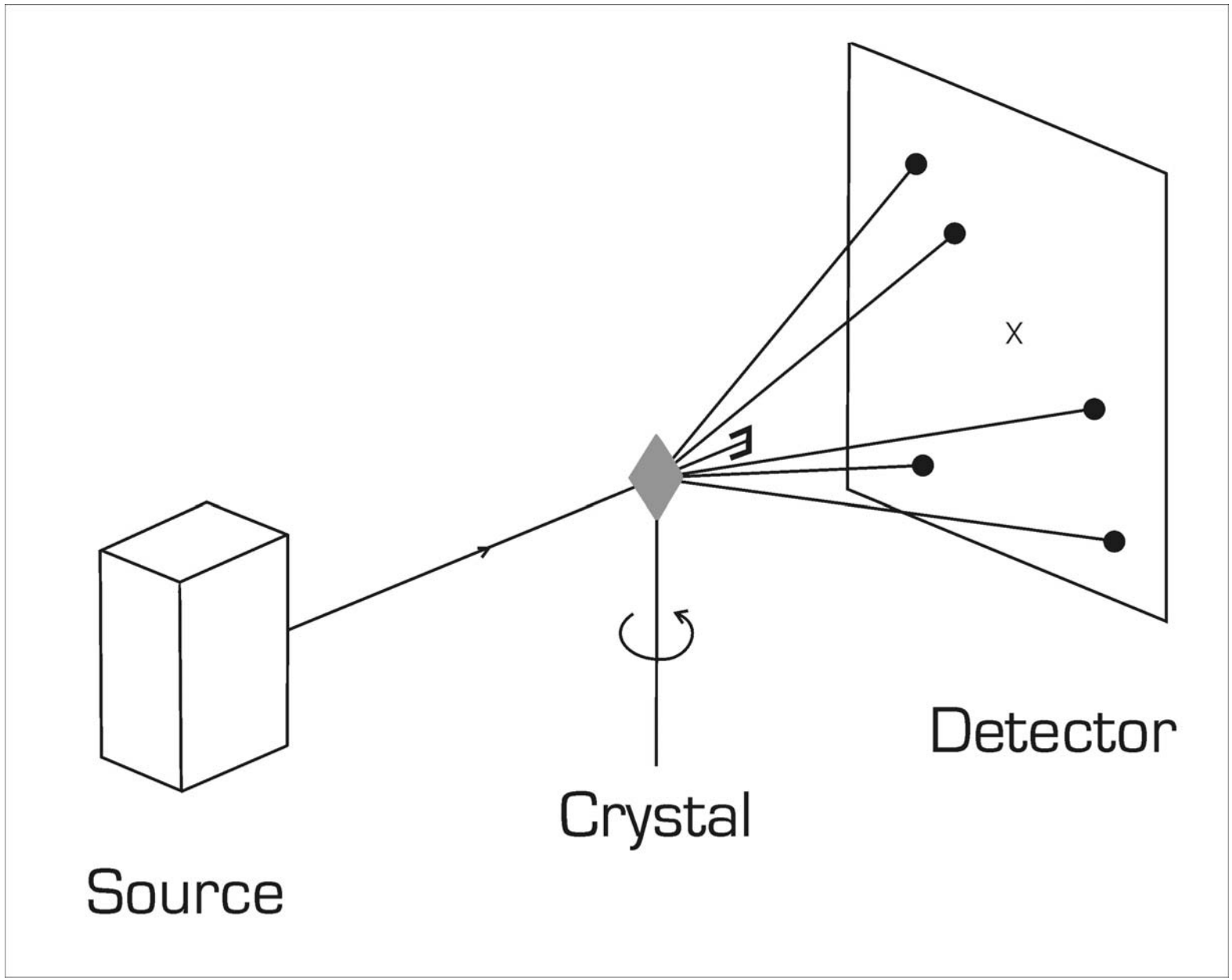

Two objectives:

- ❖ to collect a complete data set
- ❖ to collect the best possible data set

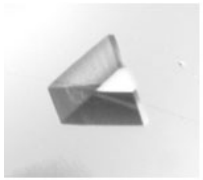
Diffraction Data Collection

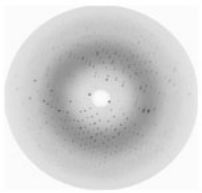


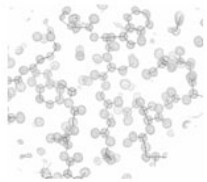



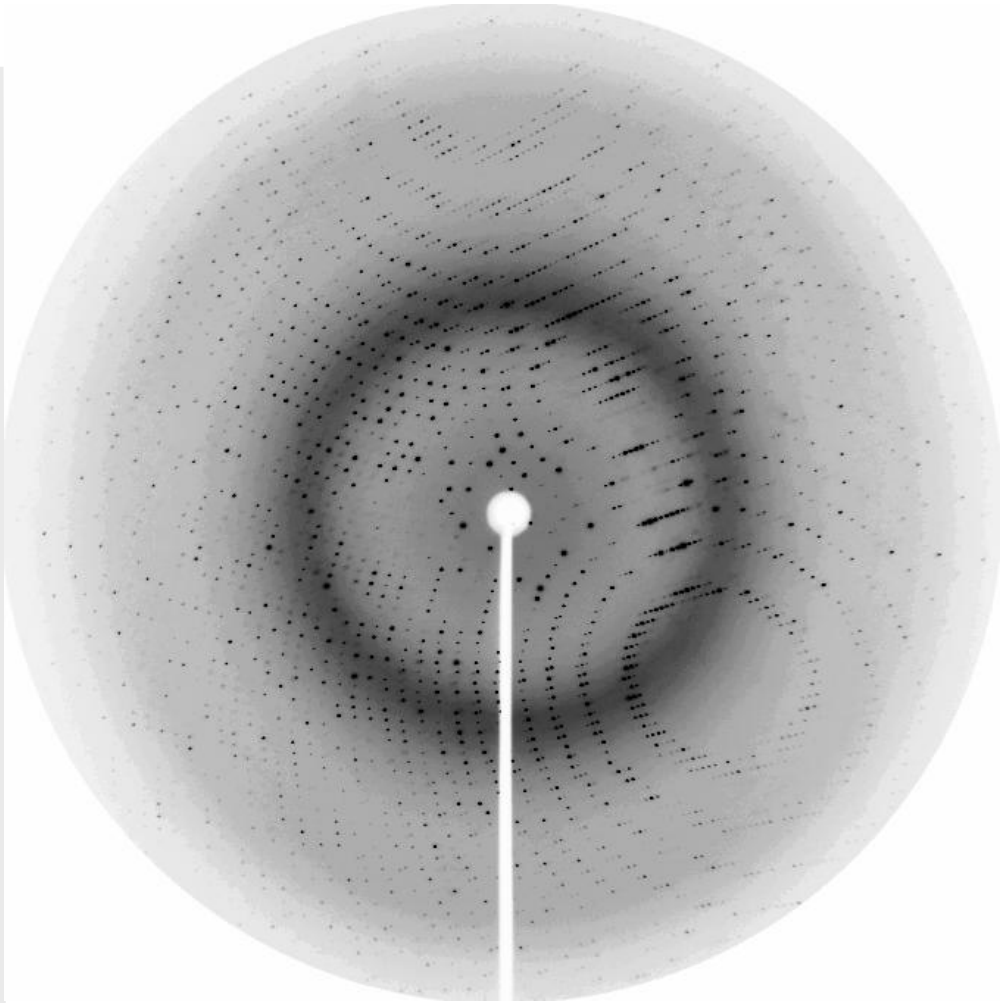



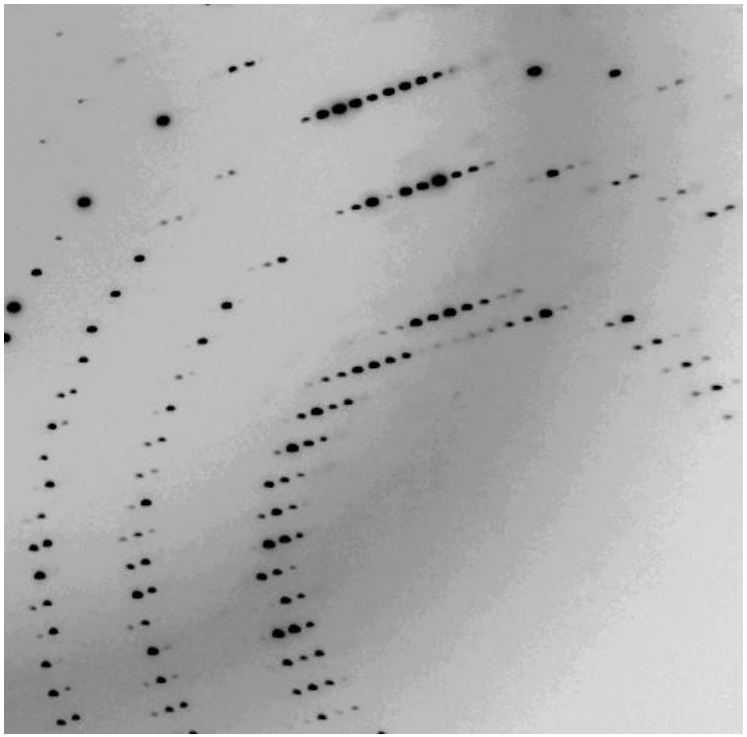
Diffraction Data Collection

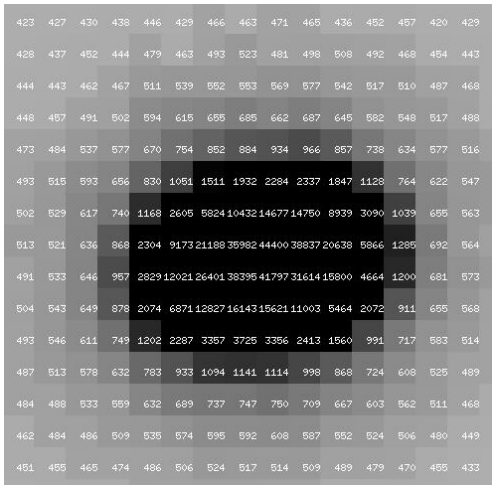










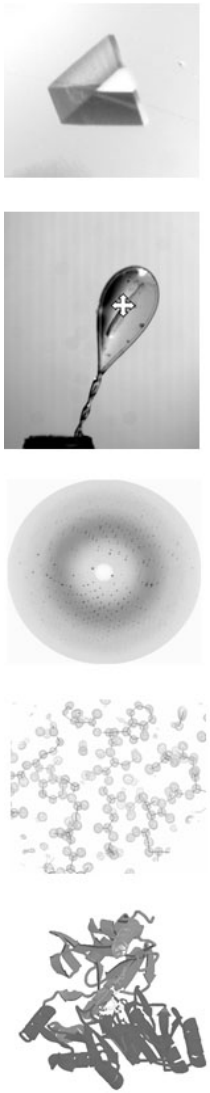


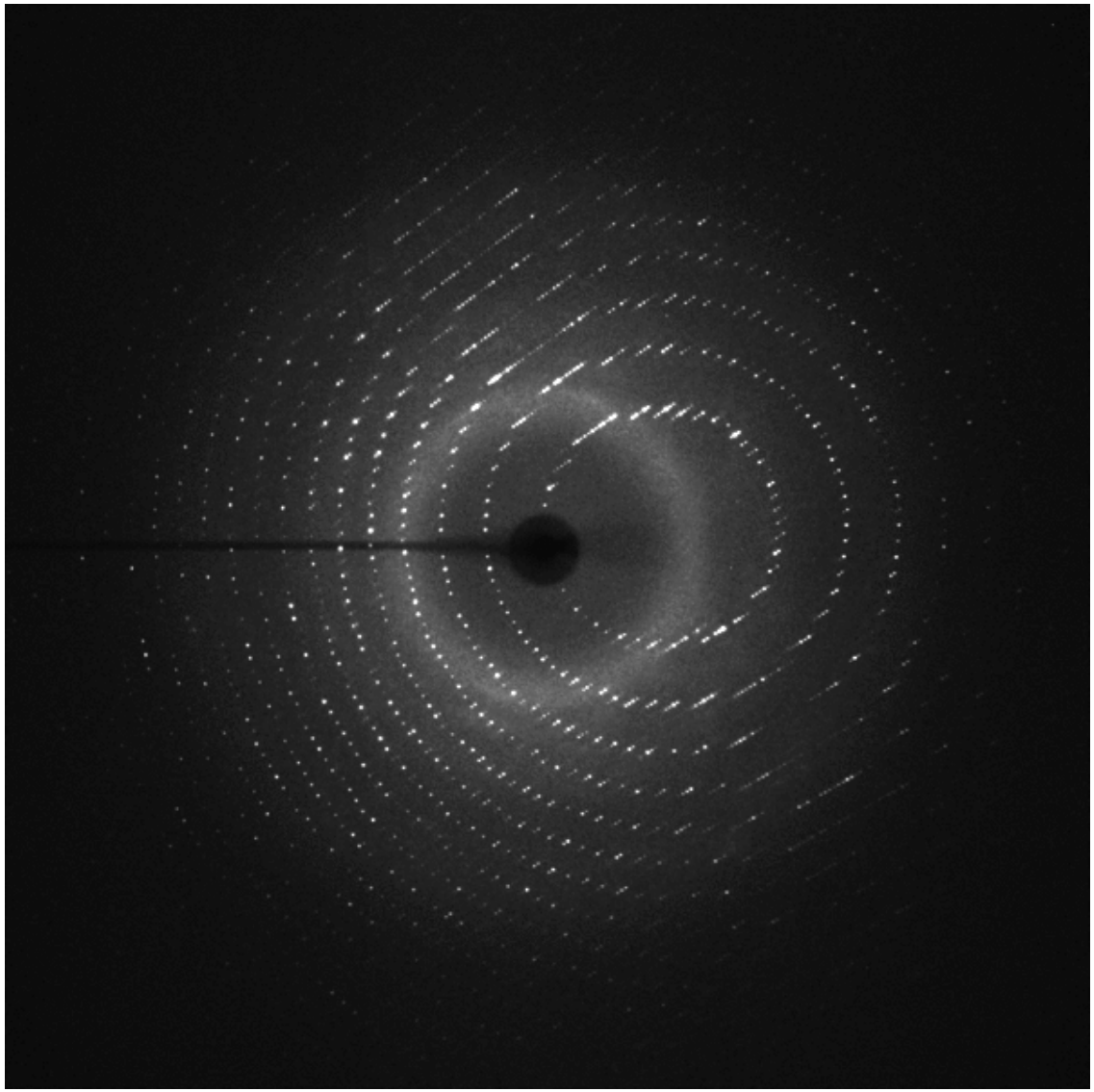
h, k, l **Miller indices**

I(h,k,l) **intensity**

σI(hkl) **error in I**

Diffraction Data Collection





HZB-MX BL14.2

MARCCD-225

λ = 0.918 Å

F = 150 mm

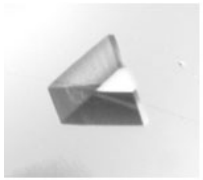
90 images

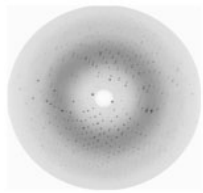
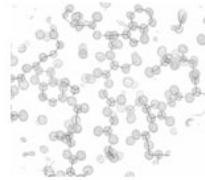
0.5°/ image

2 sec / image

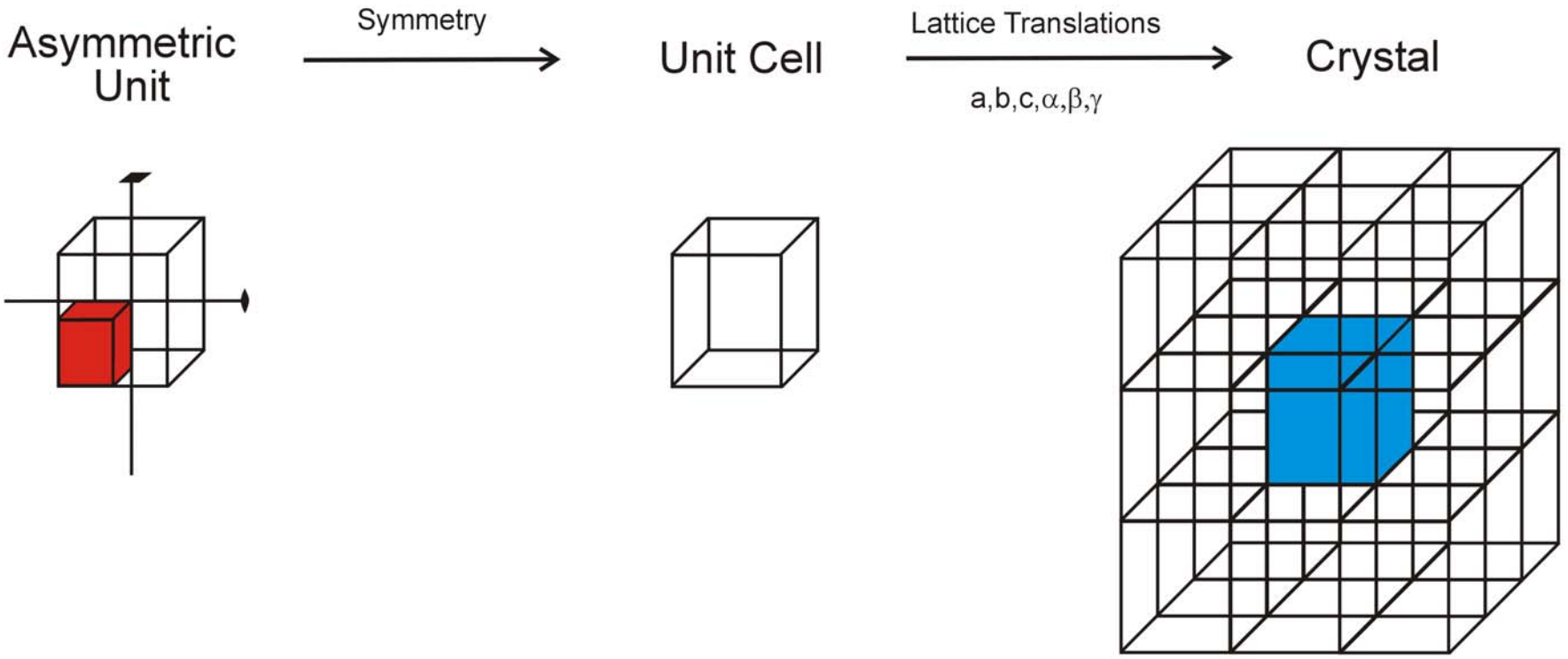
Thaumatin, space group $P4_12_12$, a=50 Å, c= 150 Å

A Crystal

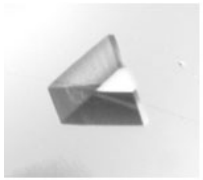


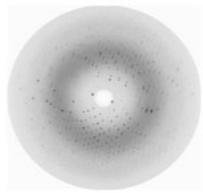
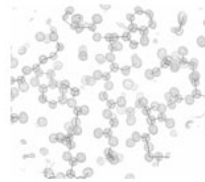



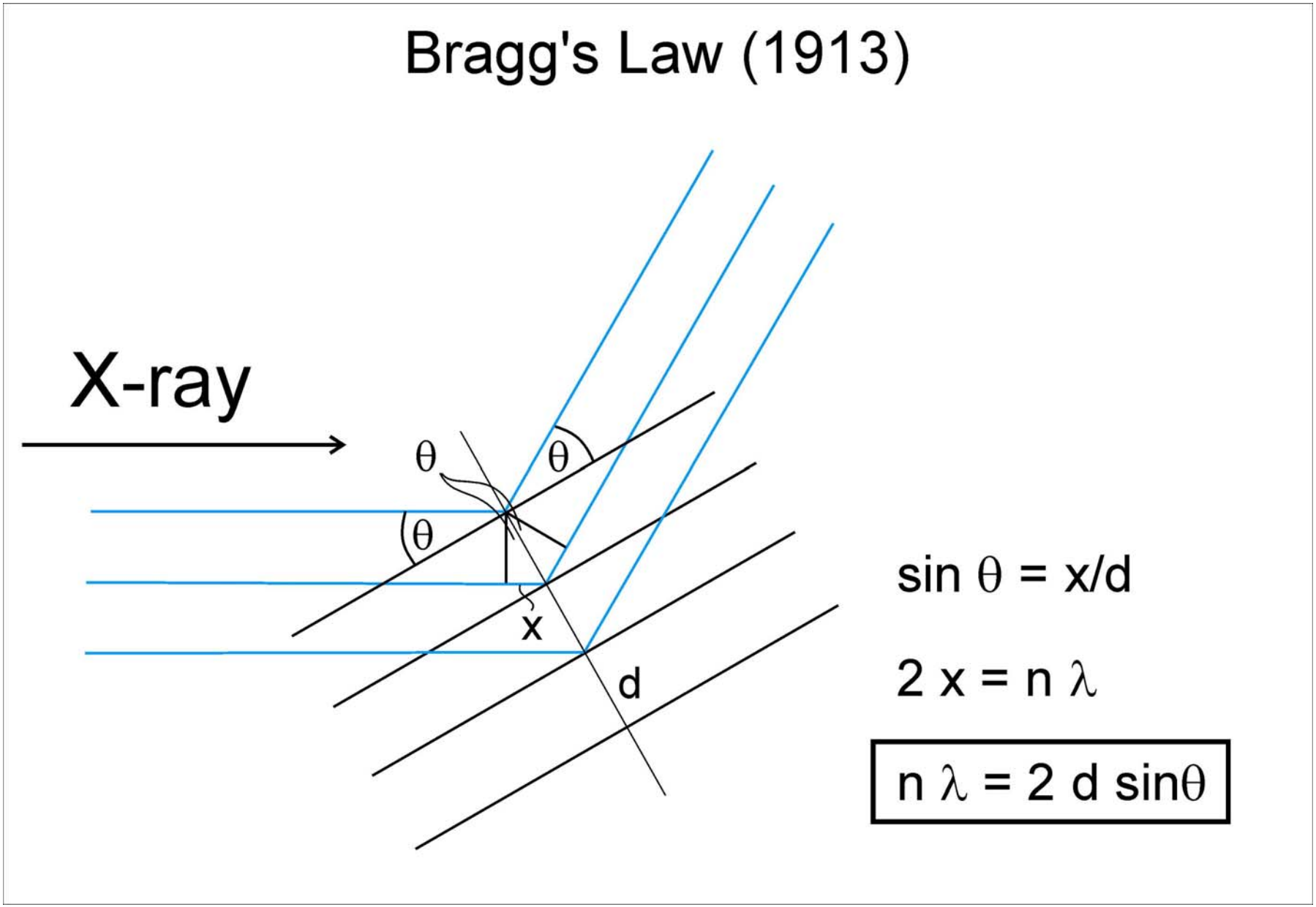

Definition: A crystal is an arrangement of building blocks, which is periodic in three dimensions.



