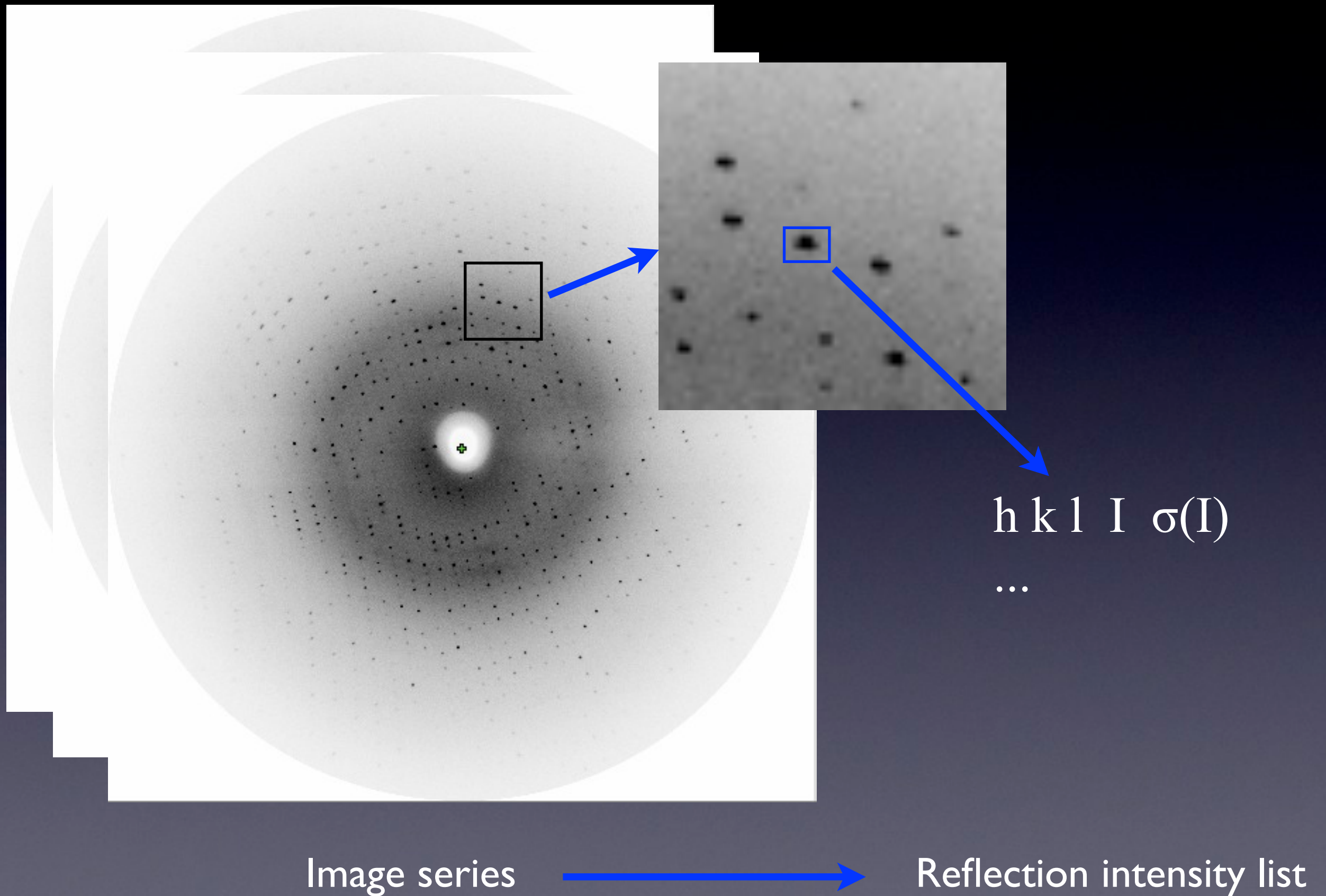


Diffraction geometry and integration of diffraction images

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Cambridge UK*

Integration



Diffraction Geometry

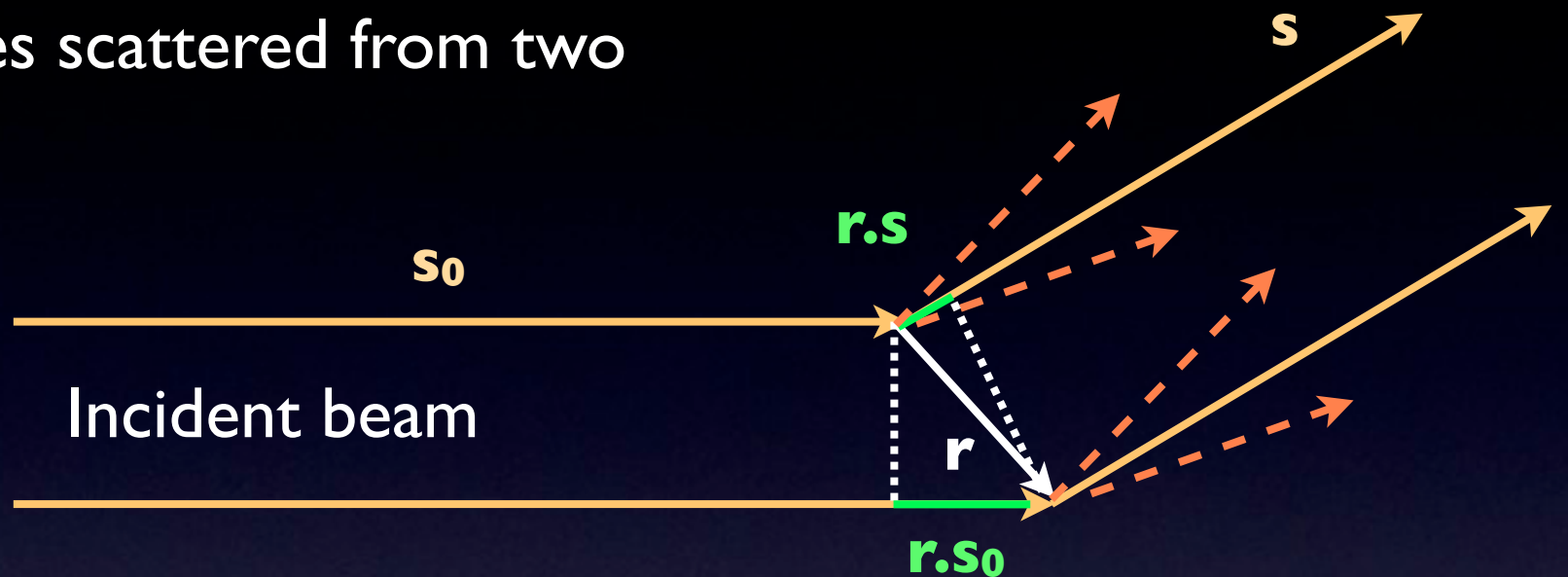
- Diffraction from a crystal - Laue equations
- Reciprocal lattice
- Ewald construction
- Data collection strategy

Diffraction conditions & explanation of the Ewald sphere construction

Scattering from two electrons

Path length difference for waves scattered from two points $\mathbf{r}$ apart in direction $\mathbf{s}$

$$\delta L = \mathbf{r} \cdot \mathbf{s} - \mathbf{r} \cdot \mathbf{s}_0 = \mathbf{r} \cdot (\mathbf{s} - \mathbf{s}_0)$$



Phase shift corresponding to path length difference δL for a wave with wavelength λ

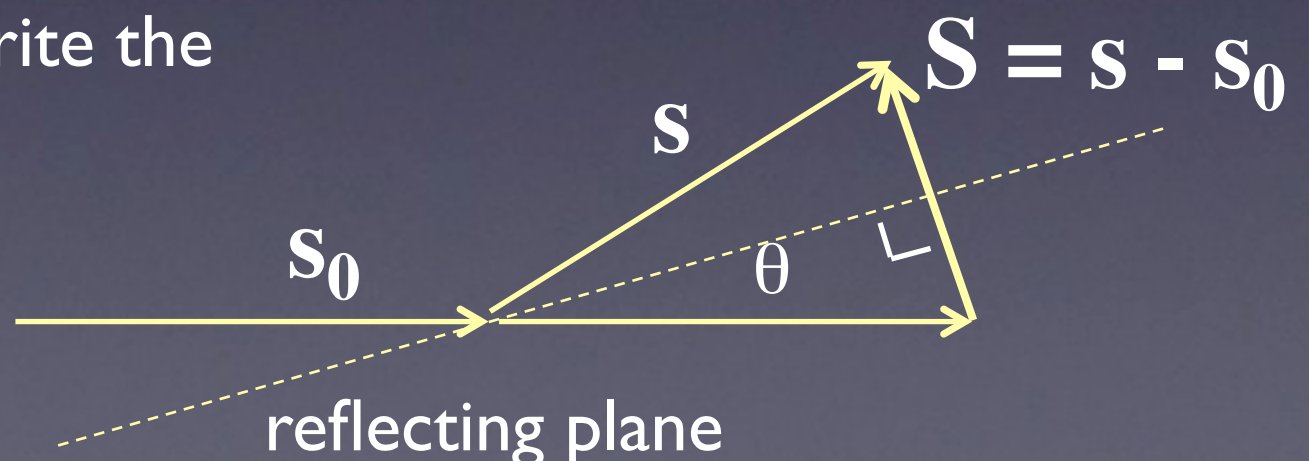
$$= 2\pi (\text{path difference}) / \lambda$$

$$= 2\pi \delta L / \lambda = 2\pi \mathbf{r} \cdot (\mathbf{s} - \mathbf{s}_0) / \lambda$$