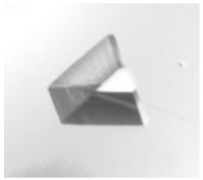
Diffraction as Reflection (Bragg)

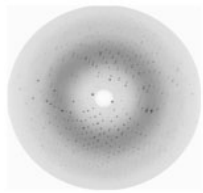
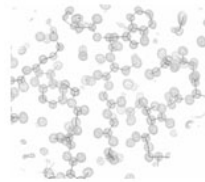


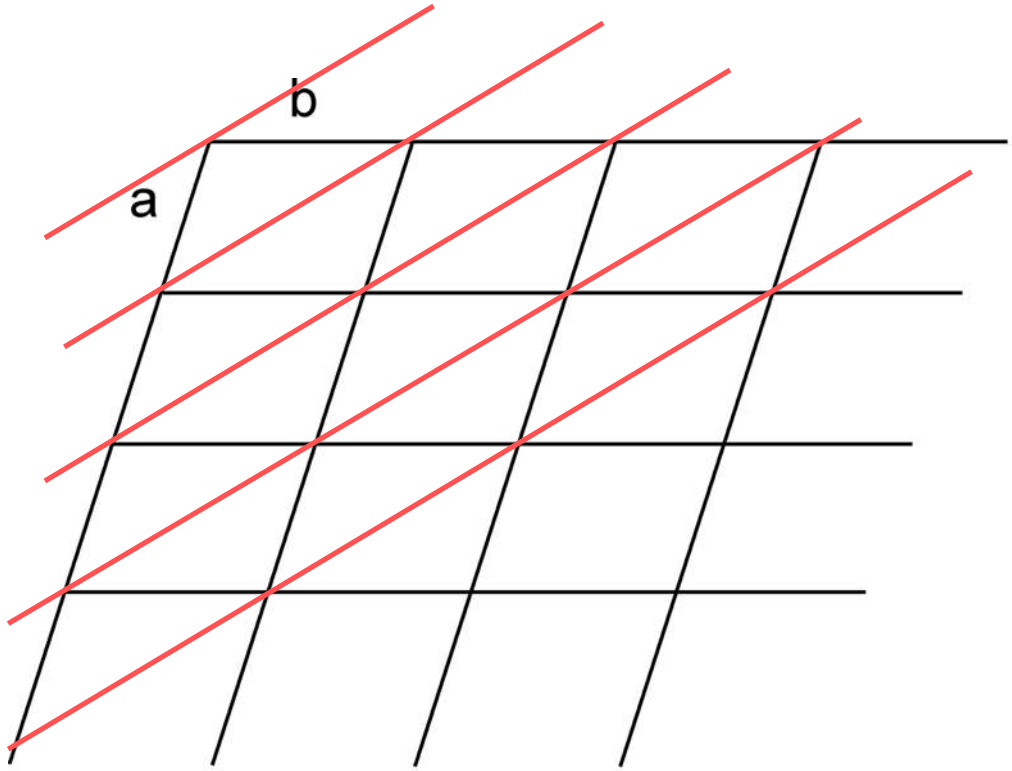



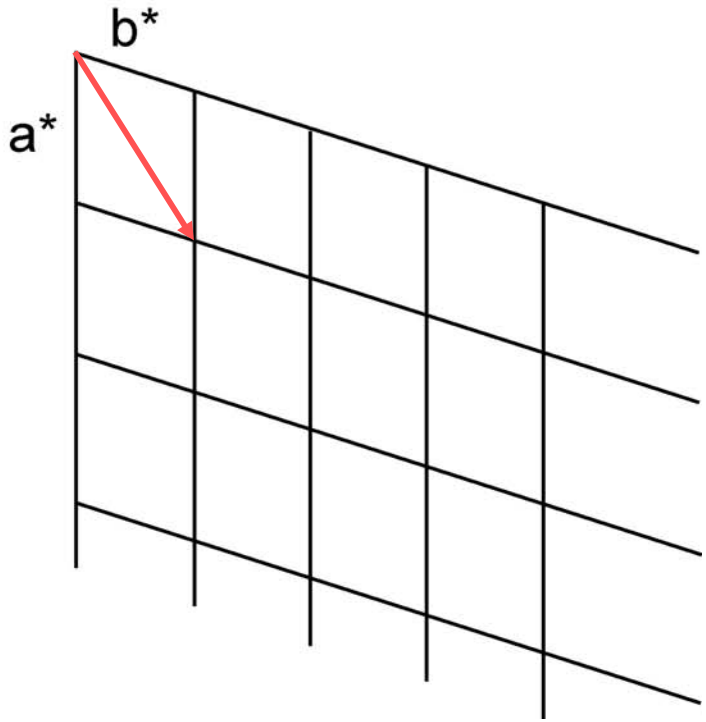



The Reciprocal Lattice (2D)





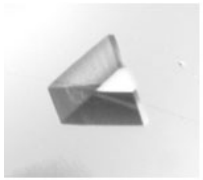
$a^* = 1/a, \quad a^* \perp b$

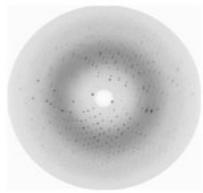
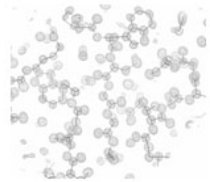
$b^* = 1/b, \quad b^* \perp a$

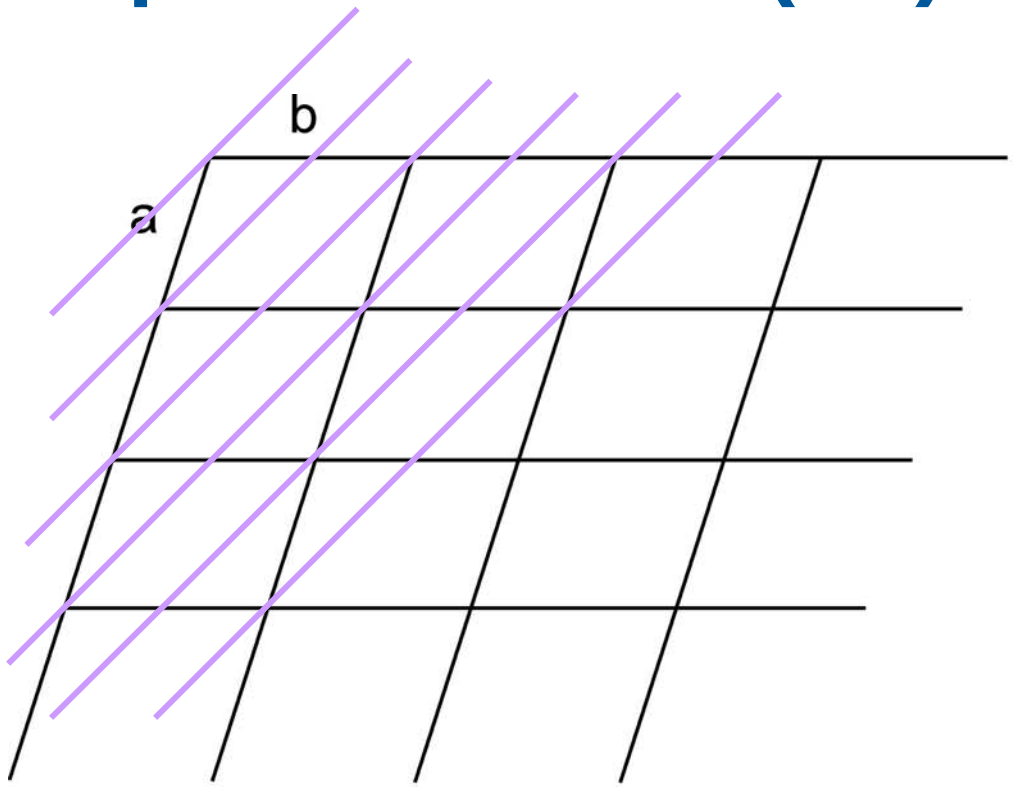
$d^* = 1\,a^* + 1\,b^*$

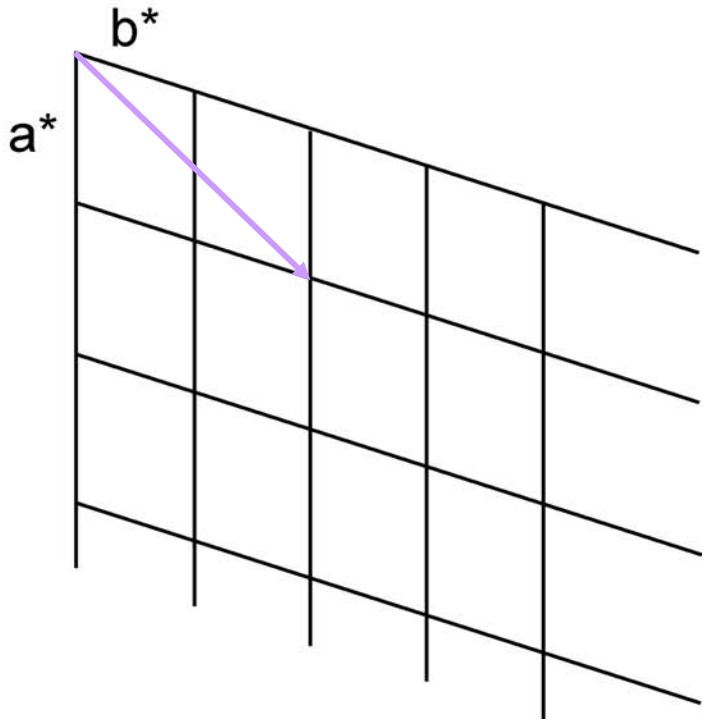
(11)

The Reciprocal Lattice (2D)





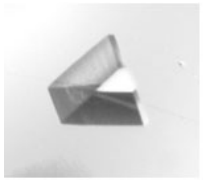
$a^* = 1/a, \quad a^* \perp b$

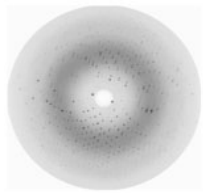
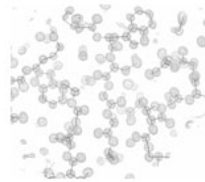
$b^* = 1/b, \quad b^* \perp a$

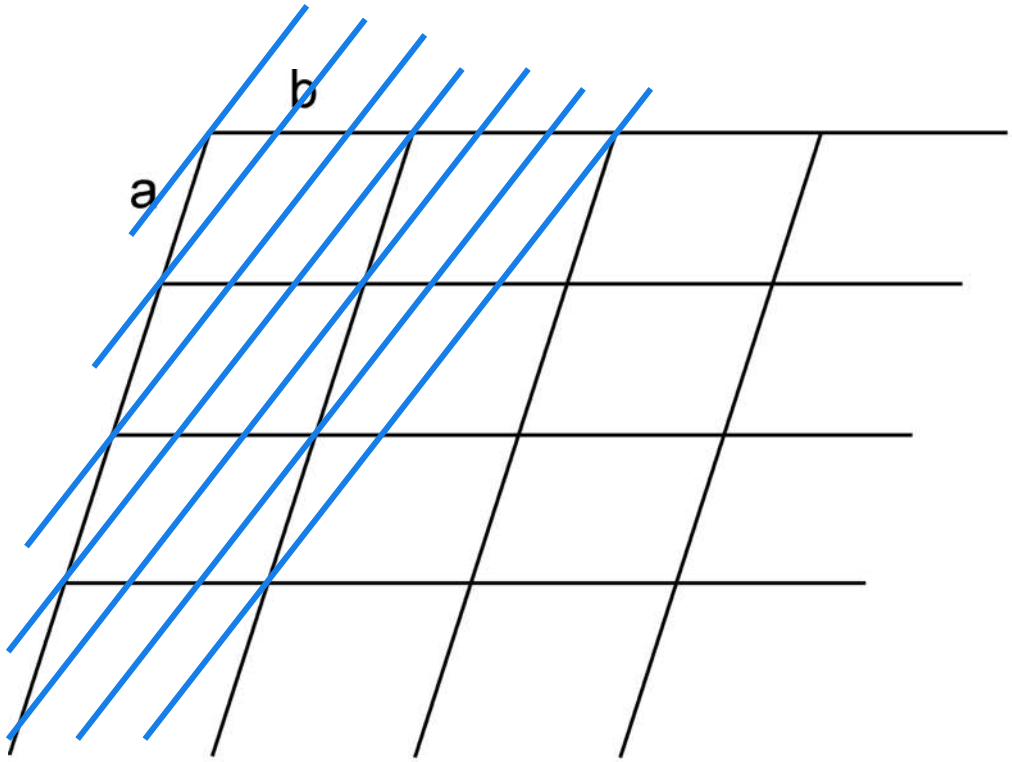
$d^* = 1\,a^* + 2\,b^*$

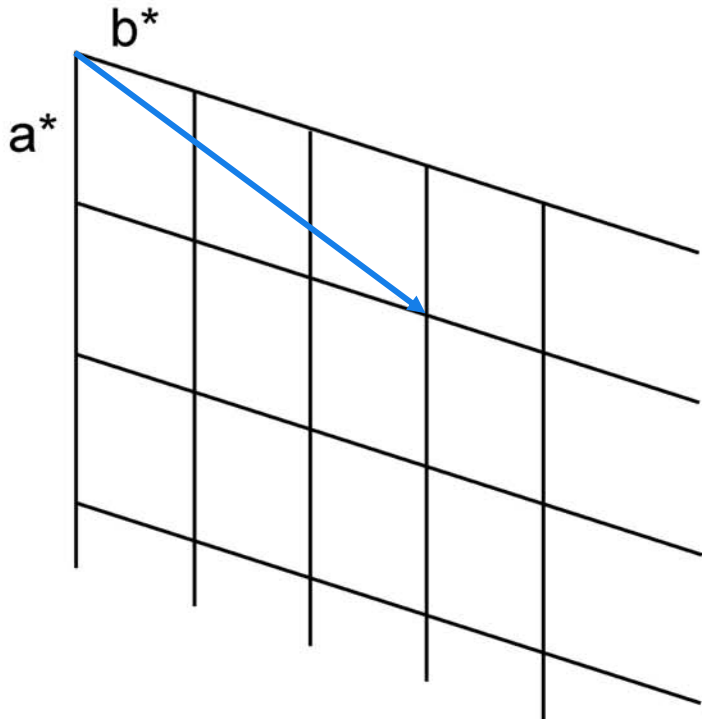
(12)

The Reciprocal Lattice (2D)





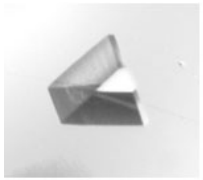
$a^* = 1/a, \quad a^* \perp b$

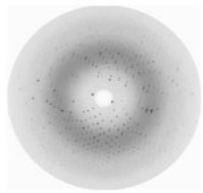
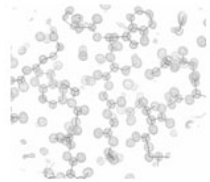
$b^* = 1/b, \quad b^* \perp a$

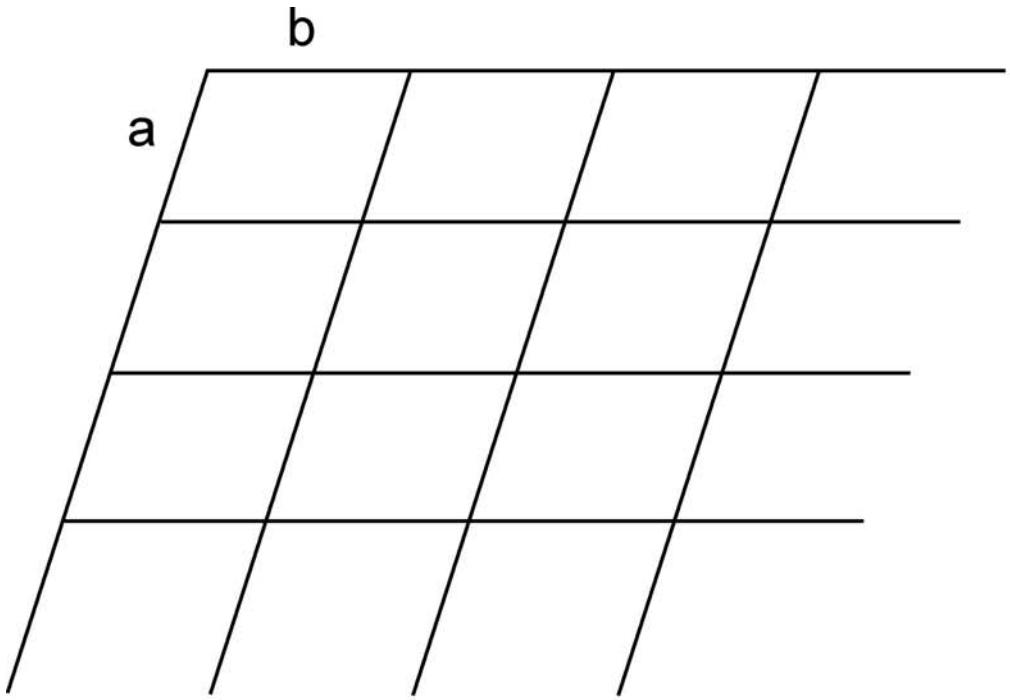
$d^* = 1\,a^* + 3\,b^*$

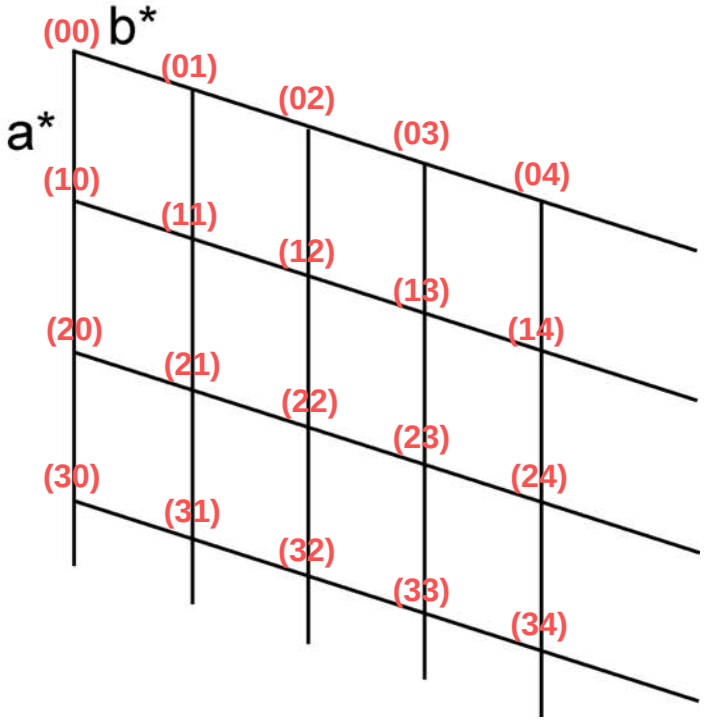
(13)

The Reciprocal Lattice (2D)



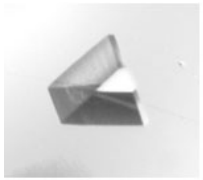



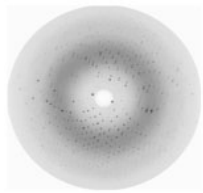
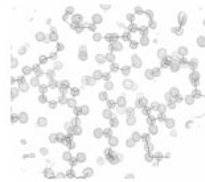


$a^* = 1/a, \quad a^* \perp b$

$b^* = 1/b, \quad b^* \perp a$

The Reciprocal Lattice (2D)



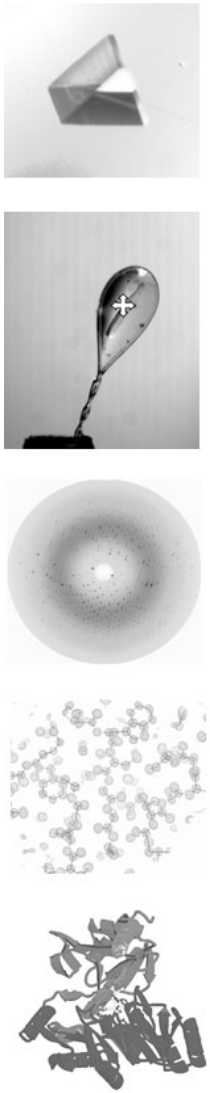




- every set of planes in the real lattice (characterized by the normal vector d) corresponds to a lattice point d* (d* = 1 / d) in the reciprocal lattice (and vice versa)

$a^* = 1/a, \quad a^* \perp b$

$b^* = 1/b, \quad b^* \perp a$

The Reciprocal Lattice (3D)



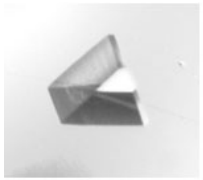
$a^* = b \times c / V, \quad a^* \perp b, c, \quad a^* \bullet a = 1$

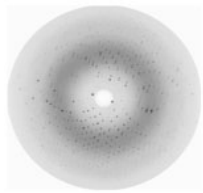
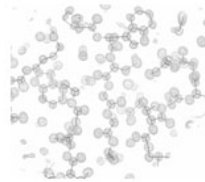
$b^* = a \times c / V, \quad b^* \perp a, c, \quad b^* \bullet b = 1$

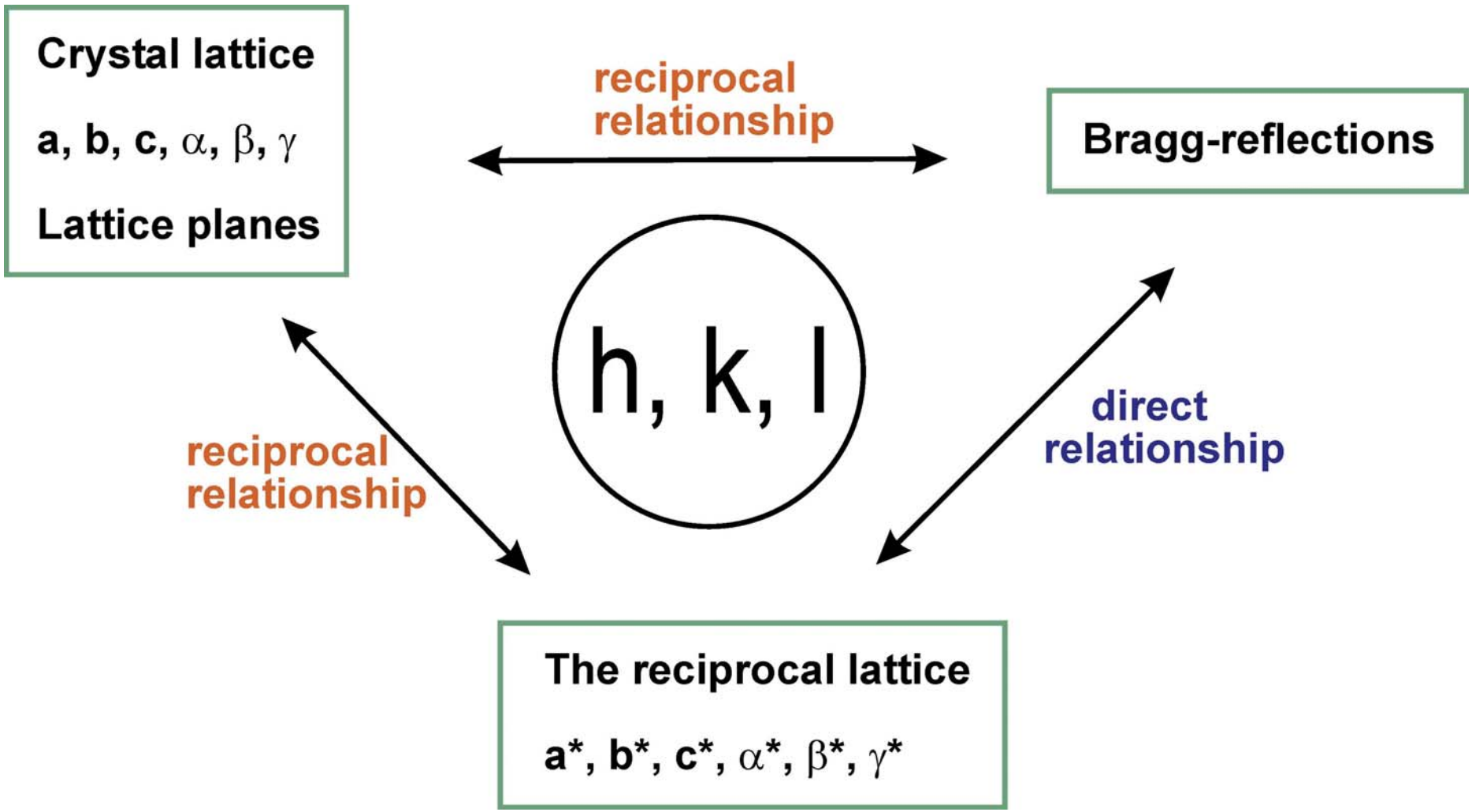
$c^* = a \times b / V, \quad c^* \perp a, b, \quad c^* \bullet c = 1$

$V^* = 1 / V$

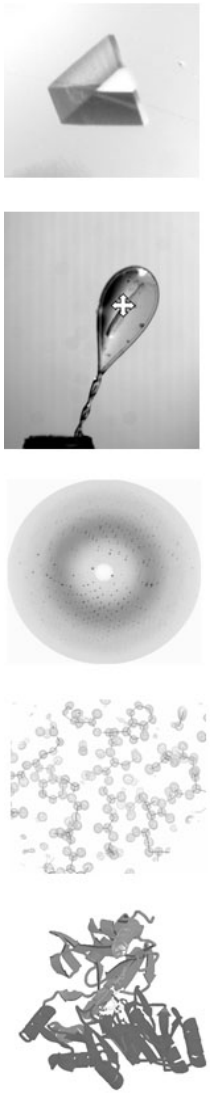
The Purpose of the Reciprocal Lattice



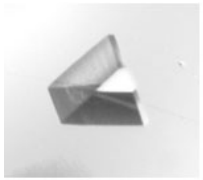



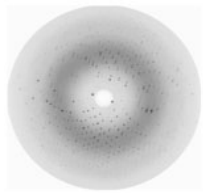
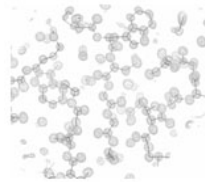
Planes, Lattice Points and Reflections



- every set of planes (characterized by the normal vector d) corresponds to a reciprocal lattice point d* (d* = 1 / d)

Planes, Lattice Points and Reflections

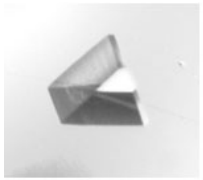


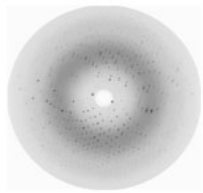
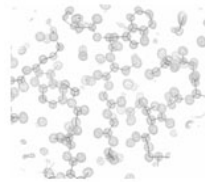




- every set of planes (characterized by the normal vector d) corresponds to a reciprocal lattice point d* (d* = 1 / d)

- d* = h • a* + k • b* + l • c* (h, k, l: Miller indices)

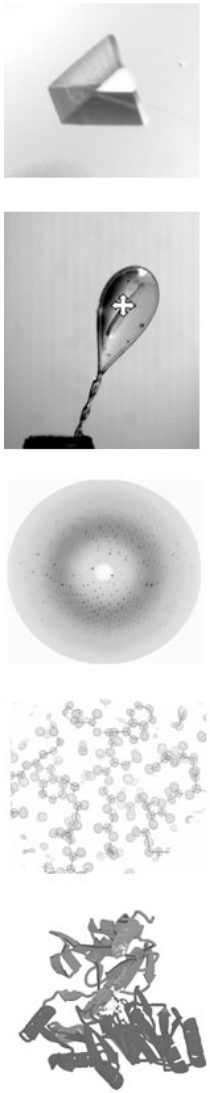
Planes, Lattice Points and Reflections



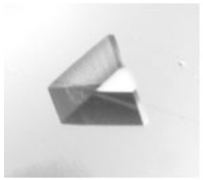

- every set of planes (characterized by the normal vector d) corresponds to a reciprocal lattice point d* (d* = 1 / d)
- d* = h • a* + k • b* + l • c* (h, k, l: Miller indices)
- every set of planes (d) corresponds to an X-ray reflection