If we make the length of the wave vectors $\mathbf{s}_0$ and $\mathbf{s} = 1/\lambda$, ie $|\mathbf{s}_0| = |\mathbf{s}| = 1/\lambda$, then we can write the phase shift $= 2\pi \mathbf{r} \cdot \mathbf{S}$ where $\mathbf{S} = \mathbf{s} - \mathbf{s}_0$

$\mathbf{S}$ is the perpendicular to an imaginary “reflecting plane” with $|\mathbf{S}| = 2 \sin \theta / \lambda$

X-rays scattered in all directions



Diffraction from a one-dimensional crystal

Total wave scattered from $n+1$ points at $\mathbf{r}_j$ ($j = 0, n$) is given by

$$\mathbf{F}(\mathbf{S}) = \sum_j \exp(i 2\pi \mathbf{r}_j \cdot \mathbf{S}) \quad \text{in the direction given by } \mathbf{S} = \mathbf{s} - \mathbf{s}_0$$

where $(2\pi \mathbf{r}_j \cdot \mathbf{S})$ is the relative phase for the wave from the j 'th point

adding up waves represented as $\exp(i \varphi) = \cos(\varphi) + i \sin(\varphi)$

A one-dimensional crystal is defined by a series of points at $\mathbf{r}_j = j \mathbf{a}$
where $\mathbf{a}$ is the vector defining the unit cell



The diagram illustrates a one-dimensional crystal lattice. It consists of a horizontal line with arrows pointing to the right, indicating the direction of the lattice vector. Below the line, the points are labeled as $0\mathbf{a}$, $\mathbf{a}$, $2\mathbf{a}$, $3\mathbf{a}$, $4\mathbf{a}$, and $= j\mathbf{a}$. The arrows are placed between the labels, showing the progression from one point to the next.

then

$$\begin{aligned} \mathbf{F}(\mathbf{S}) &= \sum_j \exp(2\pi i \mathbf{r}_j \cdot \mathbf{S}) \\ &= \sum_j \exp(2\pi i j \mathbf{a} \cdot \mathbf{S}) \end{aligned}$$

In general, this is the sum of a series of complex numbers of the same magnitude, but in random directions $\mathbf{S}$, so for large n , $|\mathbf{F}(\mathbf{S})| \approx 0$

$$\mathbf{F}(\mathbf{S}) = \sum_j \exp(2\pi i \mathbf{j} \cdot \mathbf{a} \cdot \mathbf{S}) \text{ for } j = 0, n$$

For large n , $|\mathbf{F}(\mathbf{S})|$ is only non-zero if $\mathbf{a} \cdot \mathbf{S}$ is integral, when the terms in the summation add up

$$\mathbf{a} \cdot \mathbf{S} = h \quad (h \text{ is an integer})$$

Note that this is not true for a crystal with few unit cell repeats

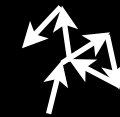
The Reciprocal Lattice

For a given cell repeat $\mathbf{a}$, $\mathbf{S}$ can only take values

$$\mathbf{S} = h \mathbf{a}^* \text{ where } \mathbf{a} \cdot \mathbf{a}^* = 1$$

$\mathbf{a}^*$ defines a lattice with spacing **inversely** proportional to the real cell spacing, since