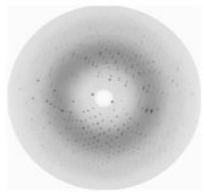
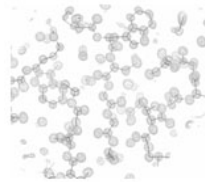
Planes, Lattice Points and Reflections

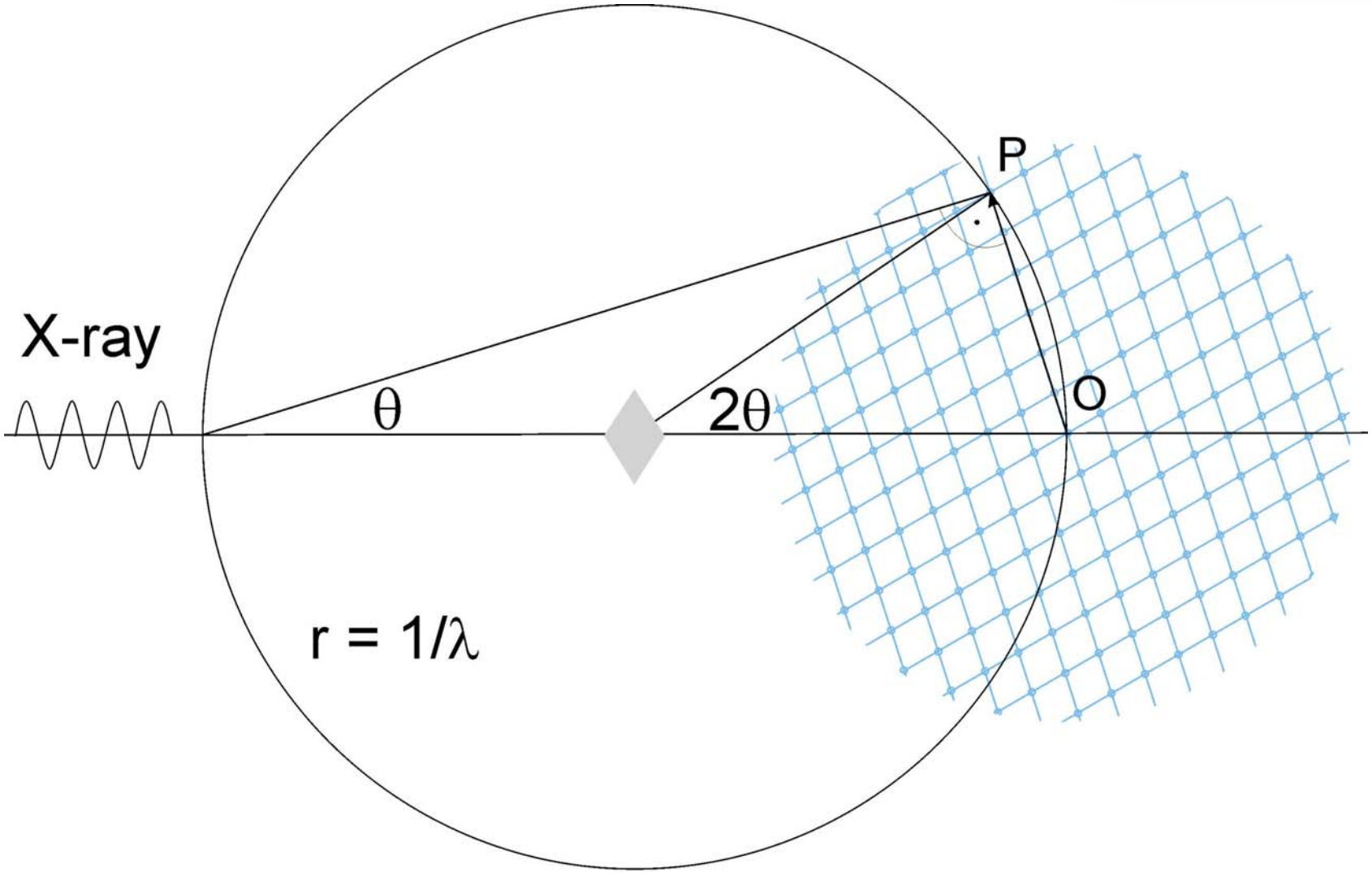


- every set of planes (characterized by the normal vector d) corresponds to a reciprocal lattice point d* (d* = 1 / d)
- d* = h • a* + k • b* + l • c* (h, k, l: Miller indices)
- every set of planes (d) corresponds to an X-ray reflection
- every reciprocal lattice point (d*) corresponds to an X-ray reflection

The Ewald Construction



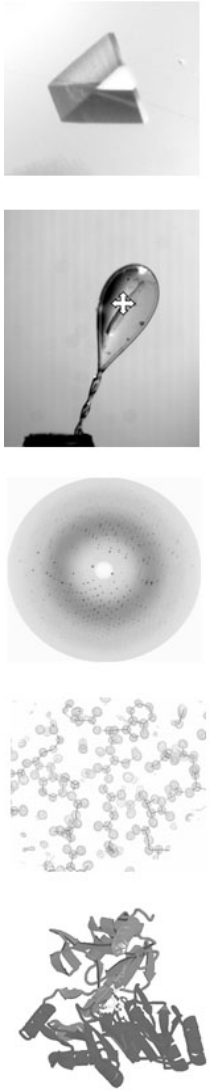



$\sin\theta = OP / (2/\lambda)$

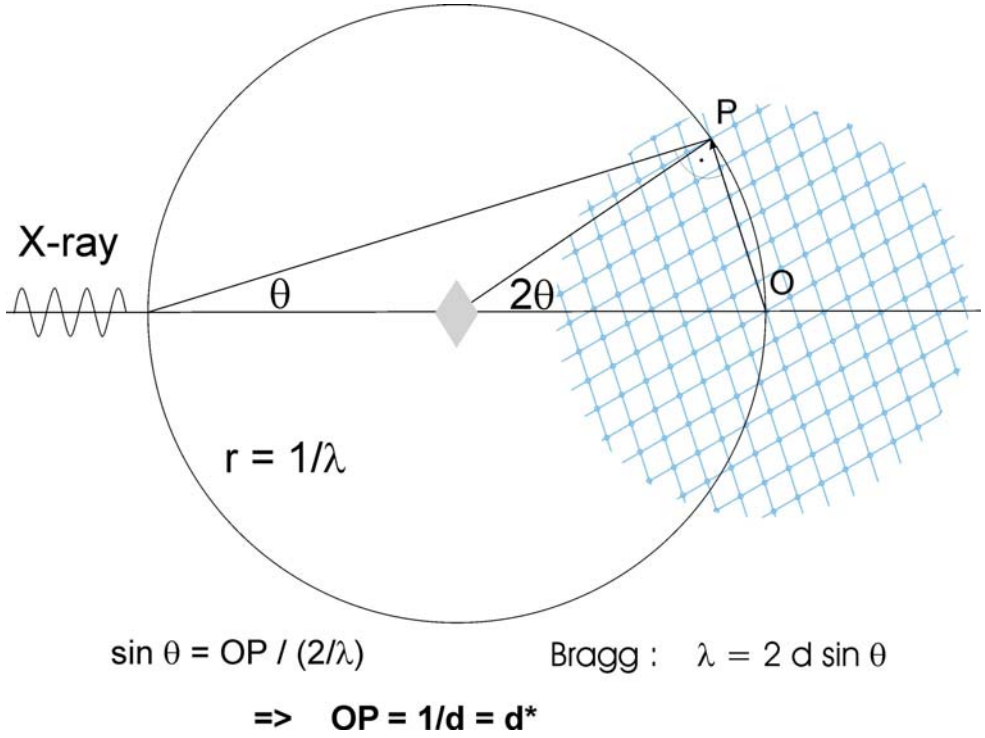
Bragg : $\lambda = 2\, d \sin\theta$

=> OP = 1/d = d*

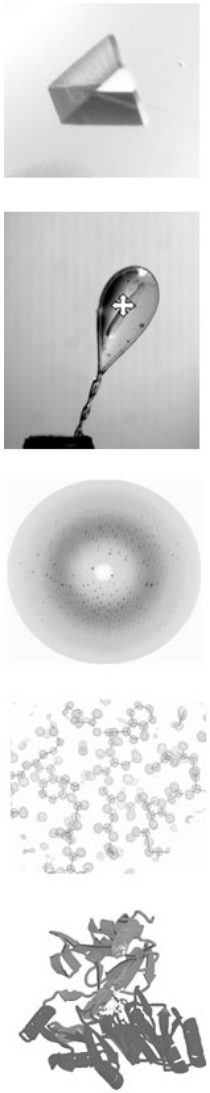
The Ewald Construction

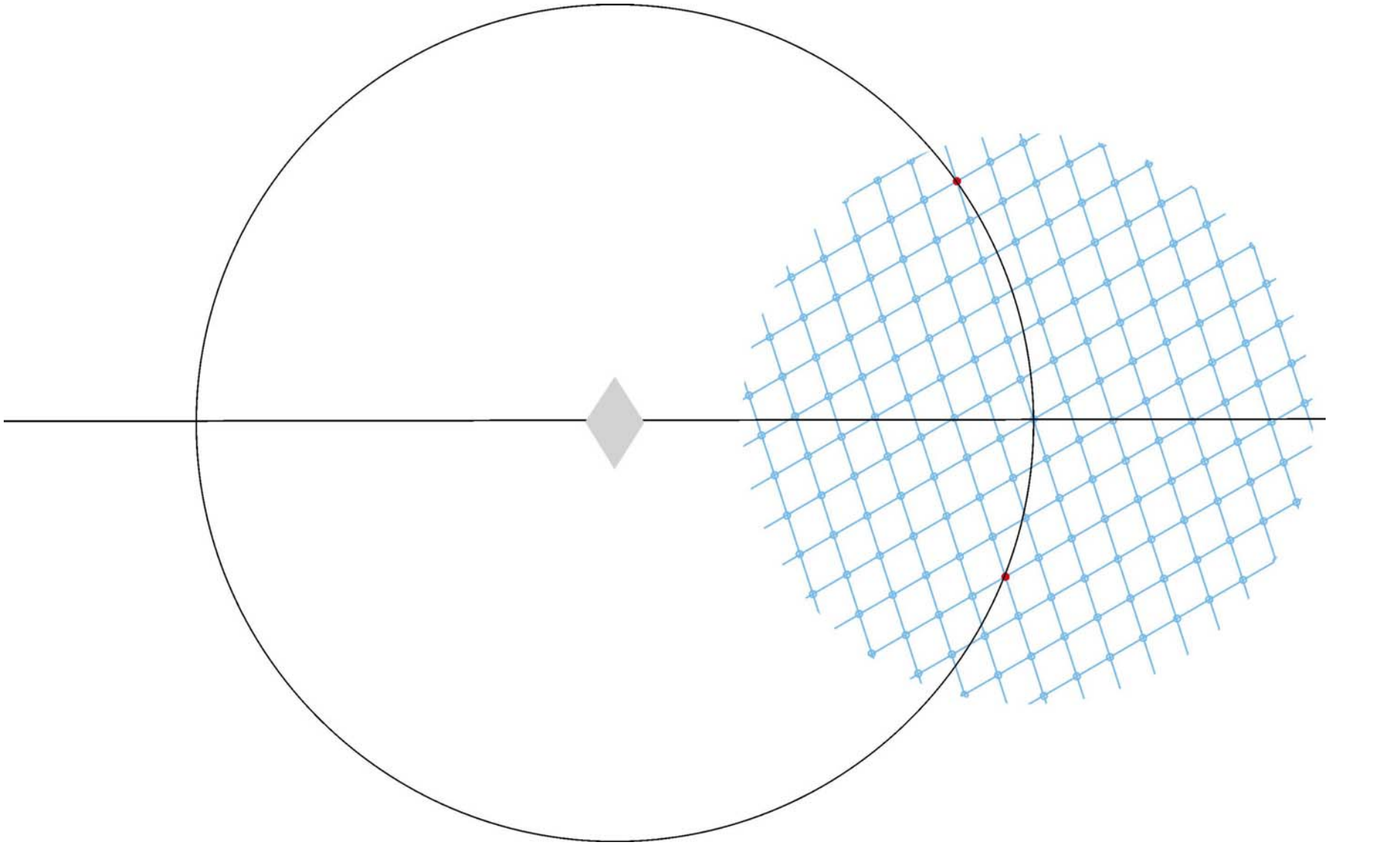


- only when OP is a reciprocal lattice point, a reflection can be observed
- the Ewald-construction is nothing but a graphical representation of Bragg's Law.

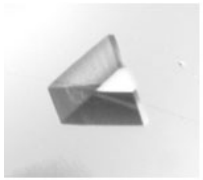


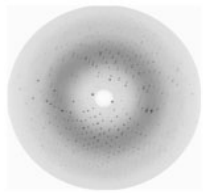
A Still Image

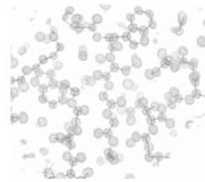


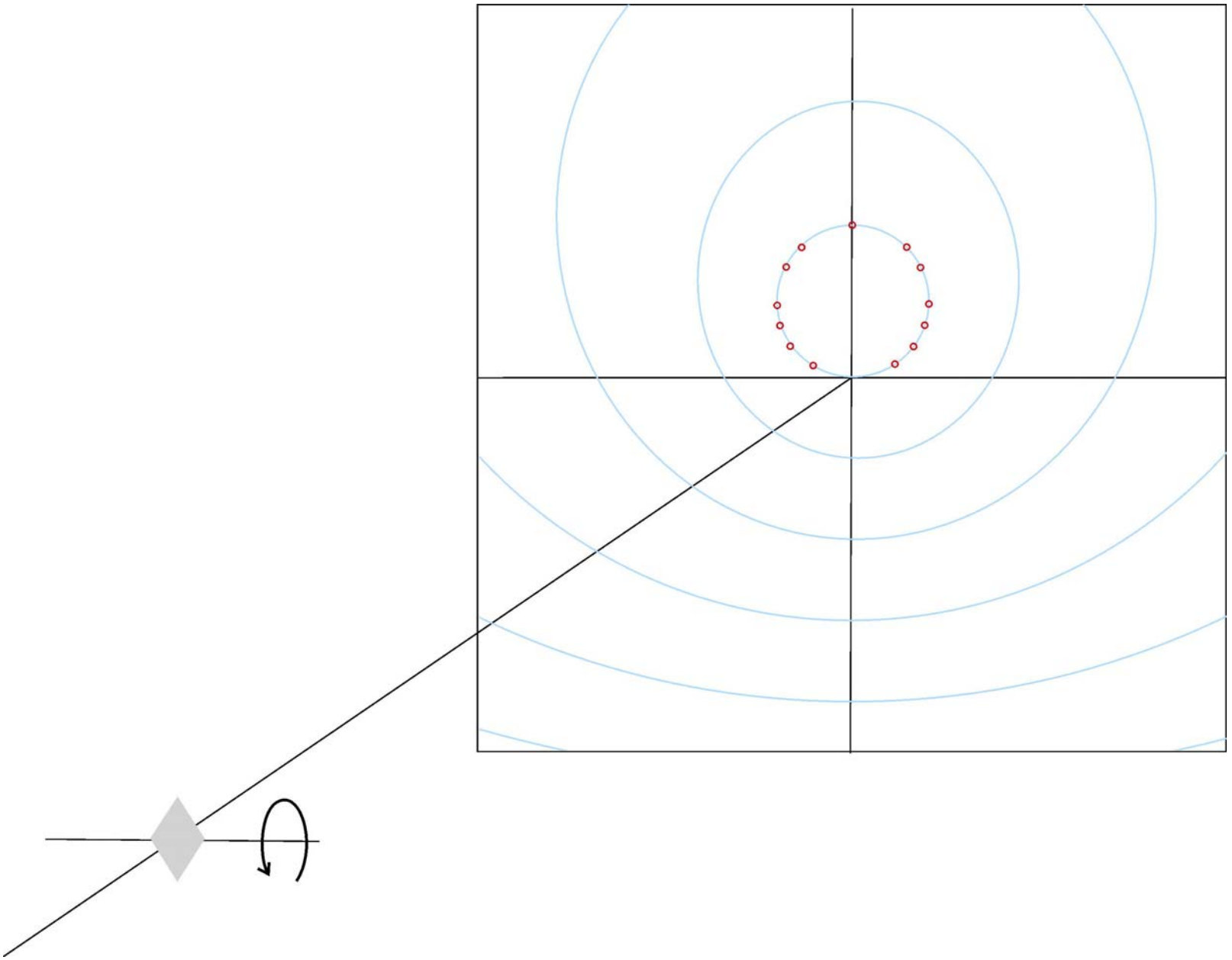


On the Detector?

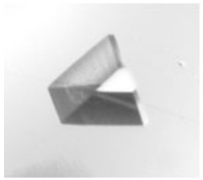


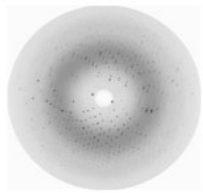
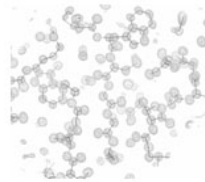


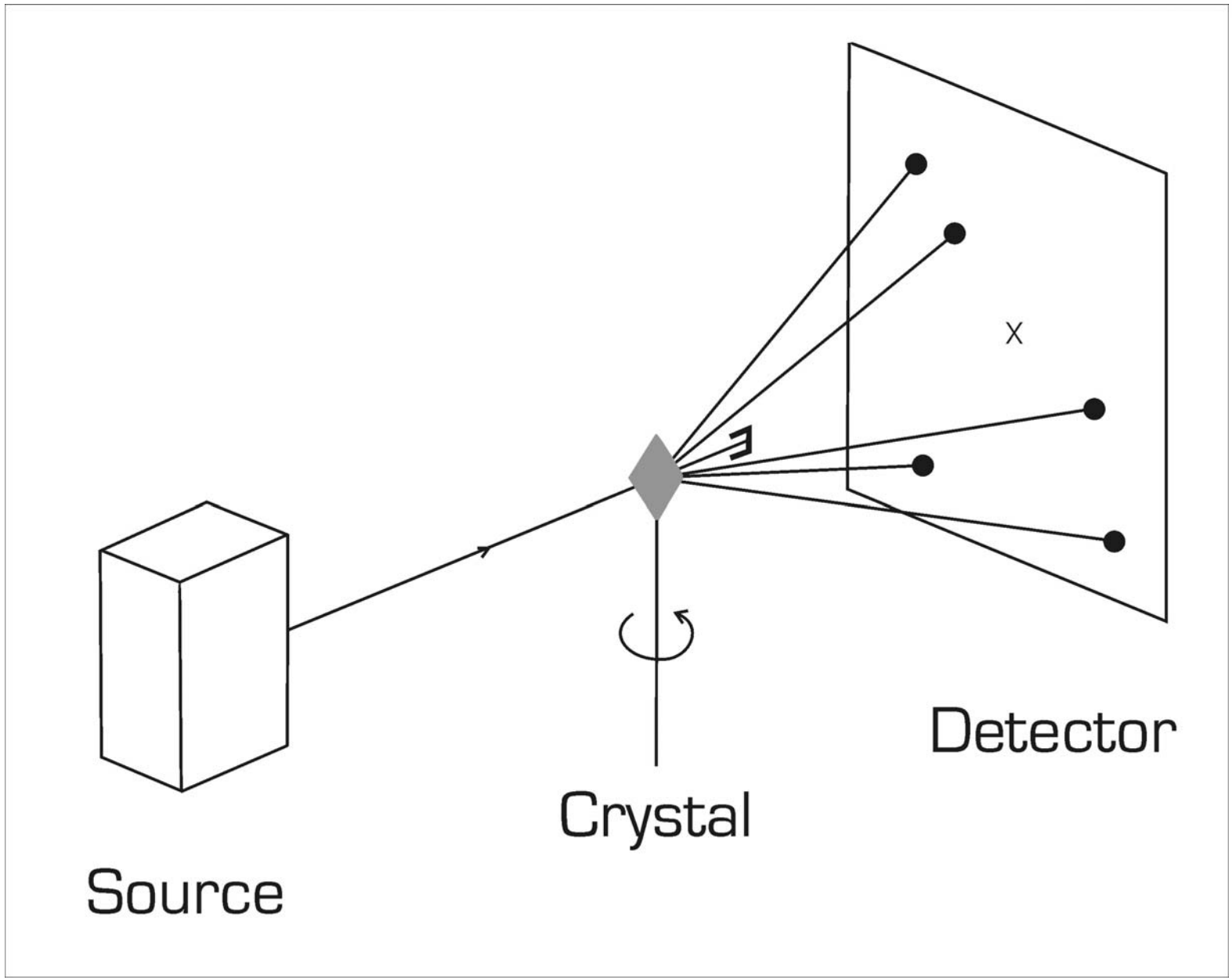




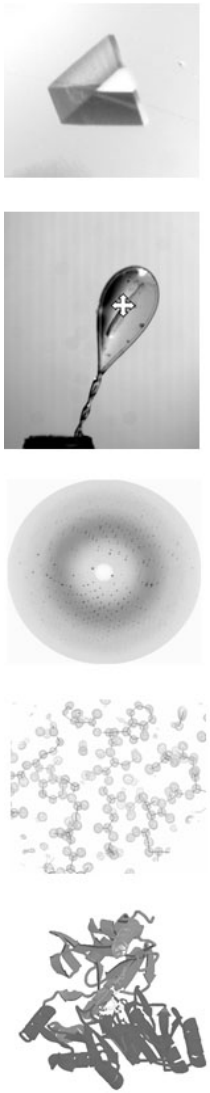
The Rotation Method



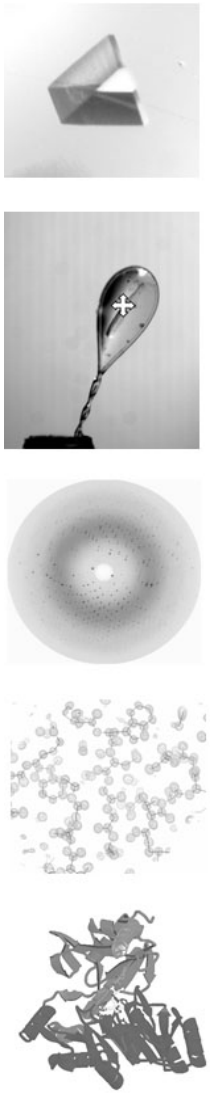



The Rotation Method



- Diffraction data are nowadays typically collected using the rotation method and an area detector.

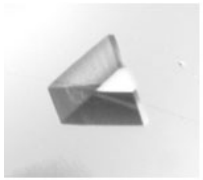
The Rotation Method

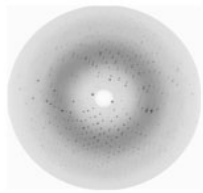


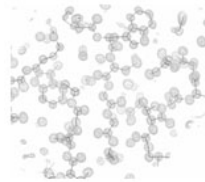
- Diffraction data are nowadays typically collected using the rotation method and an area detector.

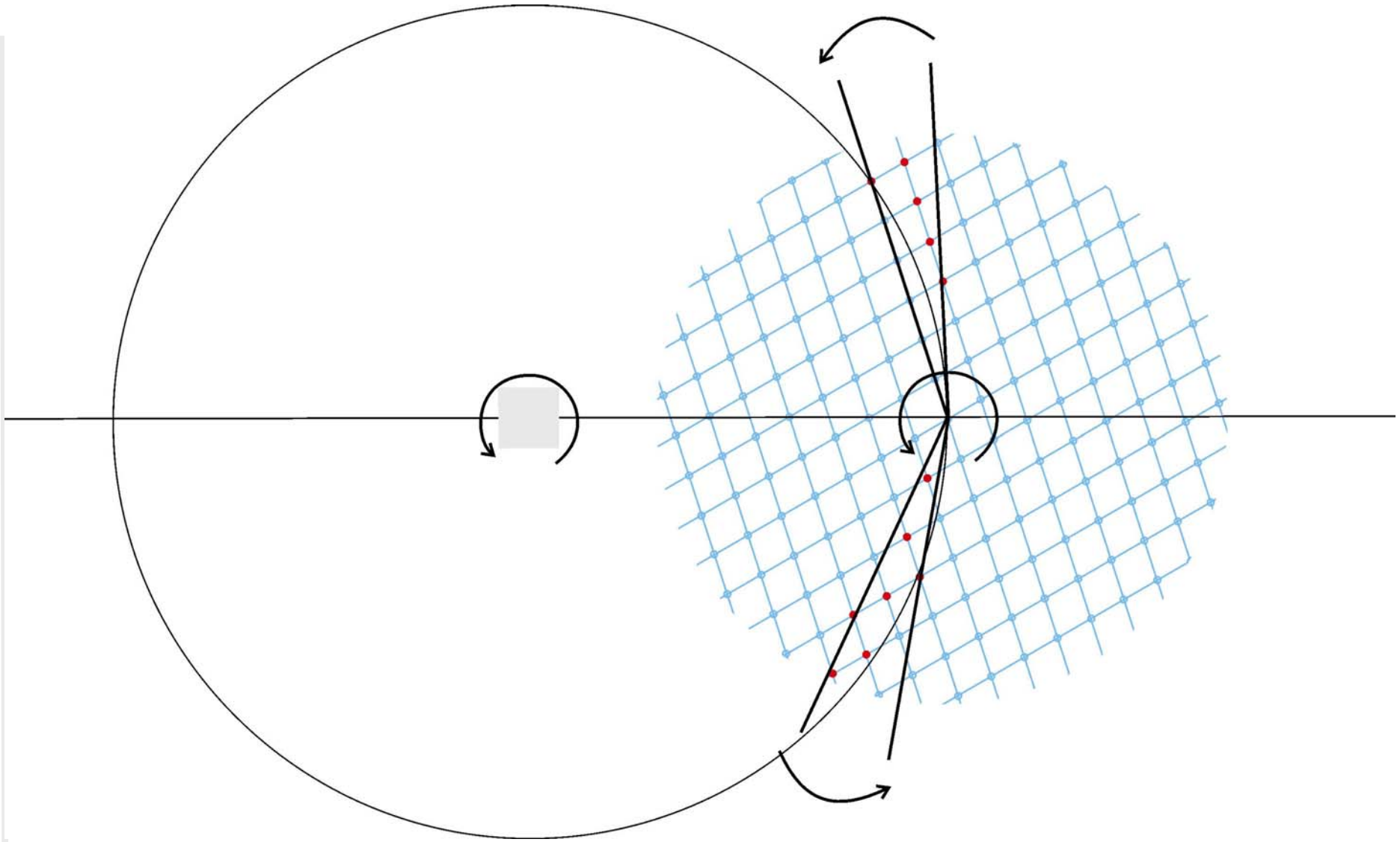
- A set of diffraction images with a small rotation increment (e.g. $\Delta\phi$ = 1.0°) is collected and constitutes the raw data.

A Small Rotation Range

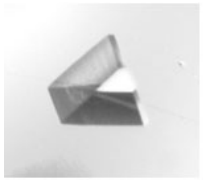


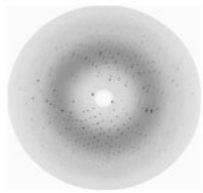


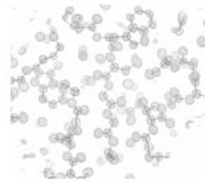


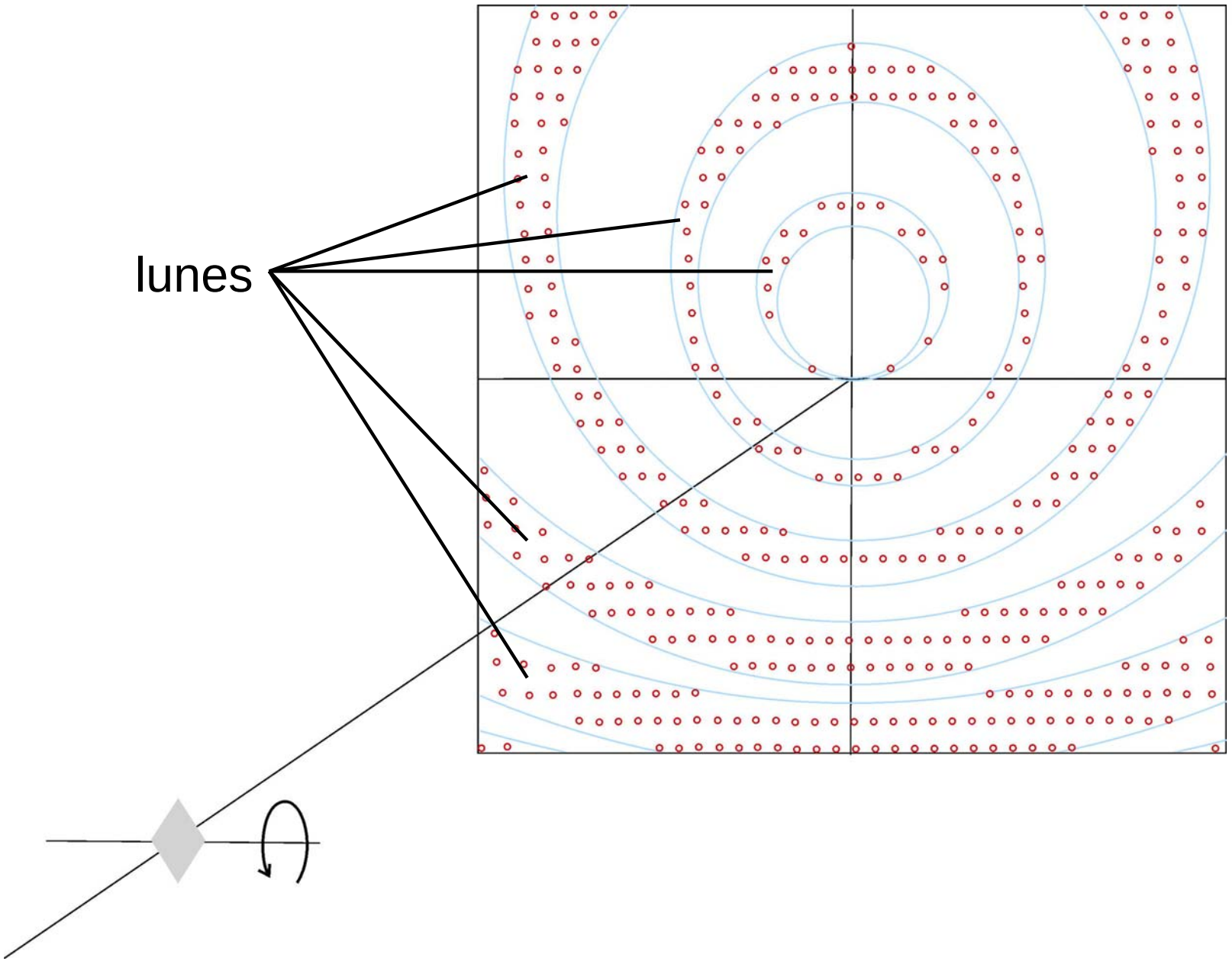


On the Detector?

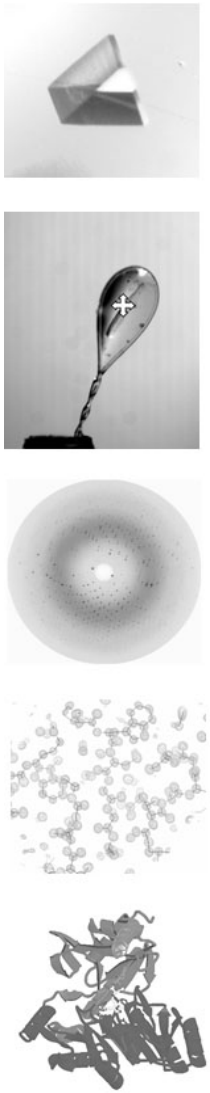


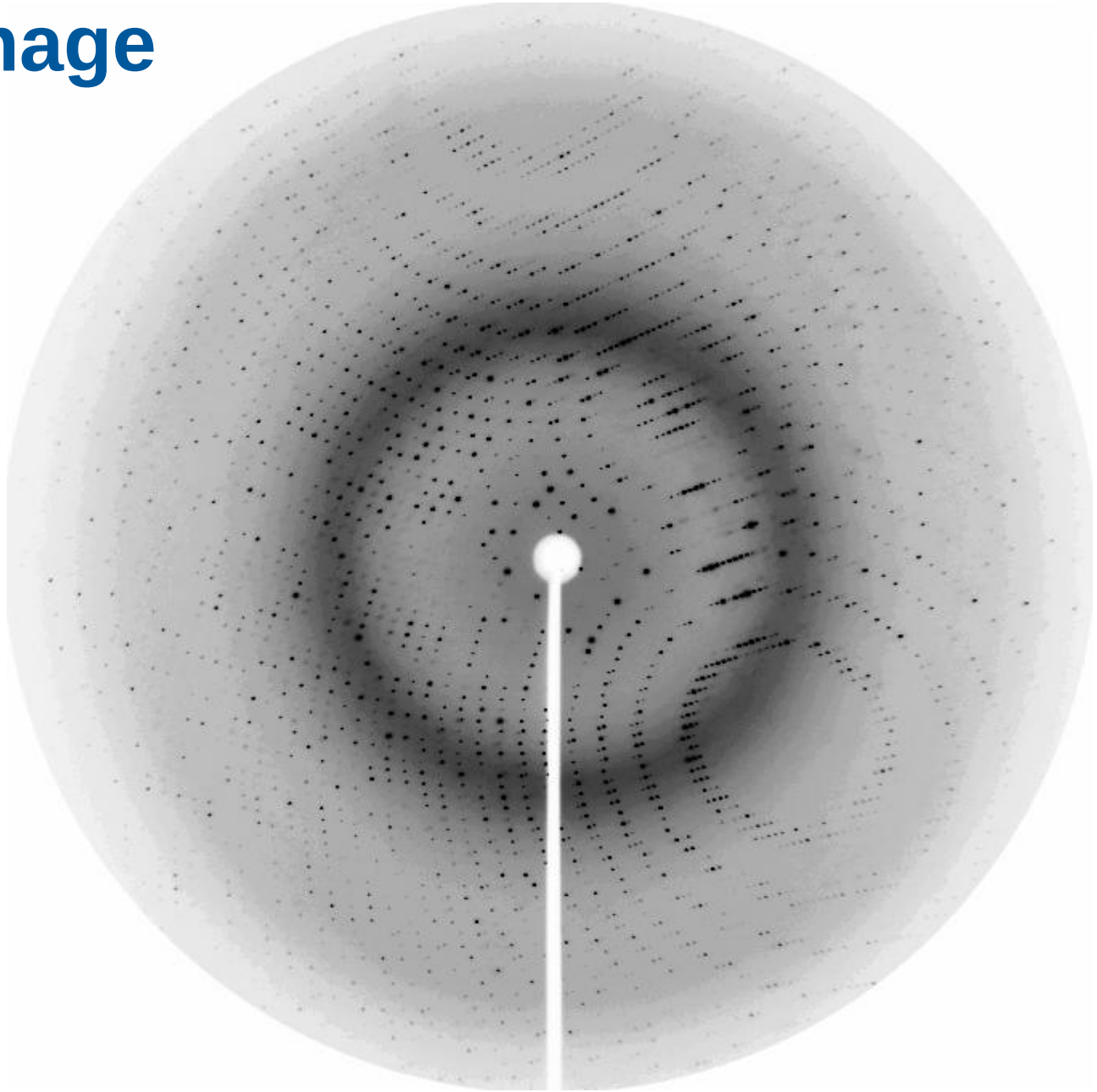




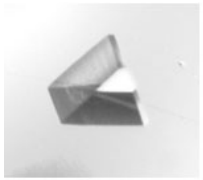


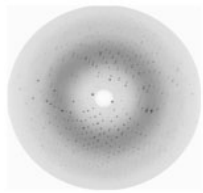
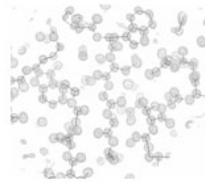
Compare this to a Real Diffraction Image



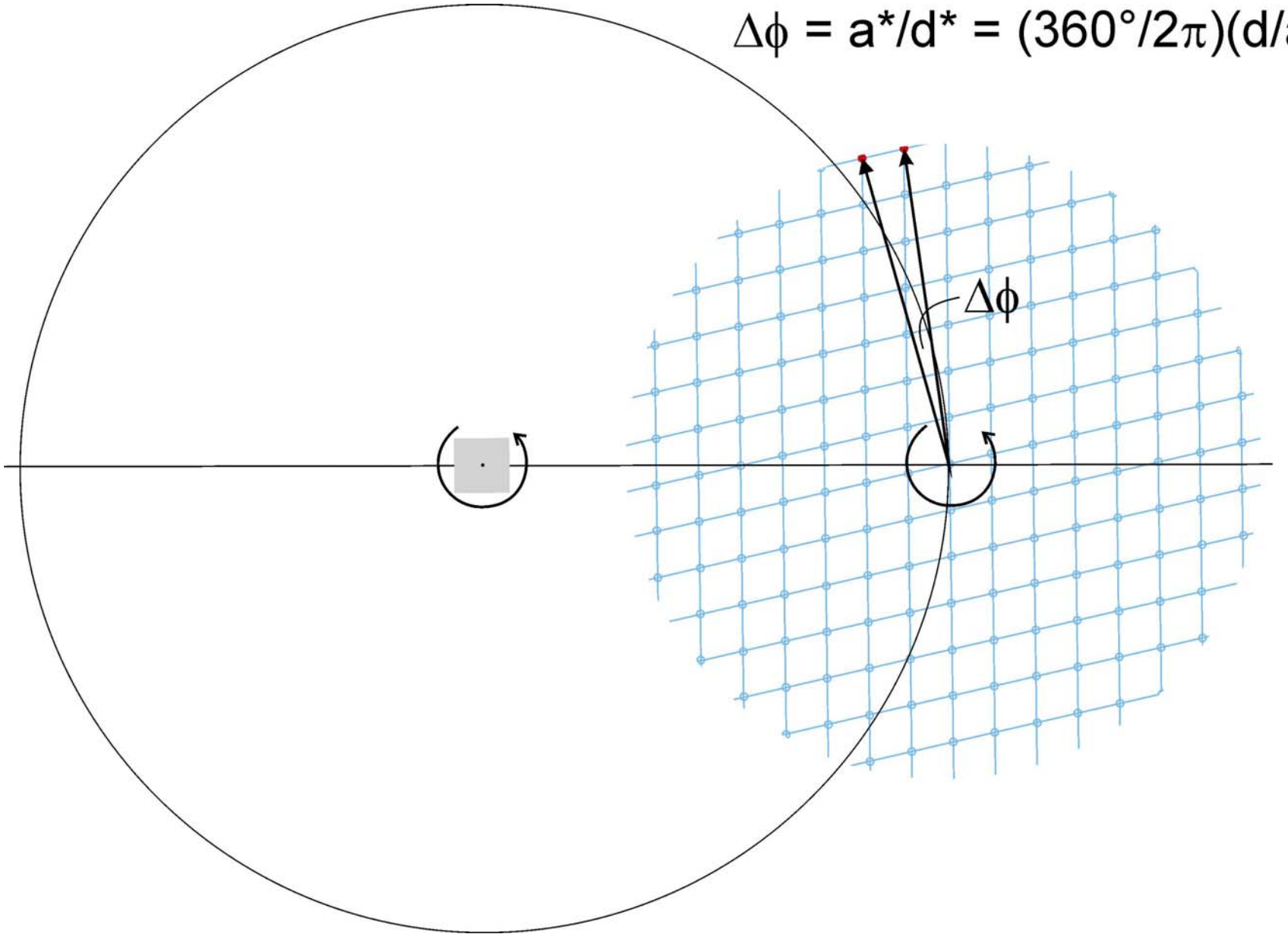


The Problem of Overlaps

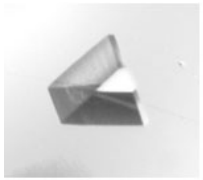


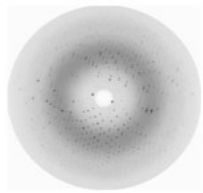
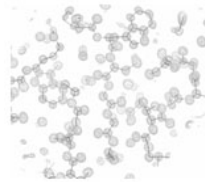




$\Delta\phi = a^*/d^* = (360°/2\pi)(d/a)$

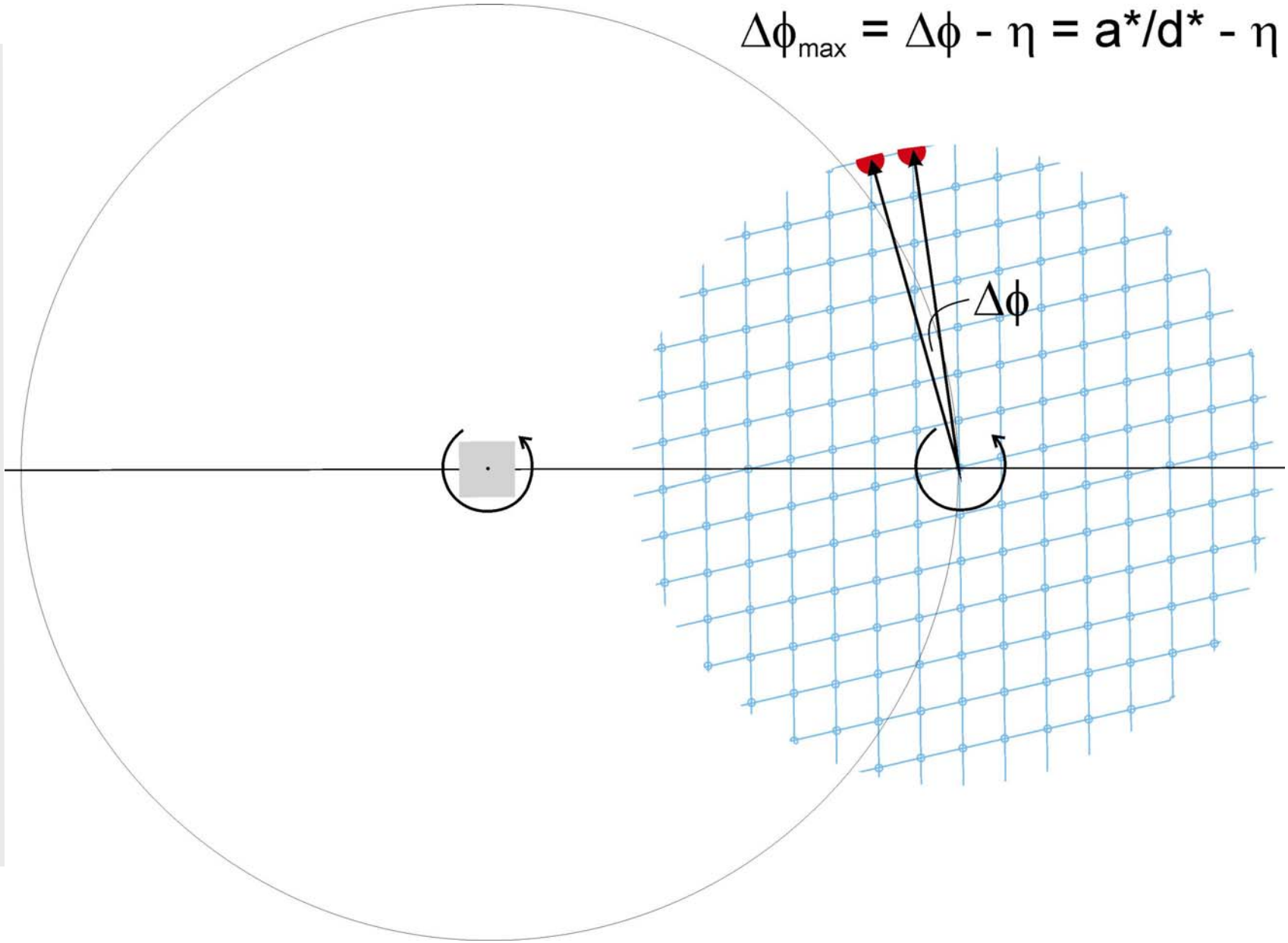


The Effect of Mosaicity

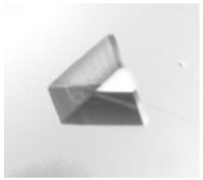


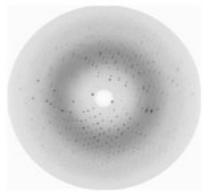
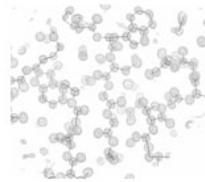



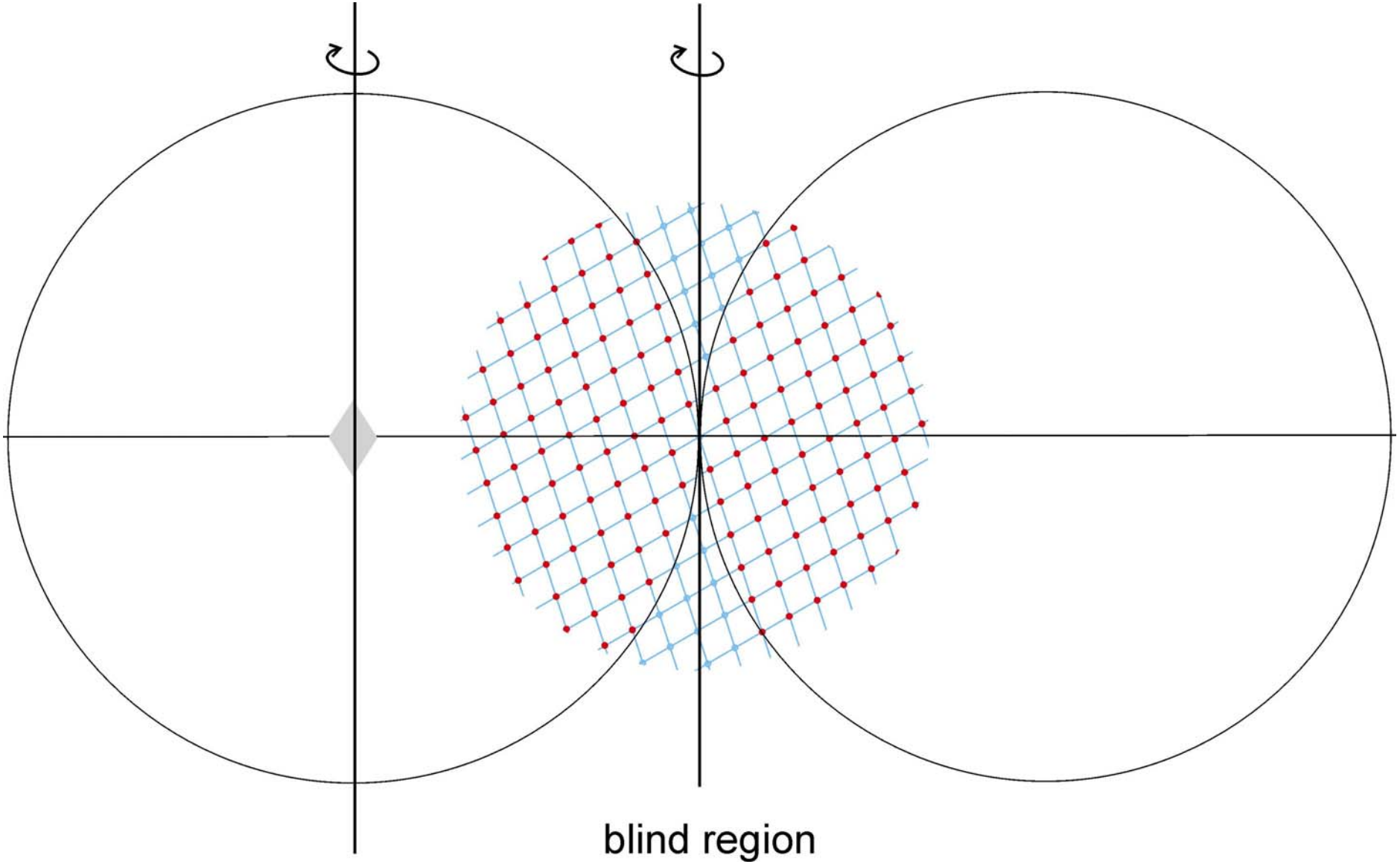

$$\Delta\phi_{max} = \Delta\phi - \eta = a^*/d^* - \eta$$



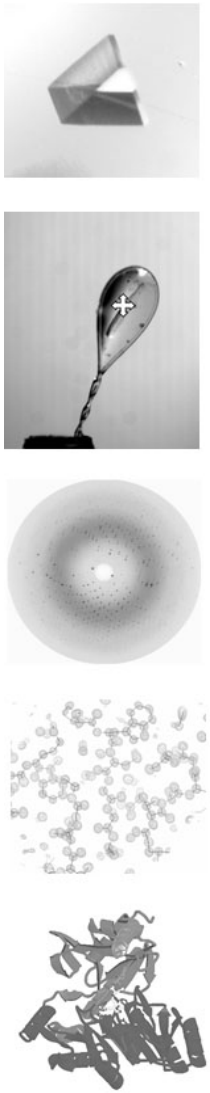
The Blind Region



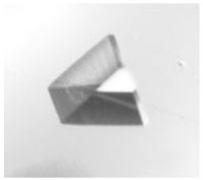



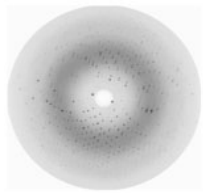
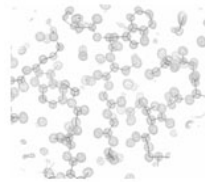
The Blind Region

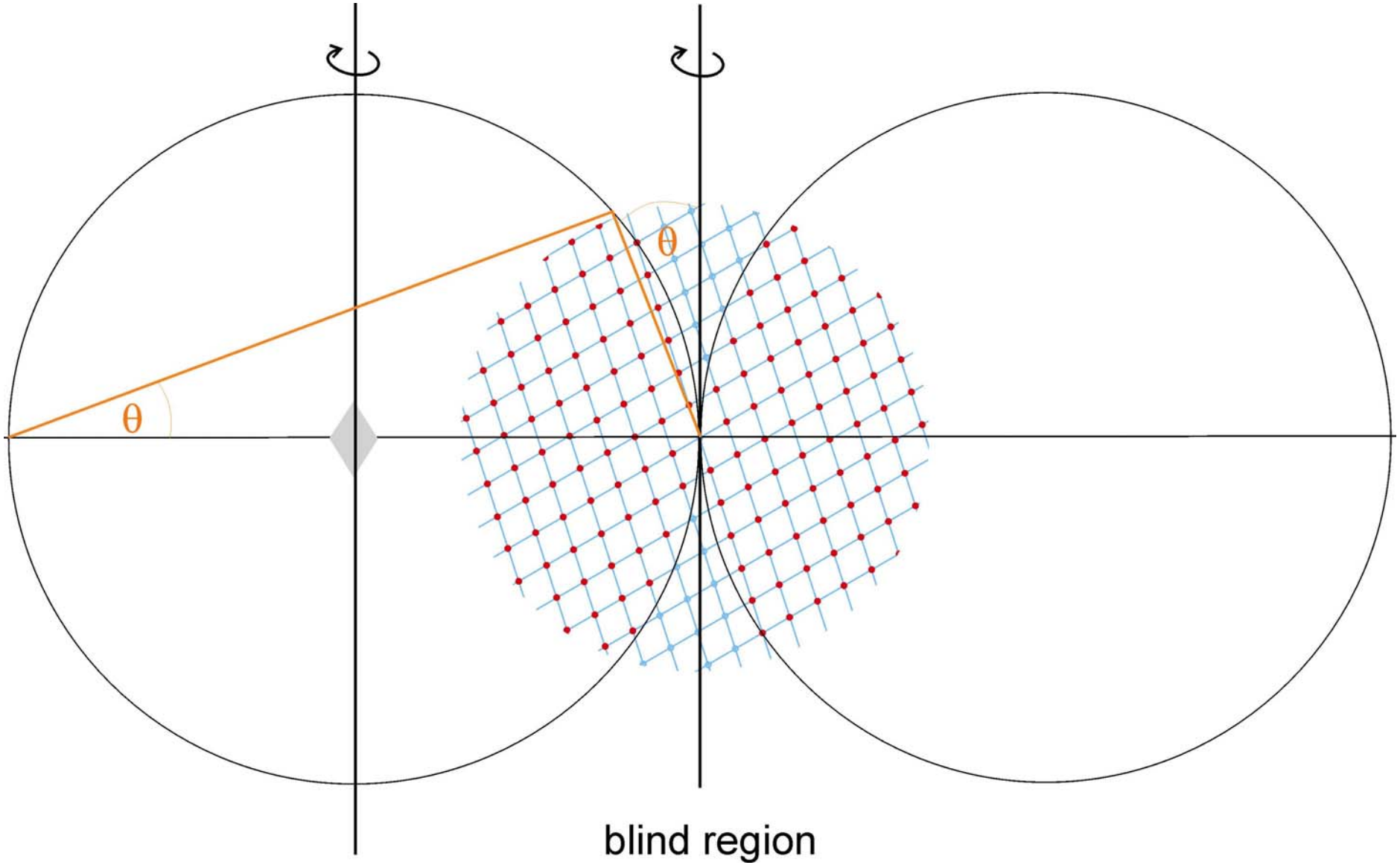


- reflections in the blind region cannot be collected by rotation around a single axis

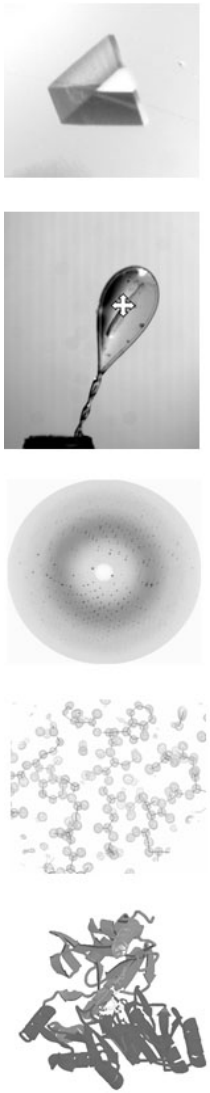
The Blind Region



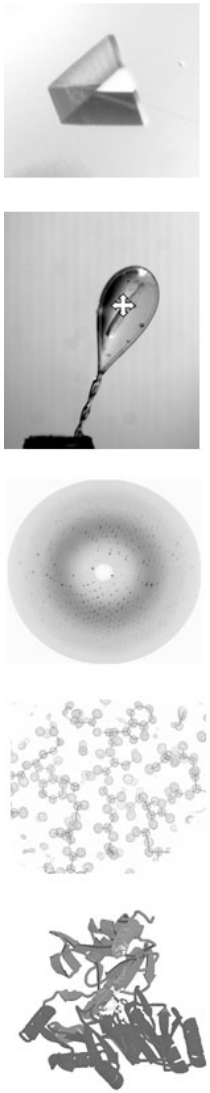



The Blind Region



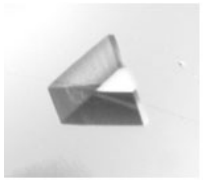
- reflections in the blind region cannot be collected by rotation around a single axis
- the size of the blind region is determined by the maximum diffraction angle θ_{max}

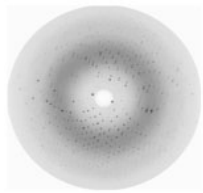
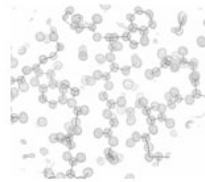
The Blind Region



- reflections in the blind region cannot be collected by rotation around a single axis
- the size of the blind region is determined by the maximum diffraction angle θ_{max}
- in order to collect a complete data set, one has to collect a pass around a second rotation axis of at least $2\theta_{max}$

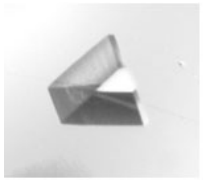
The Blind Region

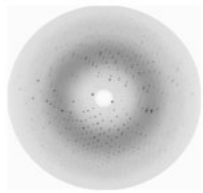
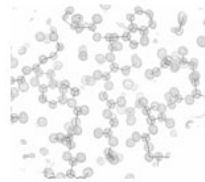



- reflections in the blind region cannot be collected by rotation around a single axis
- the size of the blind region is determined by the maximum diffraction angle θ_{max}
- in order to collect a complete data set, one has to collect a pass around a second rotation axis of at least $2\theta_{max}$
- the presence of symmetry helps unless the symmetry axis lies in the blind region

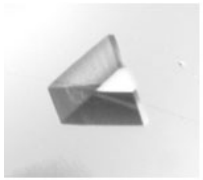
Symmetry

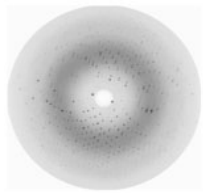
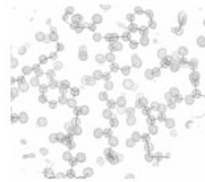



- any symmetry element present in real space will also be present in reciprocal space (a screw axis in real space will become a rotation axis in reciprocal space).

Symmetry

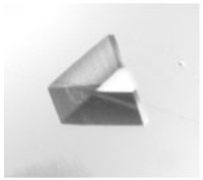


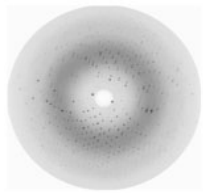
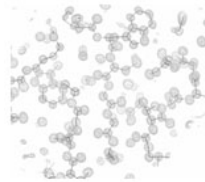



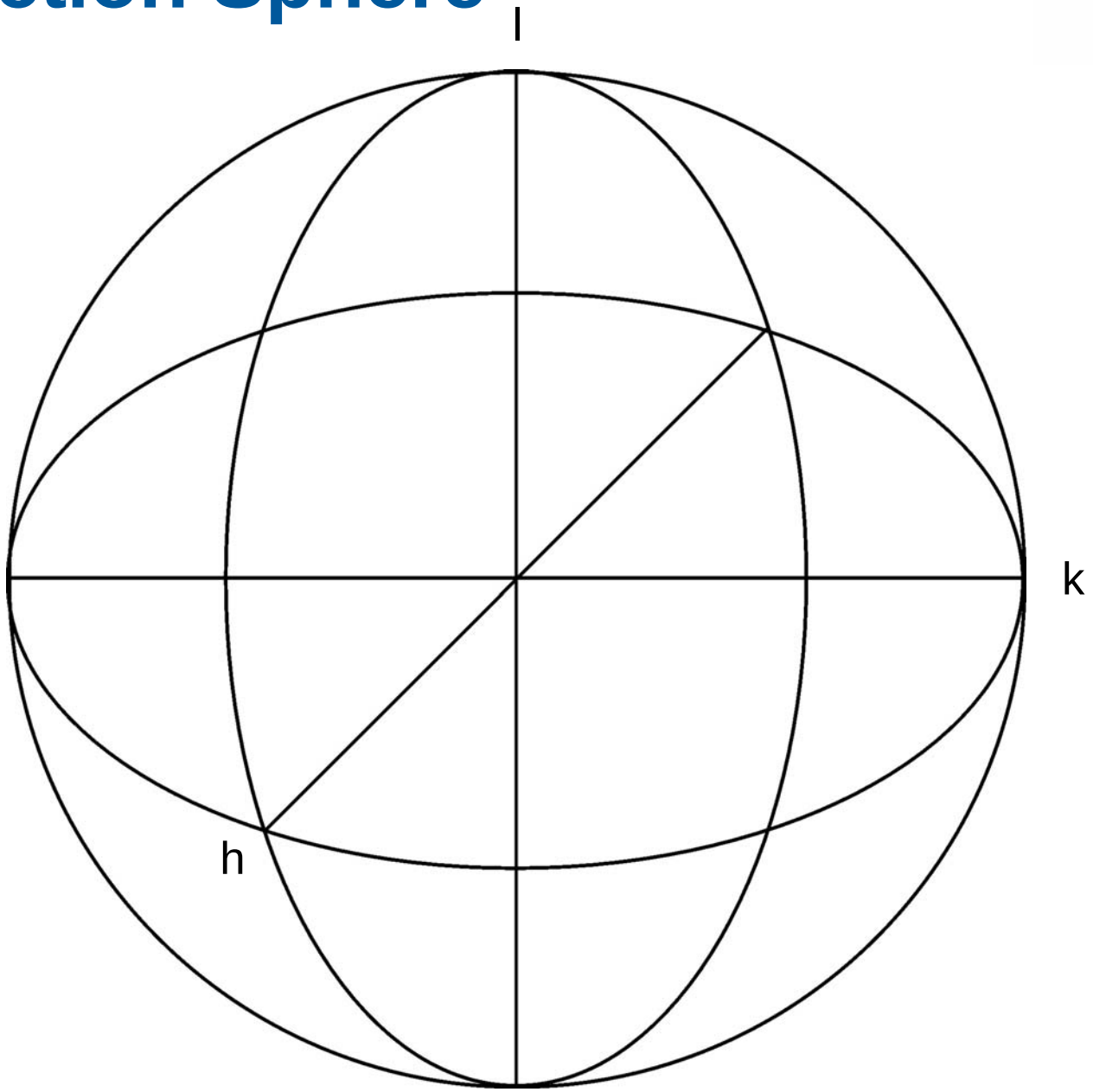

- any symmetry element present in real space will also be present in reciprocal space (a screw axis in real space will become a rotation axis in reciprocal space).

- in addition, the reciprocal space contains an inversion center in the origin (Friedel's law).

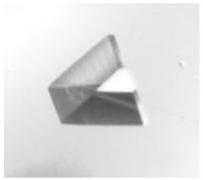
The Reflection Sphere

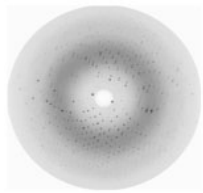
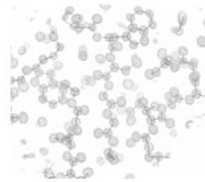


Symmetry

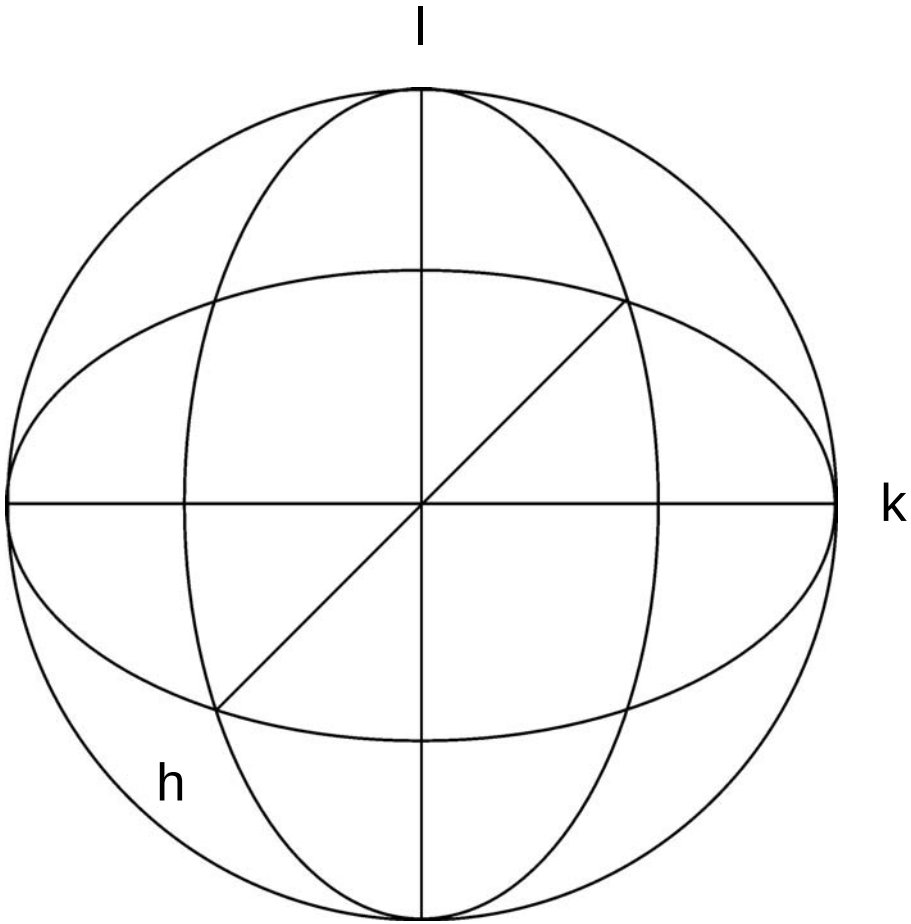


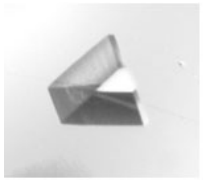

No symmetry

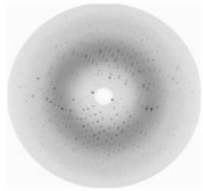
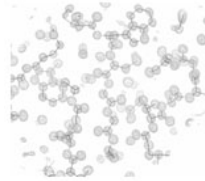
Measure the whole reflection sphere

-h → +h
-k → +k
-l → +l



Symmetry

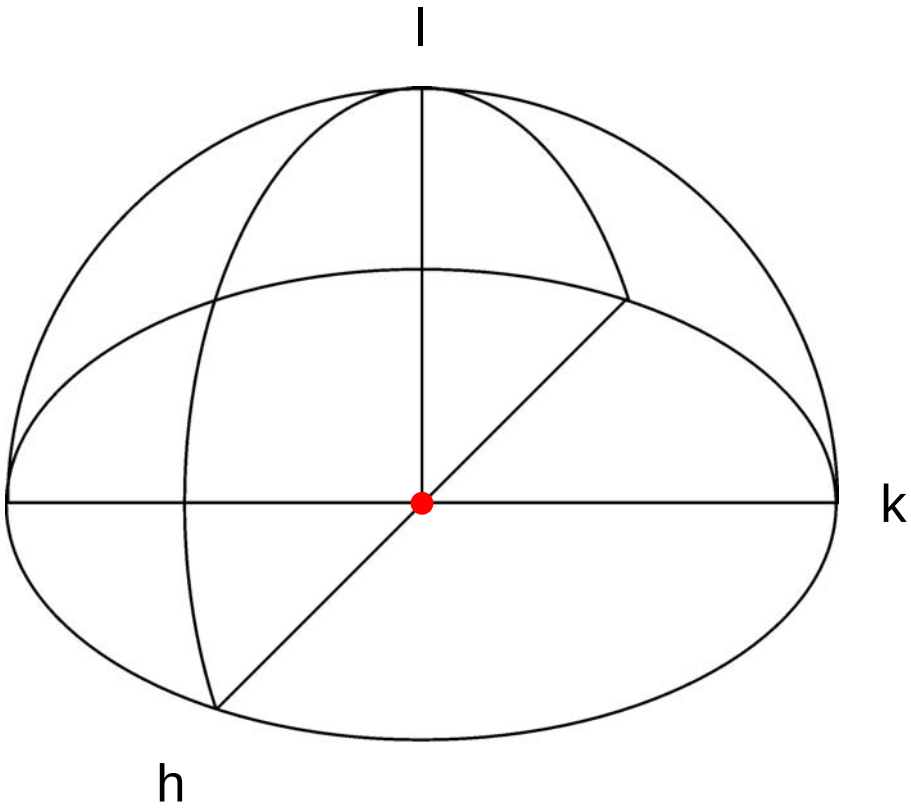


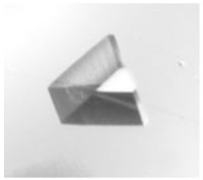

Inversion Center (Friedel)

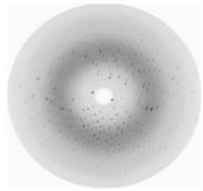
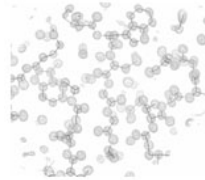
Measure half the reflection sphere

-h → +h
-k → +k
0 → +l



Symmetry

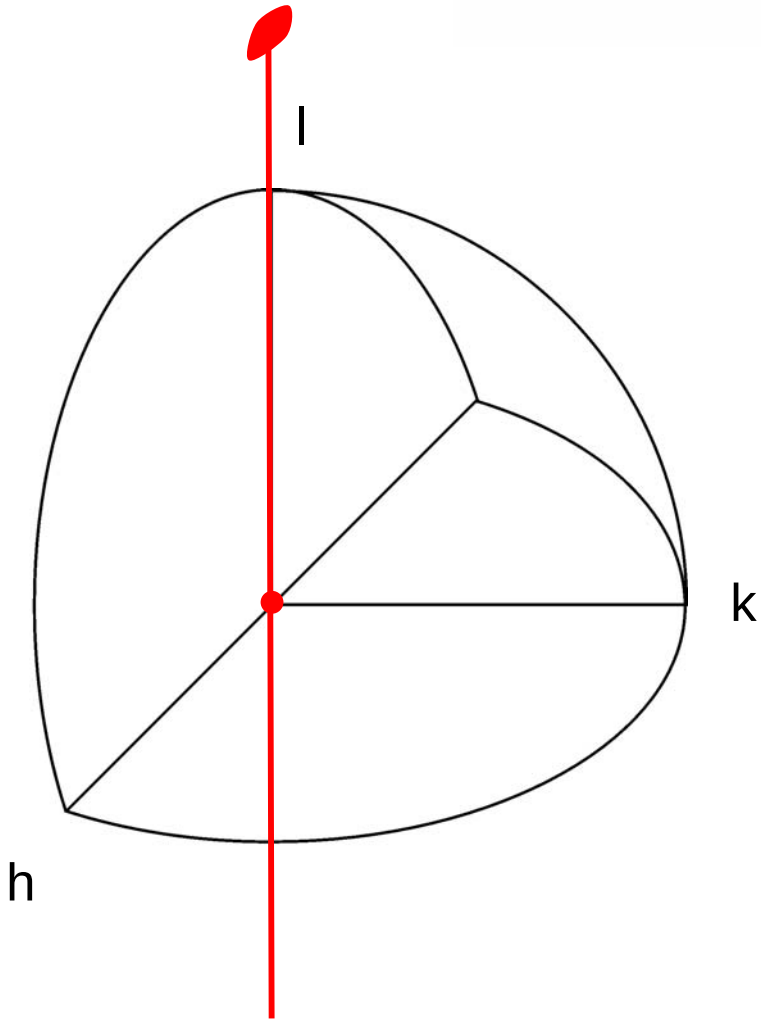


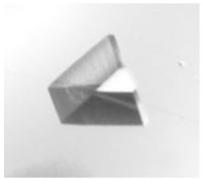

<u>Inversion Center (Friedel) +</u>
<u>2-fold rotation axis along c</u>

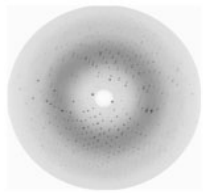
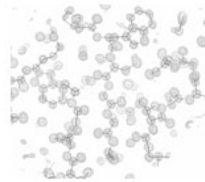
Measure a quarter of the reflection sphere

-h → +h
0 → +k
0 → +l



Symmetry

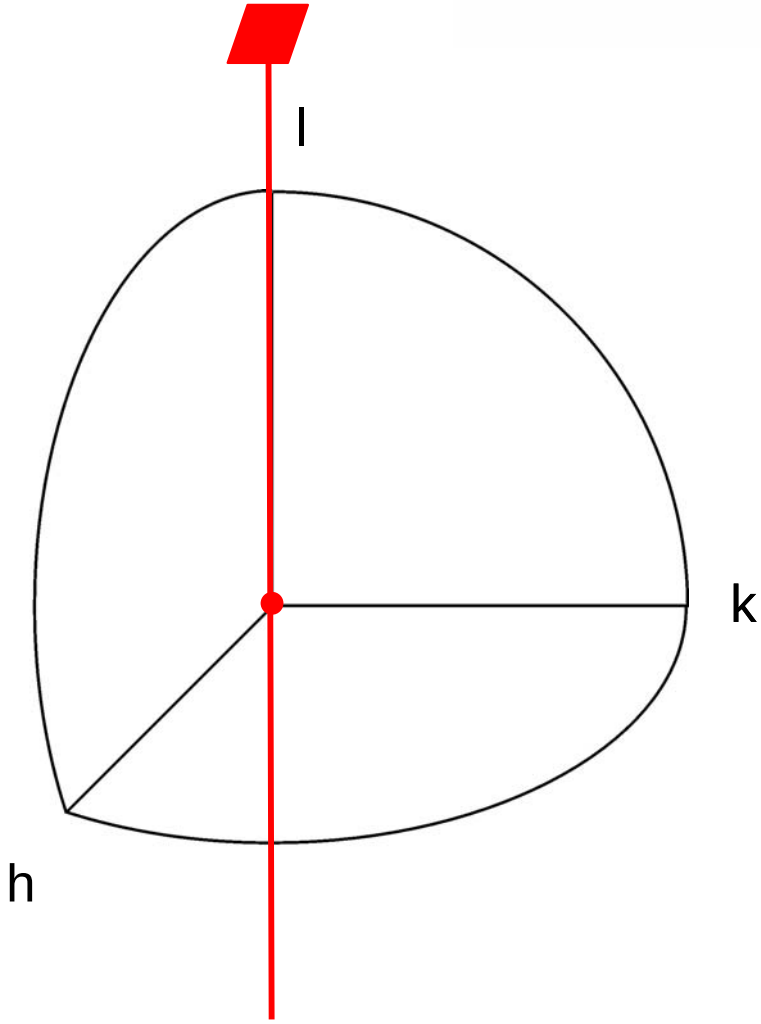


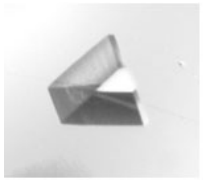

<u>Inversion Center (Friedel) +</u>
<u>4-fold rotation axis along c</u>

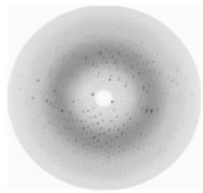
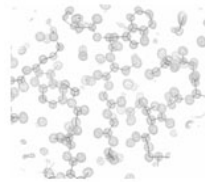
Measure an octant of the reflection sphere

0 → +h
0 → +k
0 → +l



How much do we need to collect?

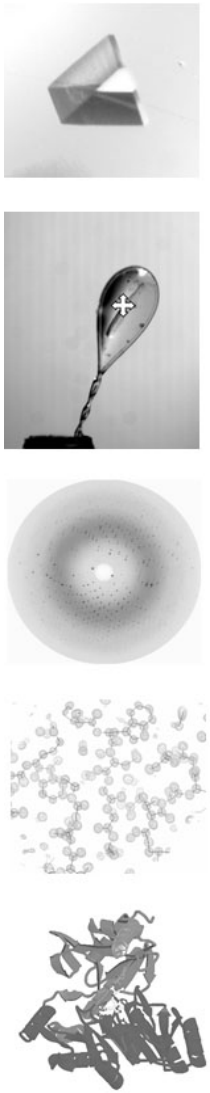



Crystal Class	Point Group	Rotation Axis	Standard Data	Anomalous Data
Triclinic	1	any	180°	180° + $2\theta_{max}$
Monoclinic	2	b*	90°	180°
		a*, c*	180°	180° + $2\theta_{max}$
Orthorhombic	222	a*, b*, c*	90°	90°
Tetragonal	4	c*	90°	90°
		a*, b*	90°	90° + θ_{max}
	422	c*	45°	45°
		a*, b*	90°	90°
Trigonal	3	c*	60°	60° + $2\theta_{max}$
		a*, b*	90°	90° + θ_{max}
	32	c*	30°	30° + θ_{max}
		a*, b*	90°	90°
Hexagonal	6	c*	60°	60°
		a*, b*	90°	90° + θ_{max}
	622	c*	30°	30°
		a*, b*	90°	90°
Cubic	23	any	≈ 60°	≈ 70°
	432	any	≈ 35°	≈ 45°

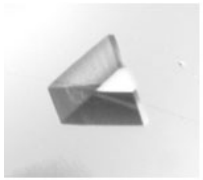
Z. Dauter (1997). *Meth. Enzymol.* **276**, 326-344.

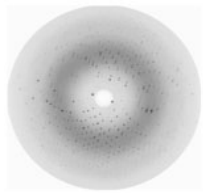
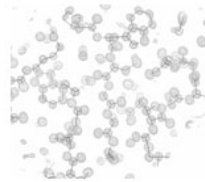
Strategy



- A decision has to be made where to start the data collection (ϕ_0), how many images to collect and which rotation increment to use ($\Delta\phi$) in order to avoid overlaps.

Strategy



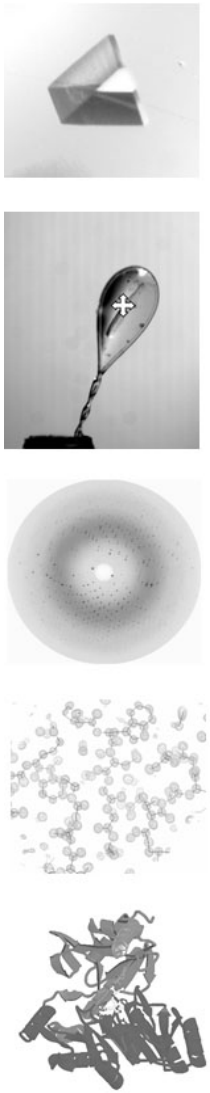

- A decision has to be made where to start the data collection (ϕ_0), how many images to collect and which rotation increment to use ($\Delta\phi$) in order to avoid overlaps.

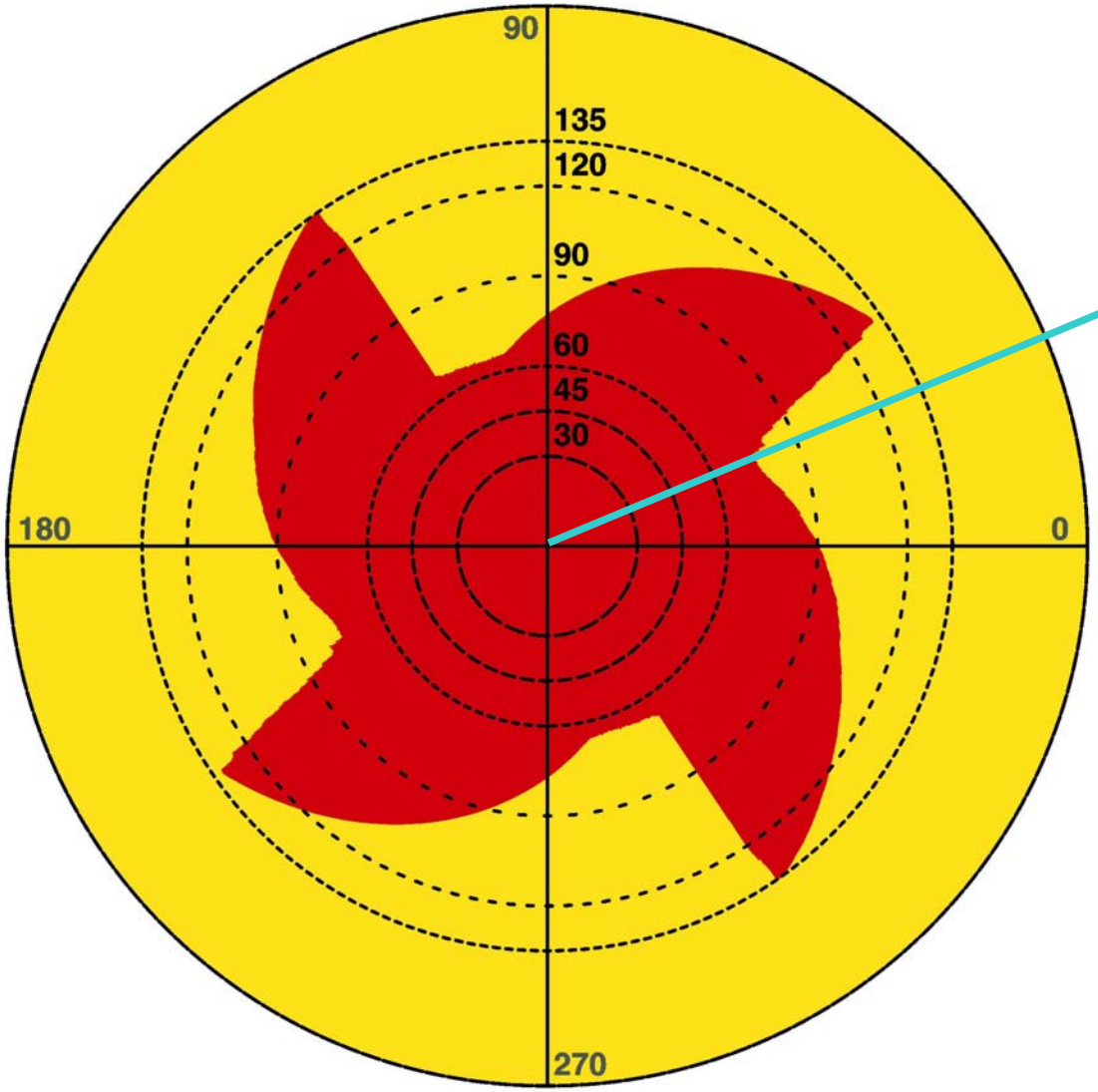
- Other decisions: maximum resolution, wavelength, detector distance, beamstop distance, exposure time, etc.

Strategy

Space group: $P2_12_12_1$

Overall completeness: 95%

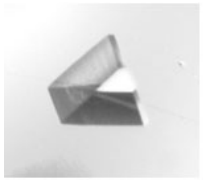


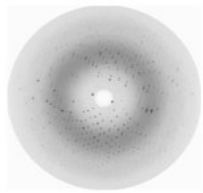
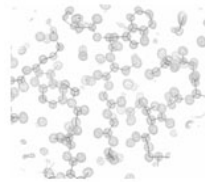


Optimal starting angle: 30°

Ravelli *et al*. (1997). *J. Appl. Cryst.* **30**, 551-554.

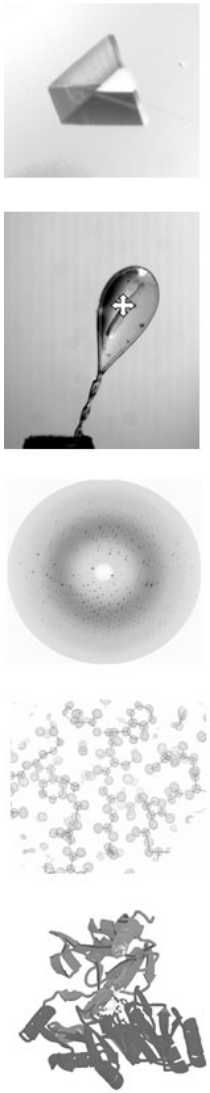
Alternative Indexing



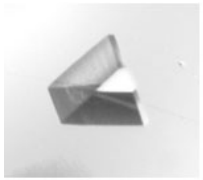

- In some space groups the reflections can be indexed in different ways.

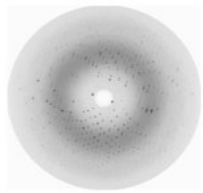
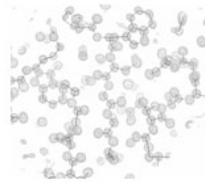
Alternative Indexing



- In some space groups the reflections can be indexed in different ways.
- It is important to take this into account, when trying to collect a complete data set from more than one crystal.

Alternative Indexing

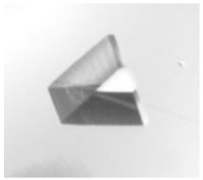


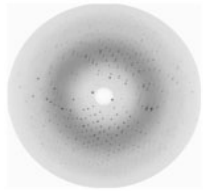
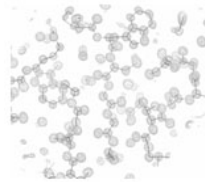




Space Group	Reindexing Transformation	Reindexing Matrix
P4, $P4_1$, $P4_2$, $P4_3$	hkl → kh-l	0 1 0 1 0 0 0 0 -1
I4, $I4_1$	hkl → hk-l	1 0 0 0 1 0 0 0 -1
P3, $P3_1$, $P3_2$	hkl → -h-kl	-1 0 0 0 -1 0 0 0 1
	or hkl → kh-l	0 1 0 1 0 0 0 0 -1
	or hkl → -k-h-l	0 -1 0 -1 0 0 0 0 -1
R3	hkl → kh-l	0 1 0 1 0 0 0 0 -1
P321, $P3_121$, $P3_221$	hkl → -h-kl	-1 0 0 0 -1 0 0 0 1
P312, $P3_112$, $P3_212$	hkl → -h-kl	-1 0 0 0 -1 0 0 0 1
P6, $P6_1$, $P6_2$, $P6_3$, $P6_4$, $P6_5$	hkl → kh-l	0 1 0 1 0 0 0 0 -1
P23, $P2_13$	hkl → k-hl	0 1 0 -1 0 0 0 0 1
I23, $I2_13$	hkl → k-hl	0 1 0 -1 0 0 0 0 1
F23	hkl → k-hl	0 1 0 -1 0 0 0 0 1

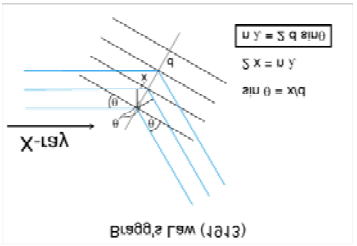
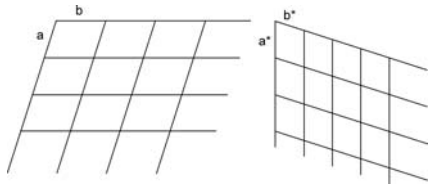
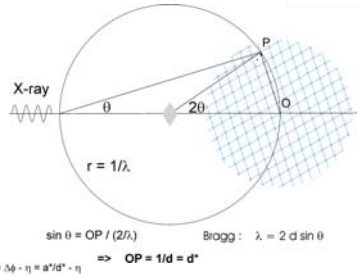
Z. Dauter (1999). *Acta Cryst.* **D55**, 1703-1717.

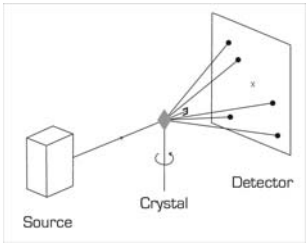
Summary – Part 1

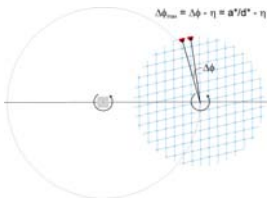
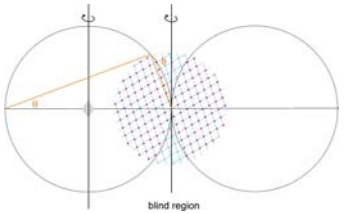


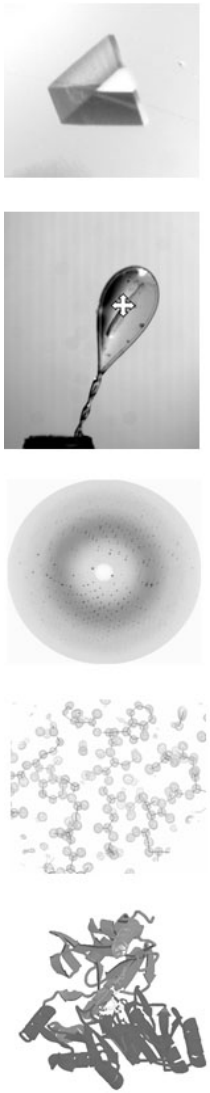

- Diffraction as Reflection (Bragg)
- Reciprocal Lattice
- Ewald Construction
- Rotation Method
- Overlaps
- Blind Region
- Data Collection Strategy
- Alternative Indexing

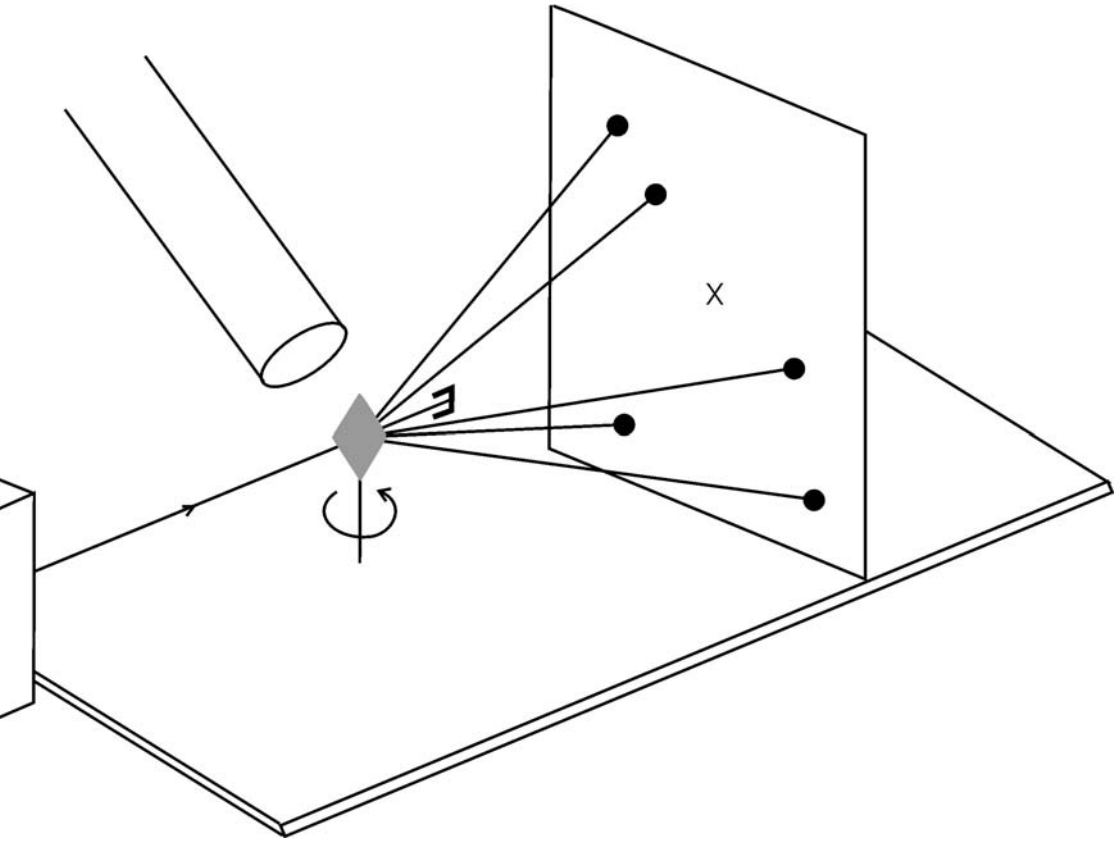






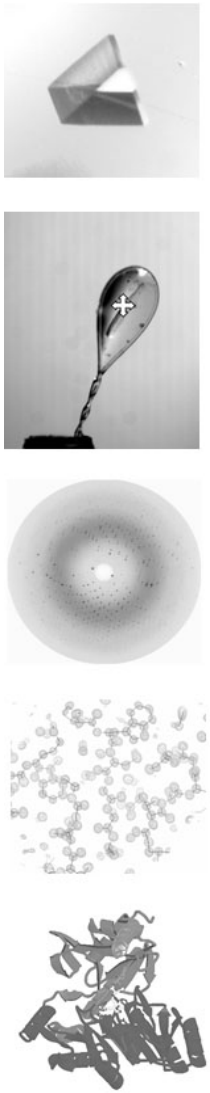



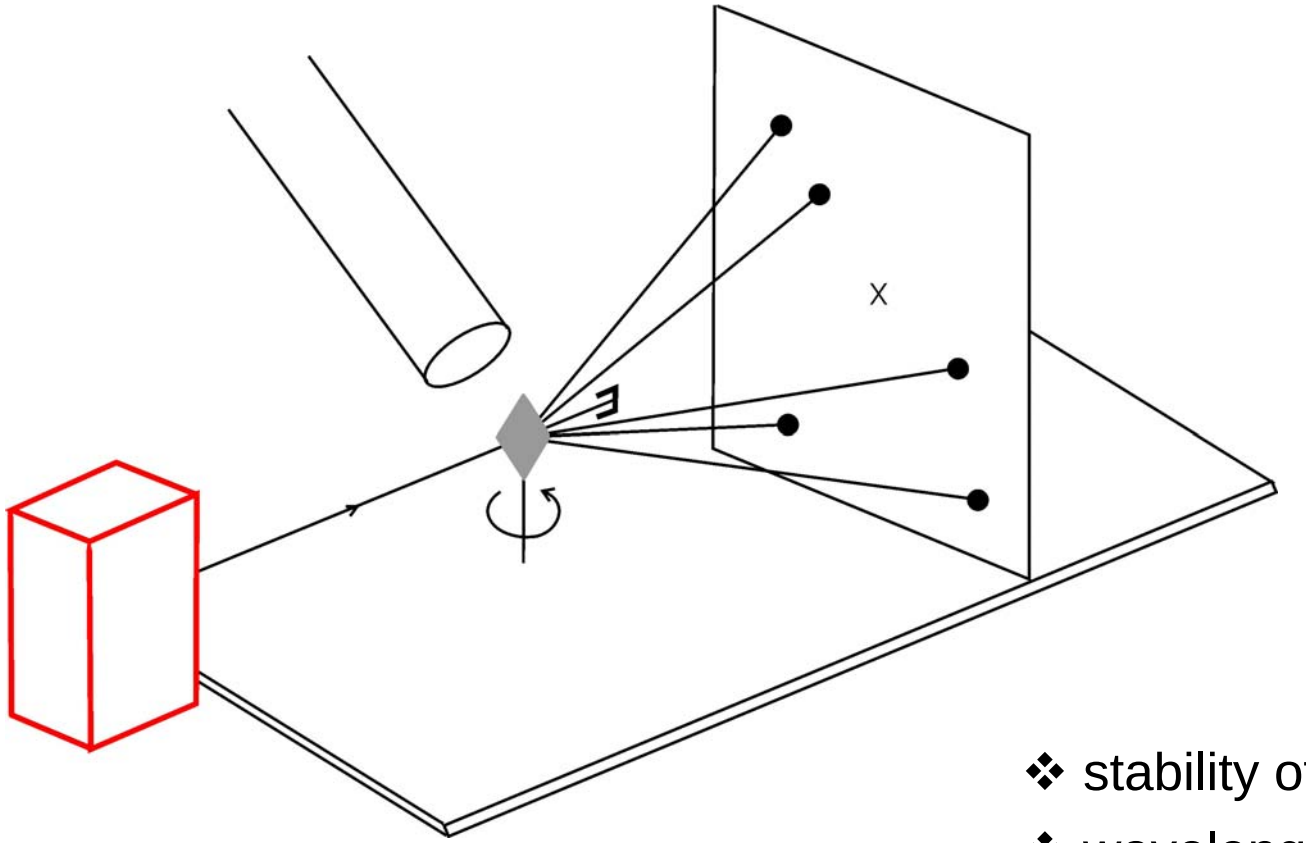
Data Collection – Sources of Error





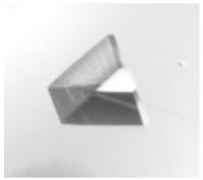
X-ray Source

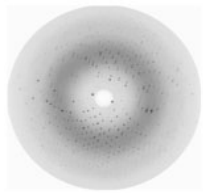
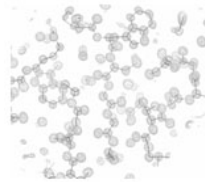


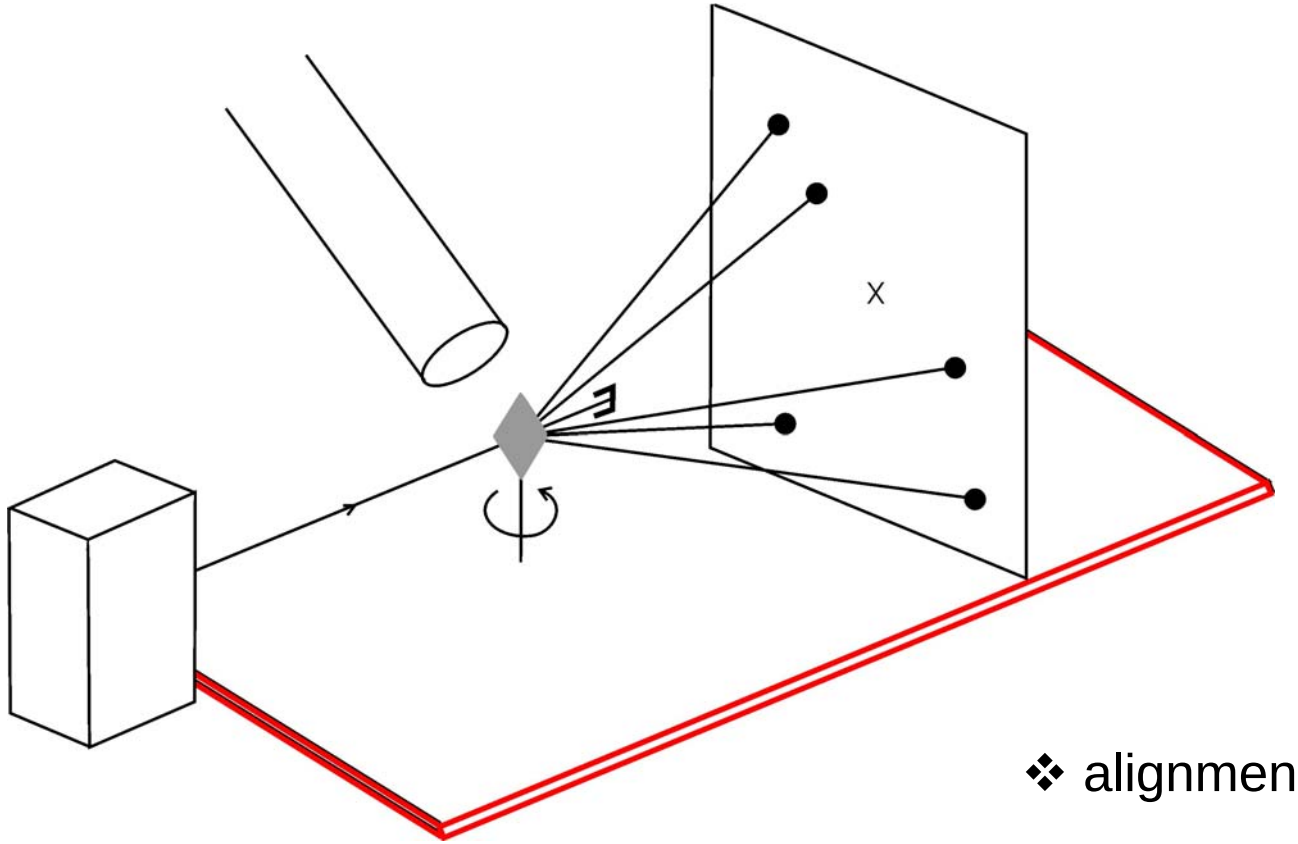


- stability of the beam
- wavelength

Experiment Table

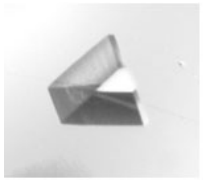


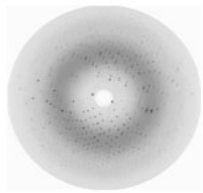
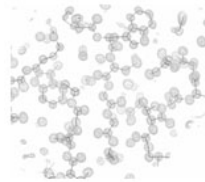



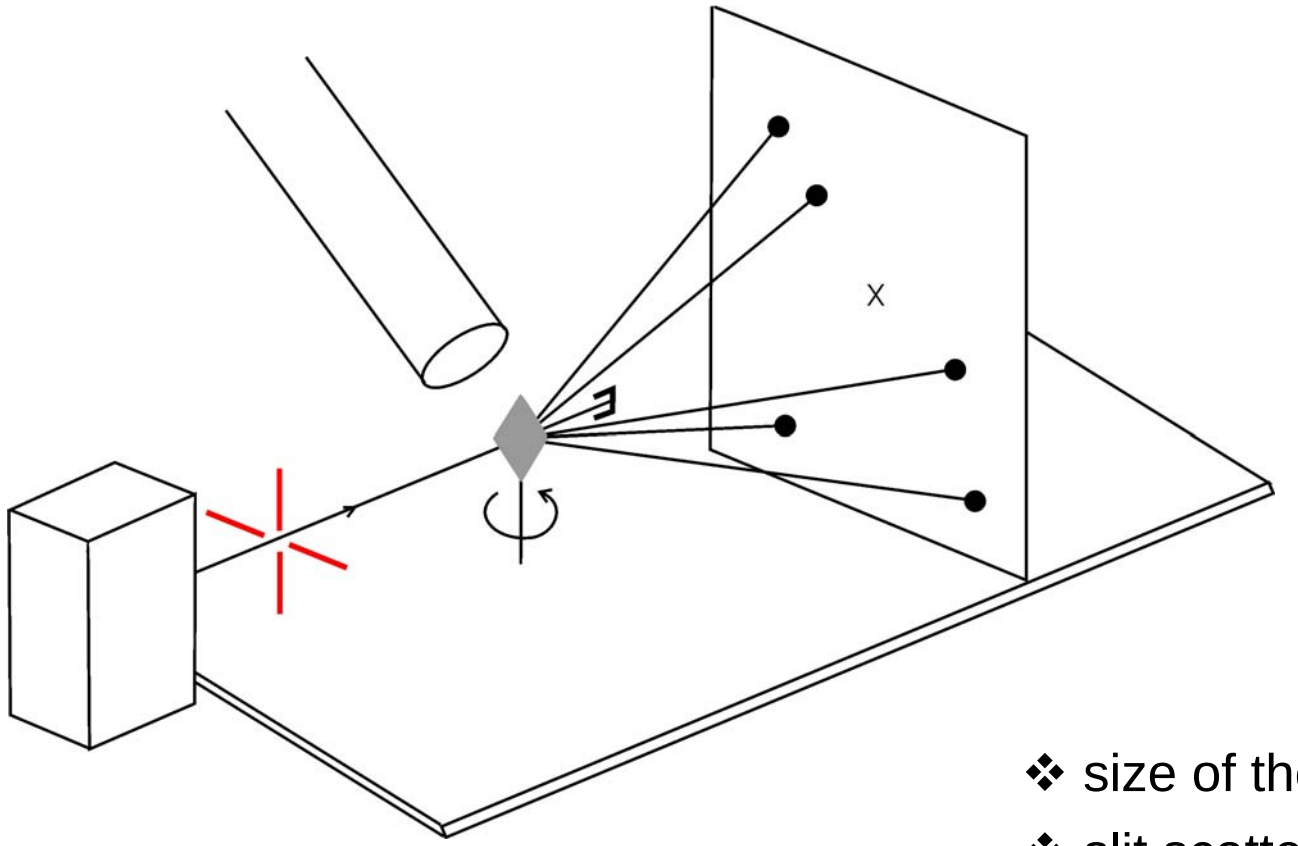



❖ alignment to beam

Slits and Collimation

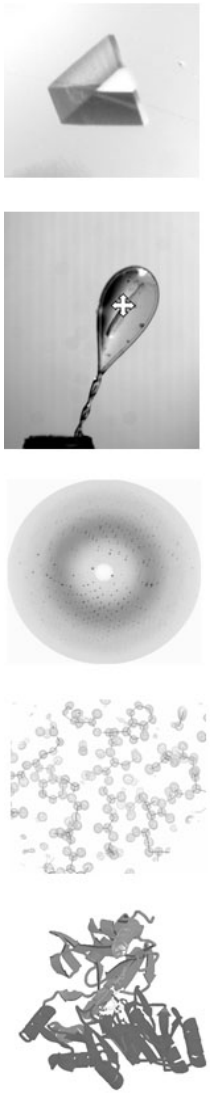


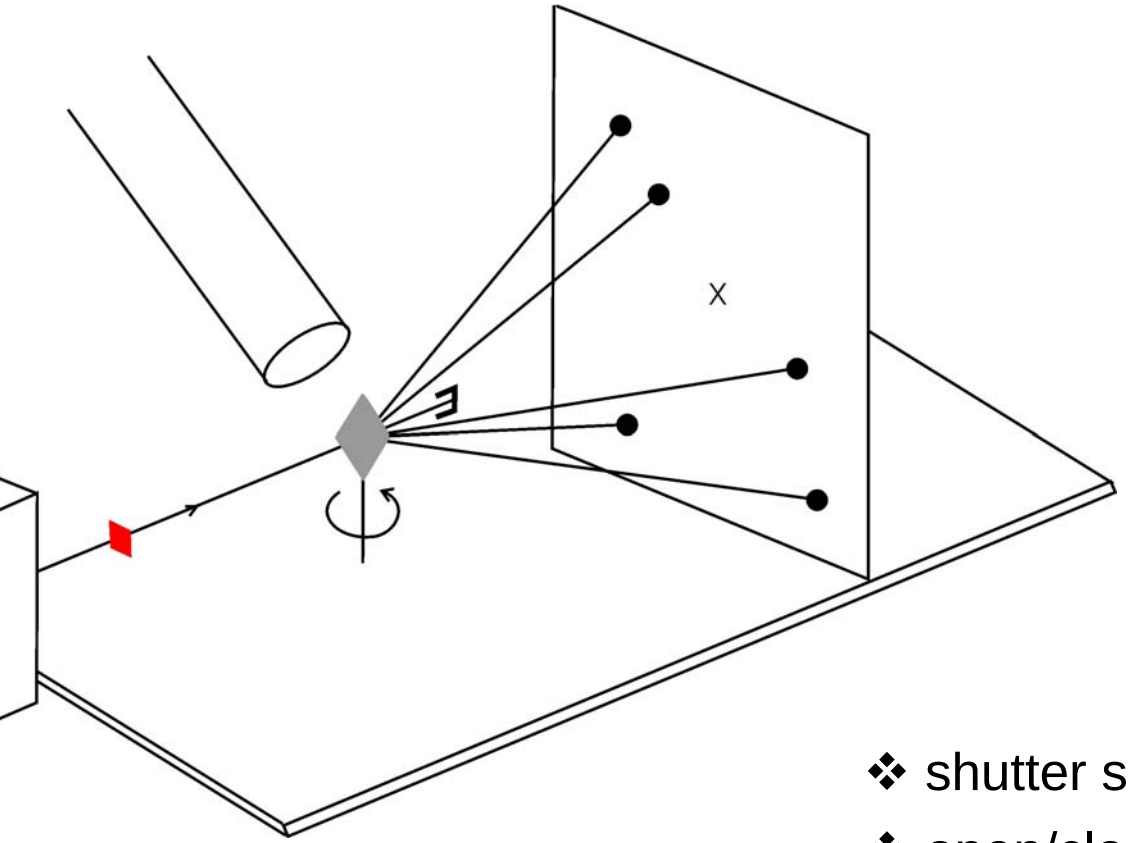



- size of the beam
- slit scattering
- slit movement

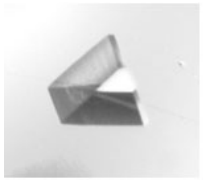
Beam Shutter

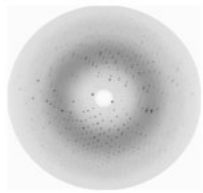
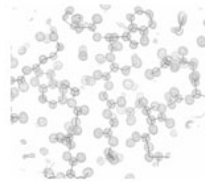


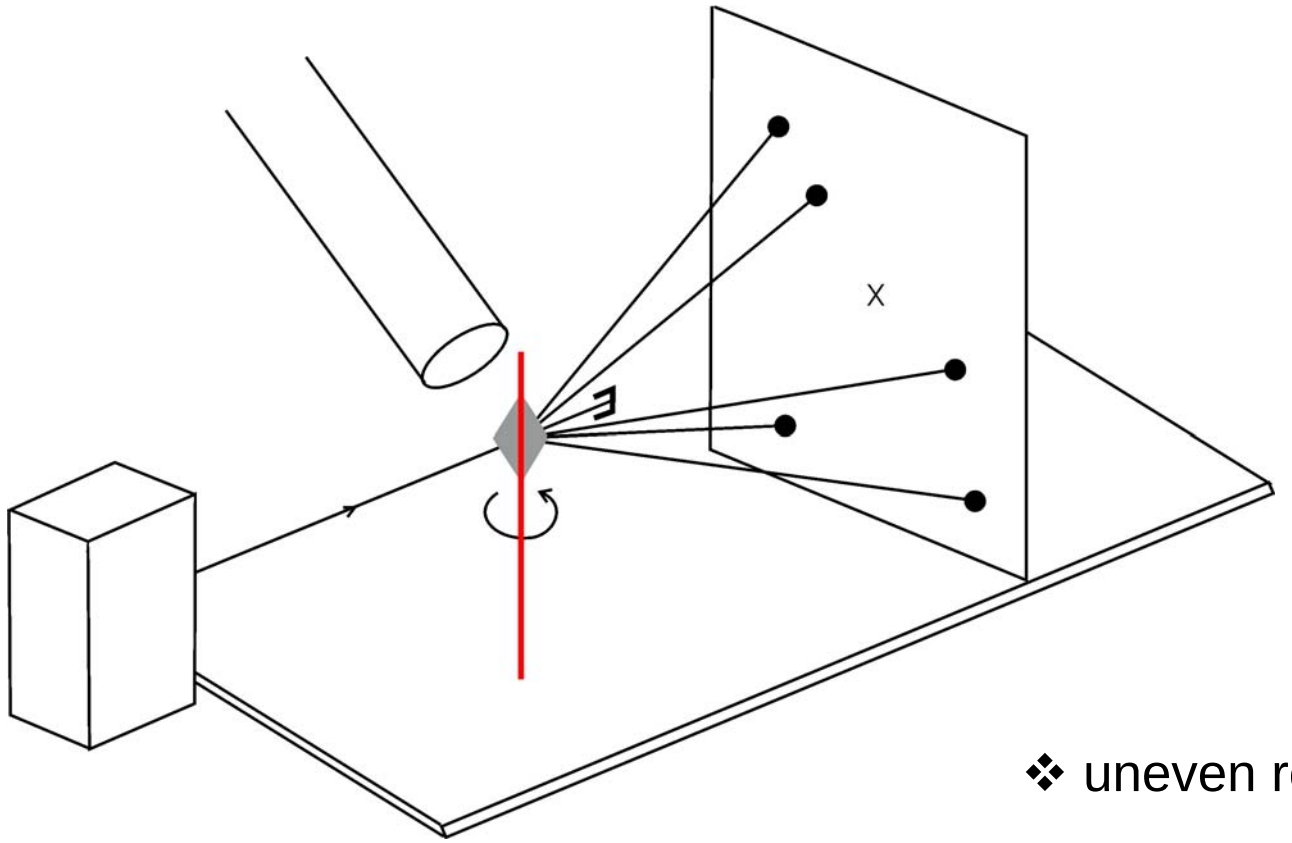


- shutter speed
- open/close movement

Rotation Axis (Spindle)

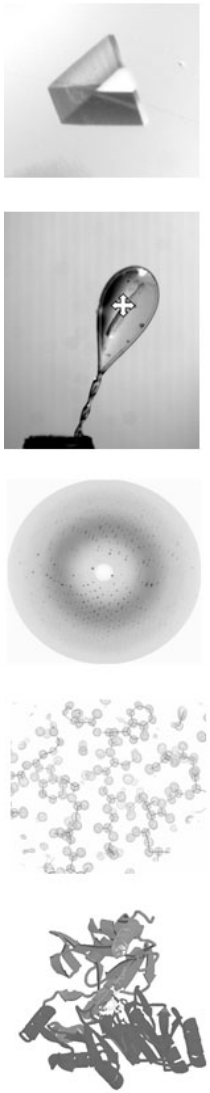


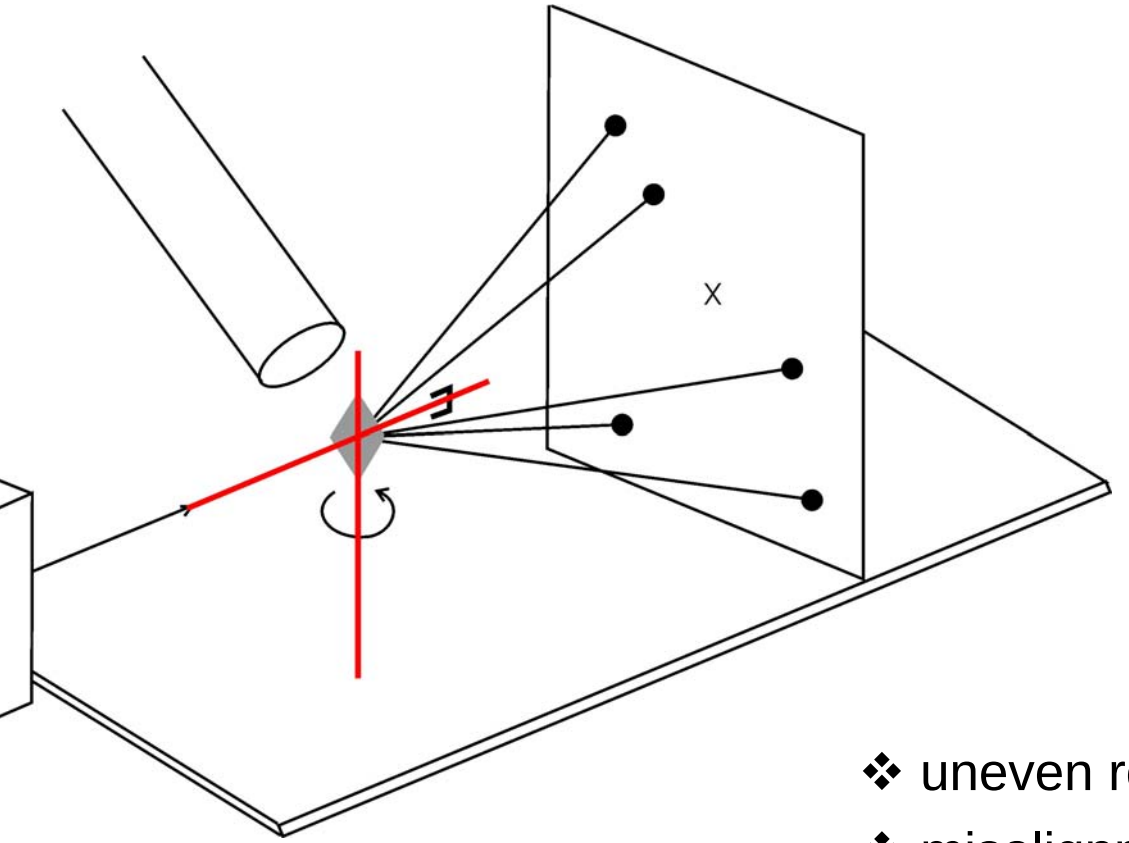



❖ uneven rotation speed

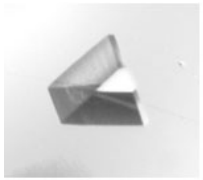
Rotation Axis (Spindle)

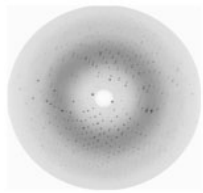
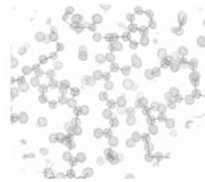


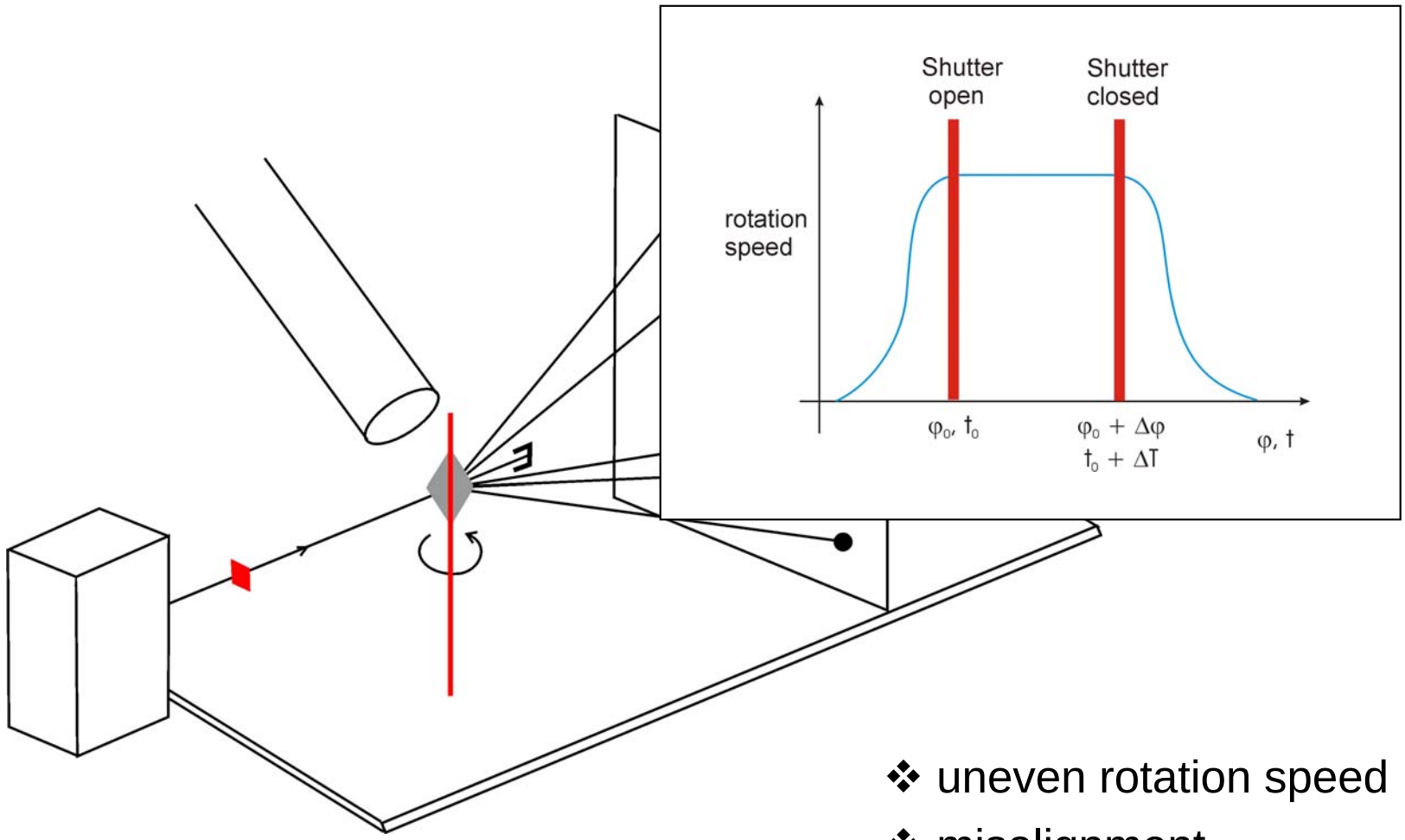


- uneven rotation speed
- misalignment

Rotation Axis (Spindle)

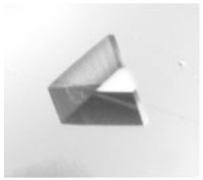


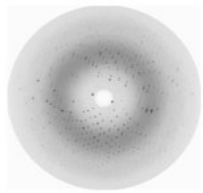
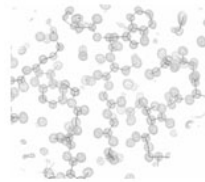



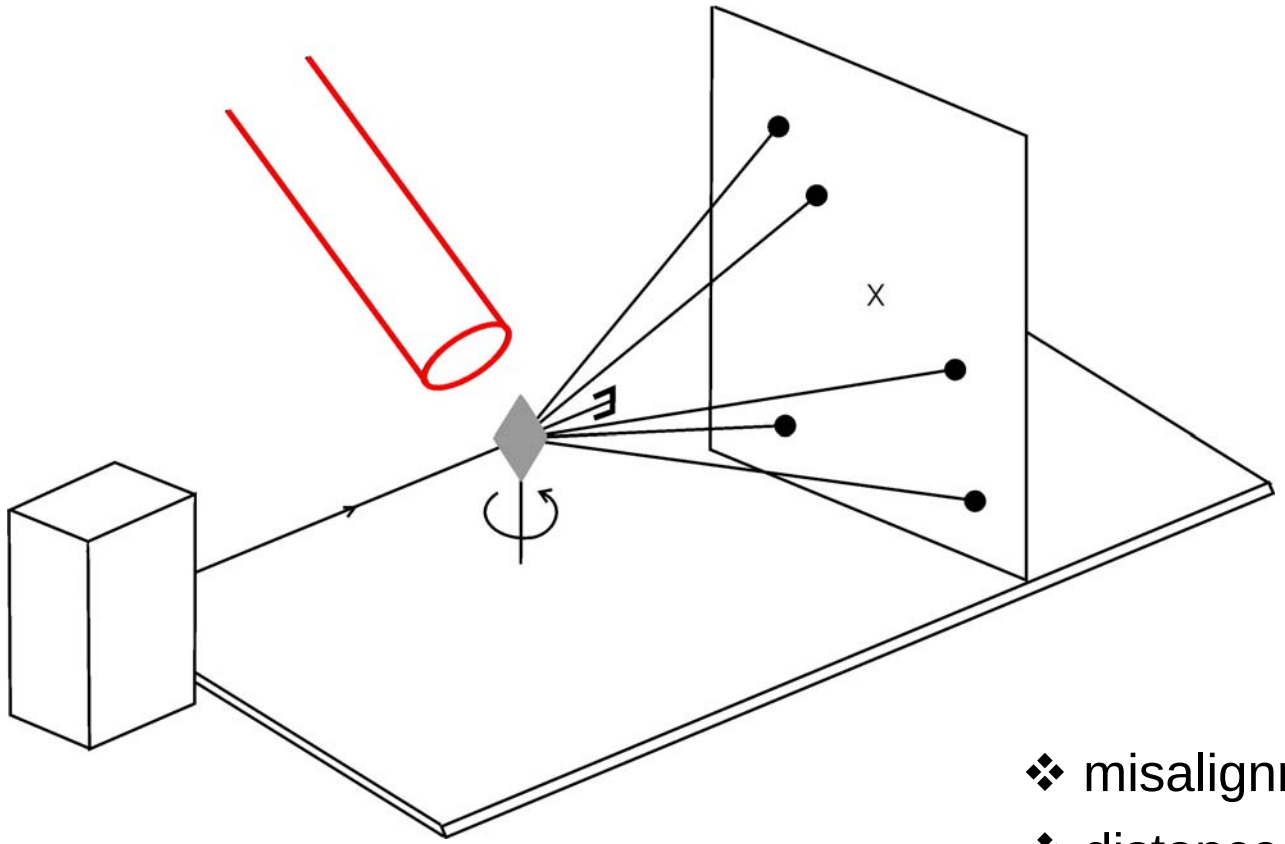



- uneven rotation speed
- misalignment
- shutter/spindle synchronization

Cryo-System

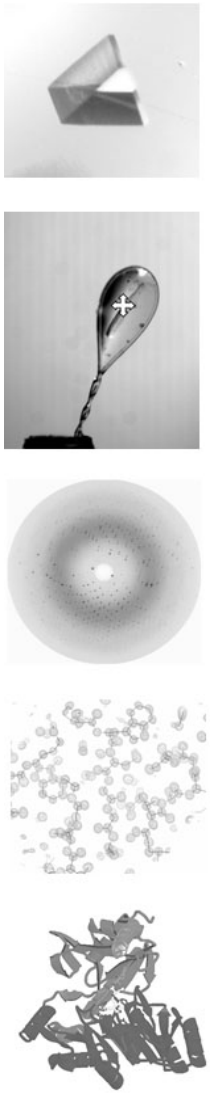


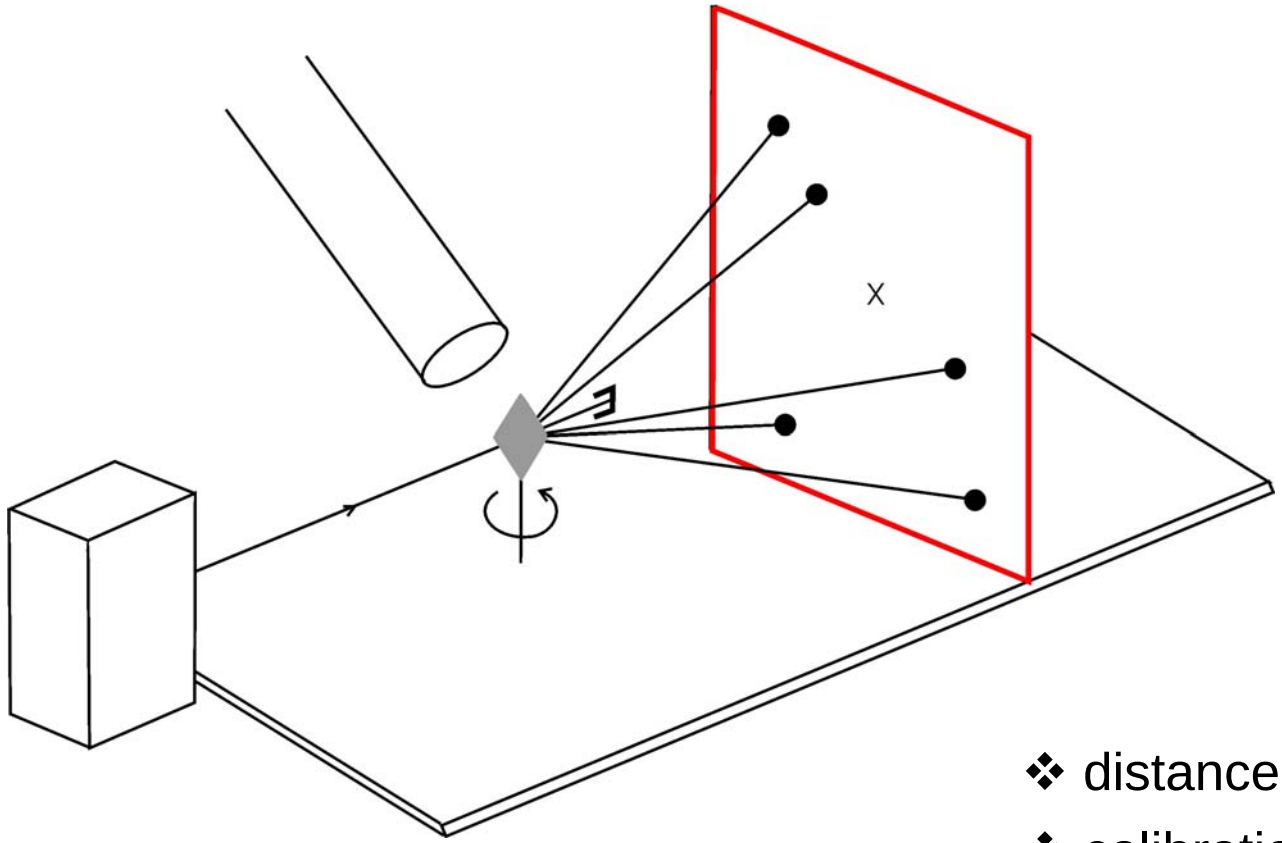



- misalignment
- distance to crystal
- T-stability

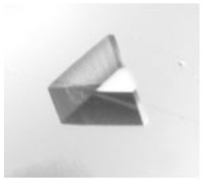
Detector

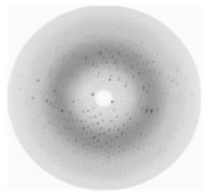
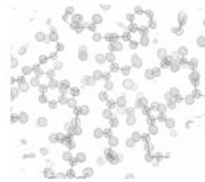


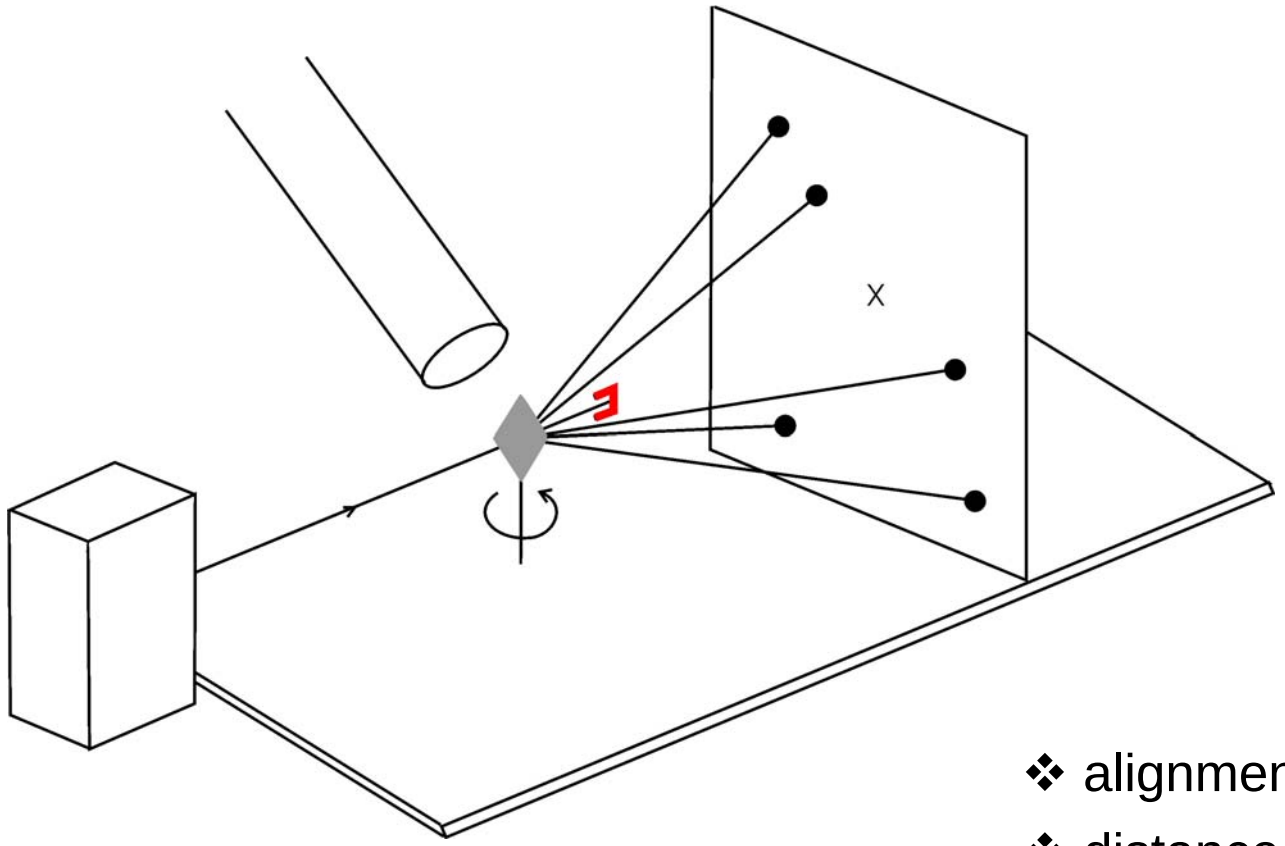


- distance
- calibration
- for CCDs: vacuum, T

Beamstop

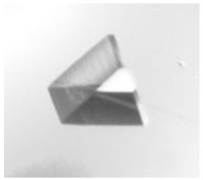


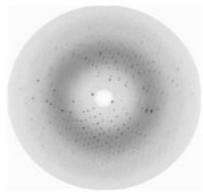
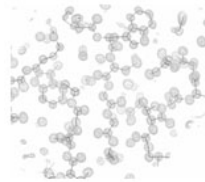



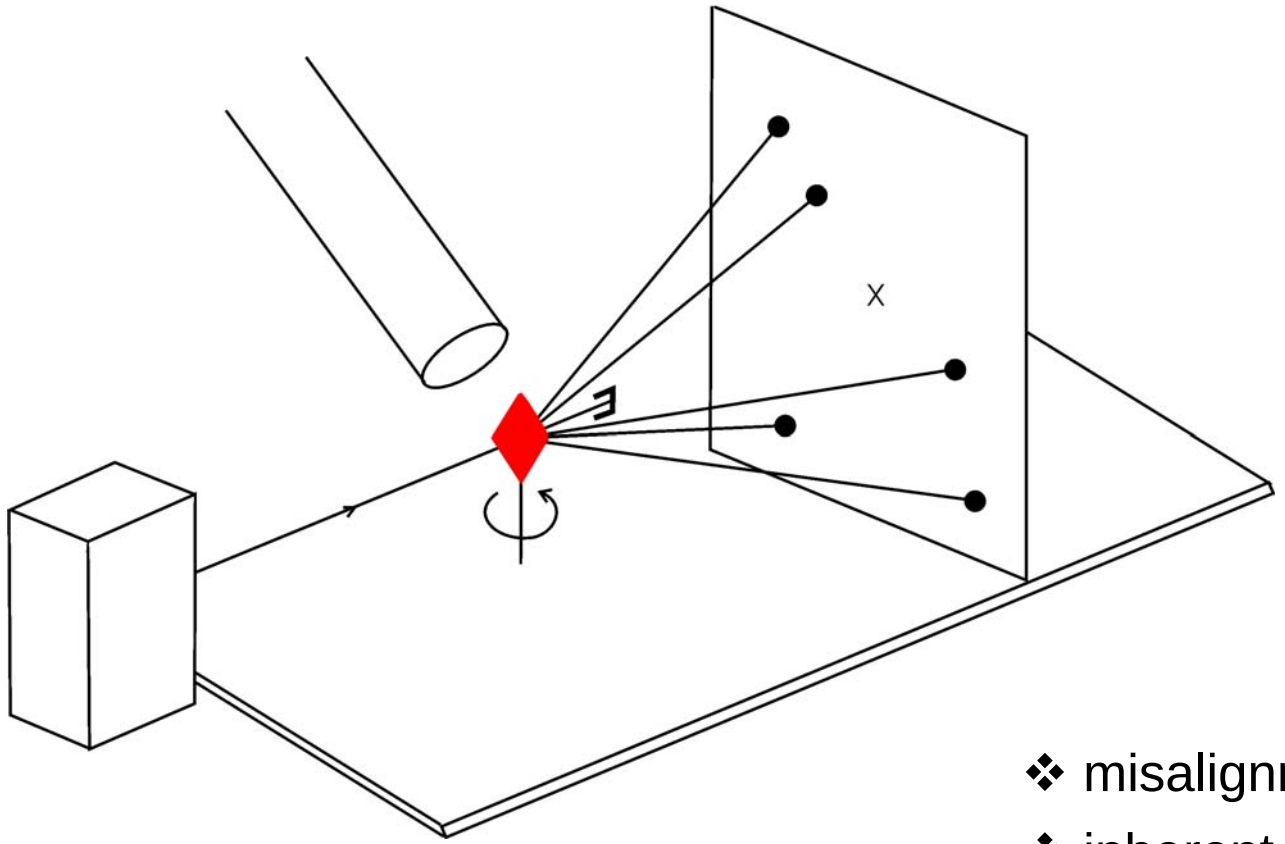



- alignment
- distance from crystal

Crystal

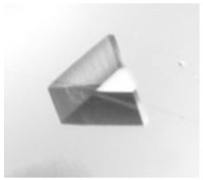


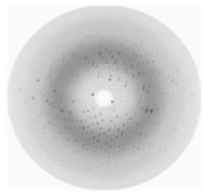



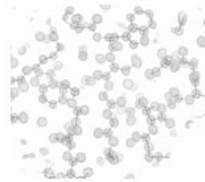



- misalignment
- inherent disorder
- damage upon freezing
- liquid around crystal
- vibration in cryostream

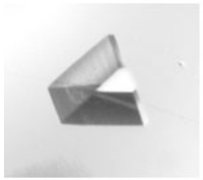
What Should You Do?

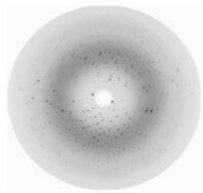
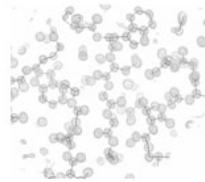






Before the Experiment

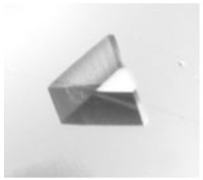


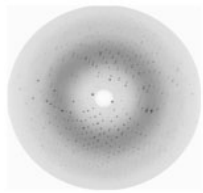
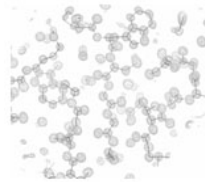




What kind of experiment do you want to do?

- ⇨ Native data collection for molecular replacement
- ⇨ Heavy atom derivative data collection for phasing
- ⇨ MAD or SAD data collection for phasing
- ⇨ High resolution native data collection
- ⇨ Screening for ligand binding
- ⇨ Other

Different Requirements

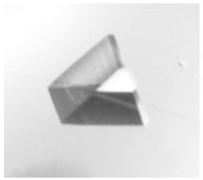


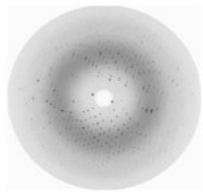



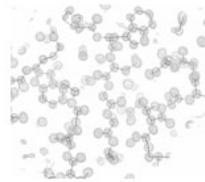

	Molecular replacement	Anomalous Phasing	High-resolution refinement	Ligand search
Accuracy	+	++++	++	++
Low-resolution completeness	+++	+++	++	++
Resolution	+	+	+++	++
Overall completeness	++	++	++	++
Automation	++	+	++	+++

Z. Dauter (2010). *Acta Cryst.* **D66**, 389-392.

Consider the Expected Signal Strength





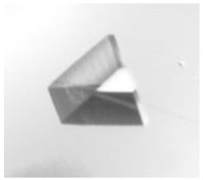


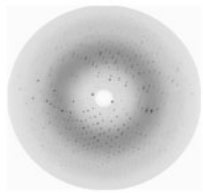
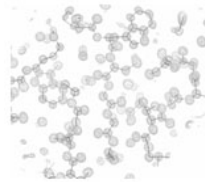
SIR: $R = 100 \bullet \Sigma_{hkl} \, | \, |F_{PH}| - |F_P| \, | \, / \, \Sigma_{hkl} \, |F_P|$ 15-30%

MAD: $R_{anom} = 200 \bullet \Sigma_{hkl} \, | \, I^+ - I^- \, | \, / \, \Sigma_{hkl} \, | \, I^+ + I^- \, |$ ~5%

S-SAD: ~1%

Before the Experiment



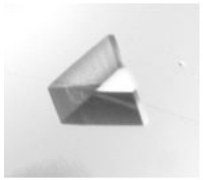

What kind of experiment do you want to do?

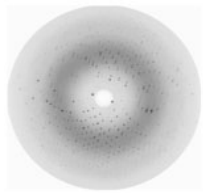
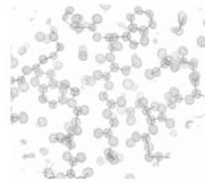
- ⇨ Native data collection for molecular replacement
- ⇨ MAD or SAD data collection for phasing
- ⇨ Heavy atom derivative data collection for phasing
- ⇨ High resolution native data collection
- ⇨ Screening for ligand binding
- ⇨ Other

How can you make sure that the beamline is ok?

- ⇨ Trust your beamline scientist
- ⇨ Carry out a test data collection

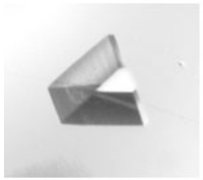
Starting the Experiment

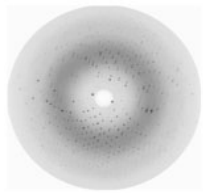
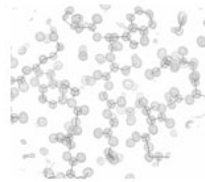



- Check cryo-system alignment and distance

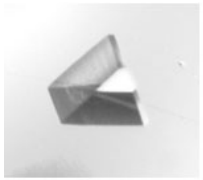
Starting the Experiment

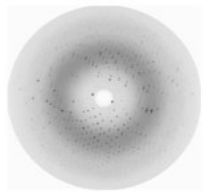
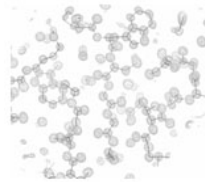


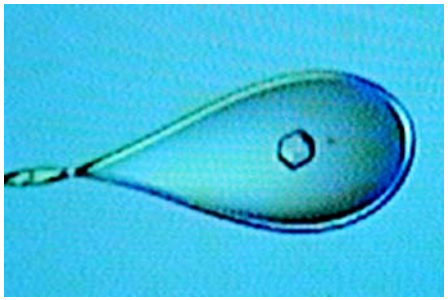
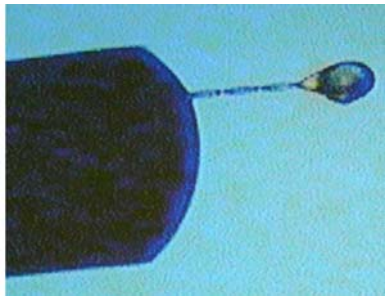

- Check cryo-system alignment and distance
- Mount crystal and center it
  - ⇨ Use the right cryo-protectant for the crystal

Starting the Experiment

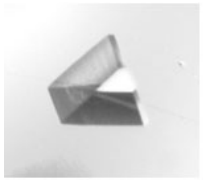


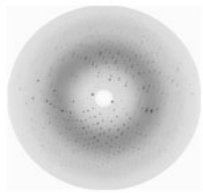
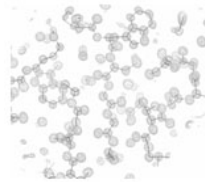




- Check cryo-system alignment and distance
- Mount crystal and center it
  - ⇨ Use the right cryo-protectant for the crystal
  - ⇨ Match loop size to crystal size

Starting the Experiment




- Check cryo-system alignment and distance
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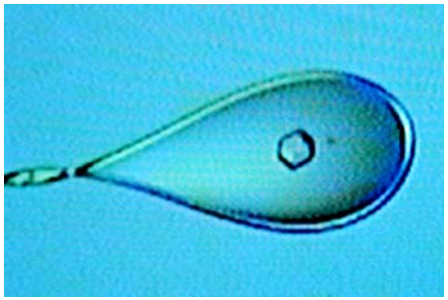
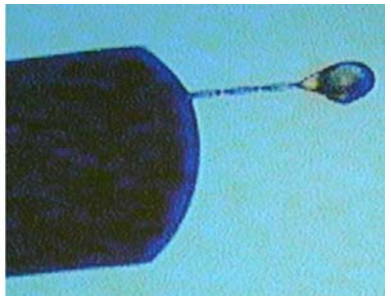
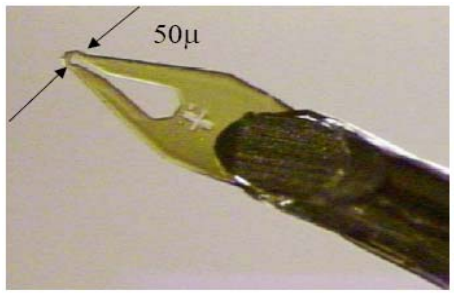
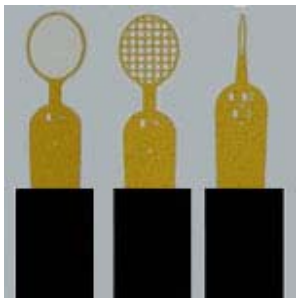
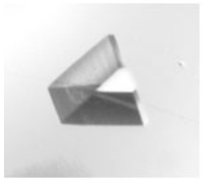



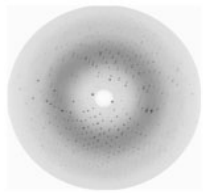
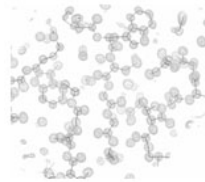
  - ⇨ consider different mounting methods





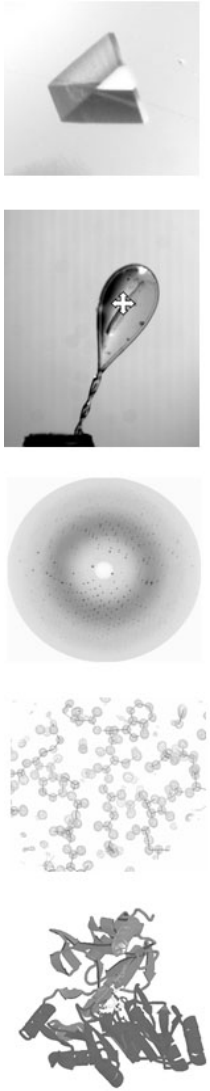
Starting the Experiment




- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size

Starting the Experiment

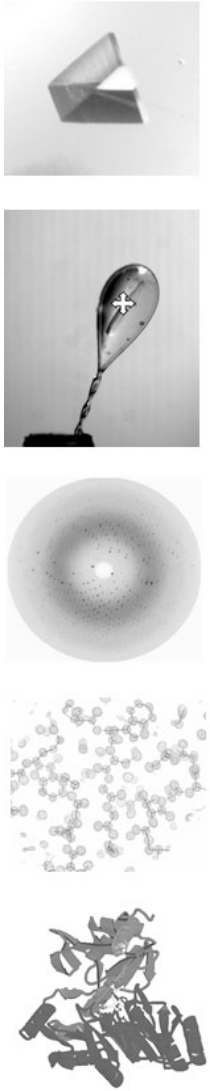


- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them

  ⇨ Inspect the diffraction pattern for split reflections or multiple lattices

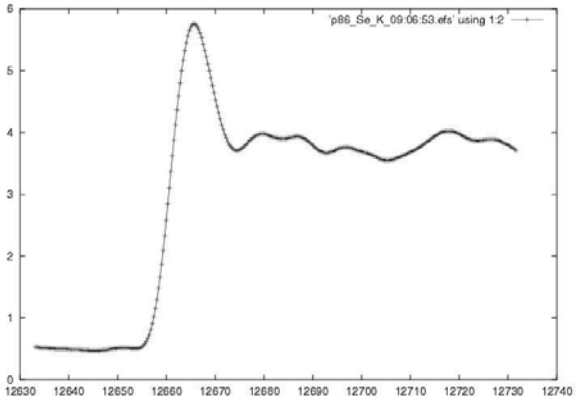
  ⇨ Check anisotropy of diffraction

Starting the Experiment

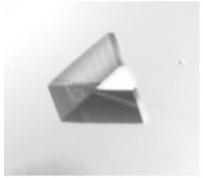


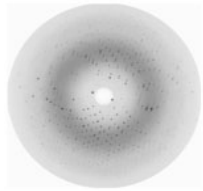
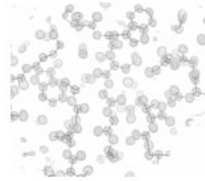
- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them
- Choose data collection wavelength

⇨ Measure an X-ray fluorescence spectrum for MAD/SAD



Starting the Experiment



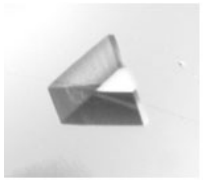



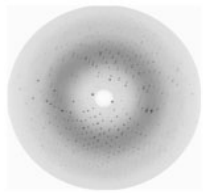
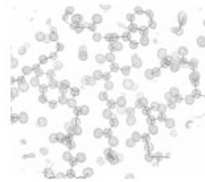

- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them
- Choose data collection wavelength
- Choose the detector distance

  ⇨ Use the whole detector surface

  ⇨ Rule of thumb: d_{min} = visible diffraction + 0.2 Å

Starting the Experiment



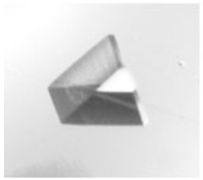



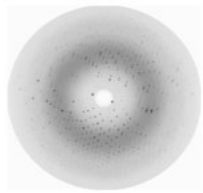
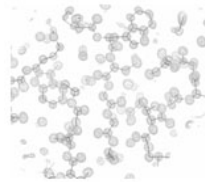

- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them
- Choose data collection wavelength
- Choose the detector distance
- Choose the total rotation range

⇨ Run a strategy program in order to get a complete data set as quickly as possible

⇨ If you have time and the crystal does not decay, collect redundant data

Starting the Experiment

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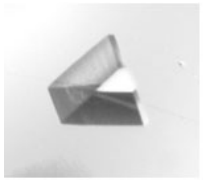
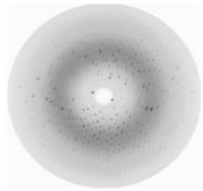
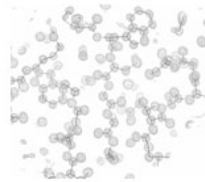
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them
- Choose data collection wavelength
- Choose the detector distance
- Choose the total rotation range
- Choose the rotation increment

  ⇨ Run a strategy program to avoid overlapping reflections

  ⇨ Fine slicing *vs.* wide slicing

Starting the Experiment

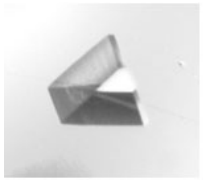


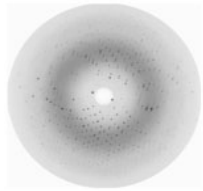
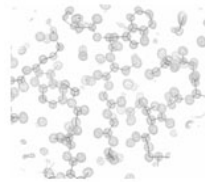




- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them
- Choose data collection wavelength
- Choose the detector distance
- Choose the total rotation range
- Choose the rotation increment
- Choose exposure time and/or attenuation

⇨ Avoid overloaded reflections

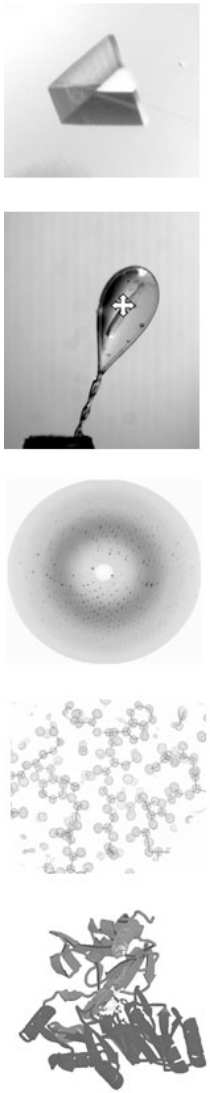
Starting the Experiment



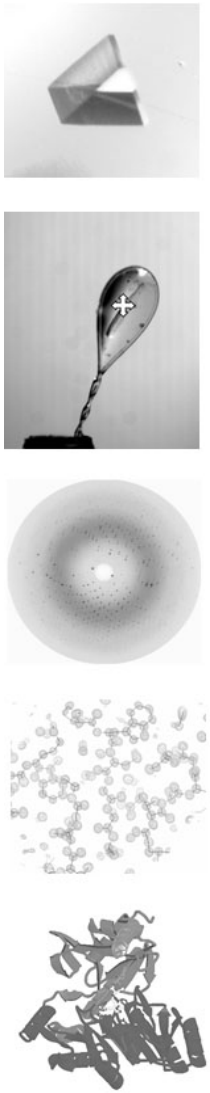

- Check cryo-system alignment and distance
- Mount crystal and center it
- Match beam size to crystal size
- Collect two test diffraction images and index them
- Choose data collection wavelength
- Choose the detector distance
- Choose the total rotation range
- Choose the rotation increment
- Choose exposure time and/or attenuation
- Start data collection

During the Experiment



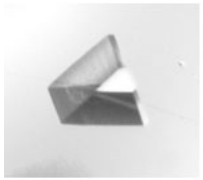
- Process the data as you collect them

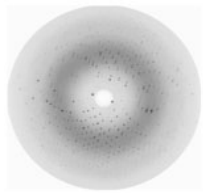
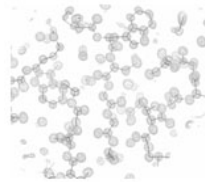
During the Experiment



- Process the data as you collect them
- Try to solve your structure as soon as possible

Summary – Part 2

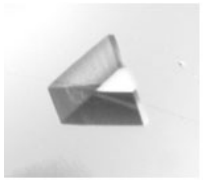


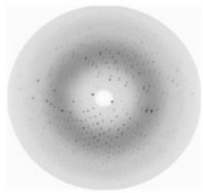
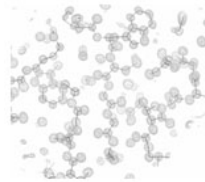




The collection of diffraction data is the last real **experiment** that is conducted before the determination and refinement of the structure.

The factors involved in diffraction data collection are complex and require some thought in order to produce the highest quality data set possible.

The quality of the diffraction data ultimately determines the quality of the resulting structure.




Thank you for your attention