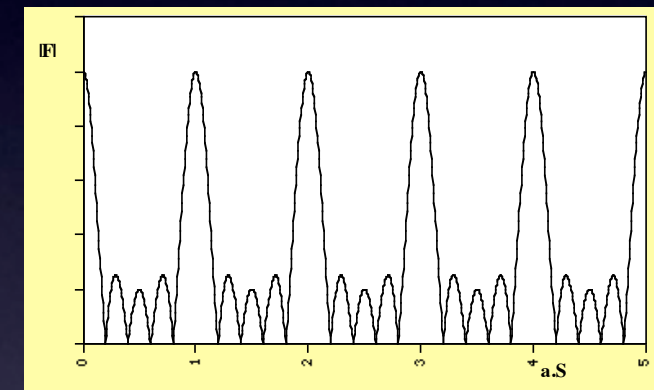
$$|\mathbf{a}^*| = 1 / |\mathbf{a}|$$



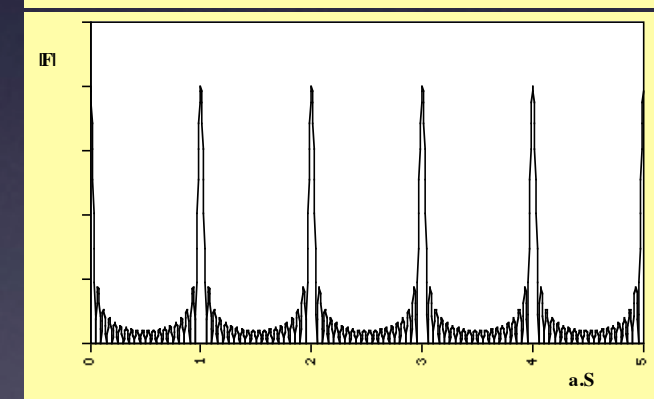
Random



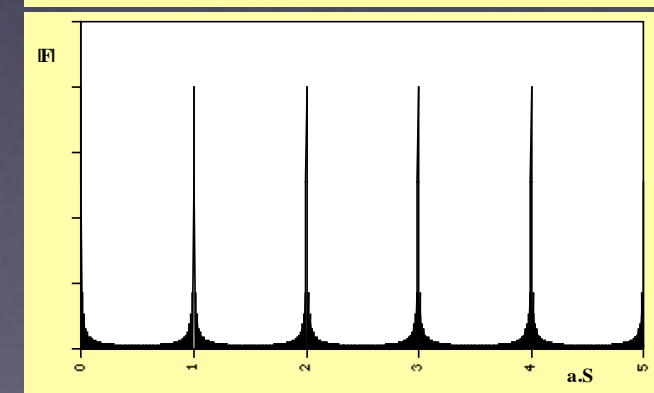
In phase



$n=4$



$n=19$



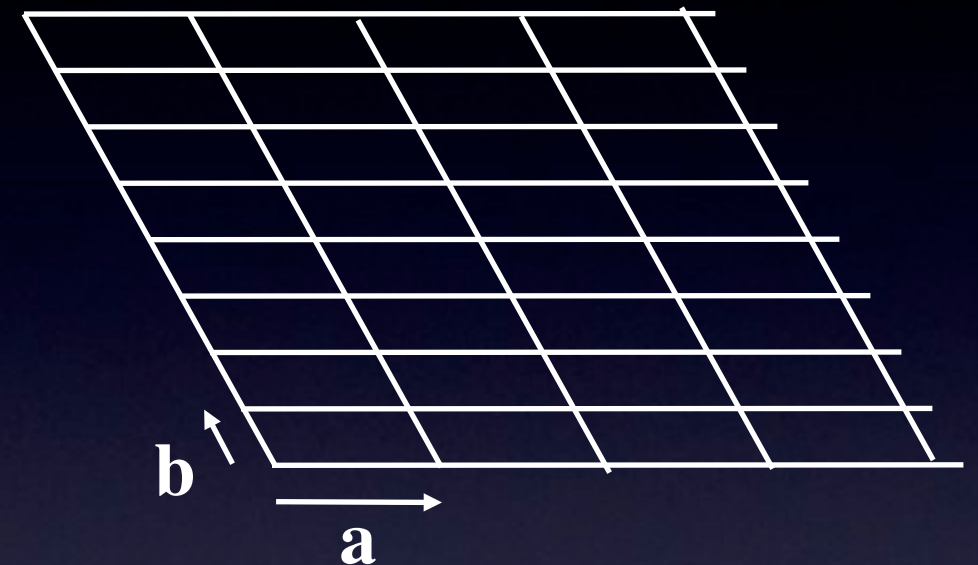
$n=99$

Three dimensional crystals

A 3-dimensional crystal is defined by three vectors, **a**, **b**, **c**

The coordinates of a general unit cell relative to a fixed origin is given by

$$\mathbf{r}_{uvw} = u \mathbf{a} + v \mathbf{b} + w \mathbf{c} \text{ where } u, v, w \text{ are integers}$$



so total scattering from one point in each cell is given by

$$\begin{aligned} \mathbf{F}(\mathbf{S}) &= \sum_u \sum_v \sum_w \exp(2\pi i \mathbf{r}_{uvw} \cdot \mathbf{S}) \\ &= \sum_u \exp(2\pi i u \mathbf{a} \cdot \mathbf{S}) \sum_v \exp(2\pi i v \mathbf{b} \cdot \mathbf{S}) \sum_w \exp(2\pi i w \mathbf{c} \cdot \mathbf{S}) \end{aligned}$$

As in the 1-dimensional case, $|\mathbf{F}(\mathbf{S})|$ is only non-zero for large numbers of unit cells if $\mathbf{a} \cdot \mathbf{S}$, $\mathbf{b} \cdot \mathbf{S}$, and $\mathbf{c} \cdot \mathbf{S}$ are all integral

$$\text{ie } \mathbf{a} \cdot \mathbf{S} = h \quad \mathbf{b} \cdot \mathbf{S} = k \quad \mathbf{c} \cdot \mathbf{S} = l$$

These are the Laue equations

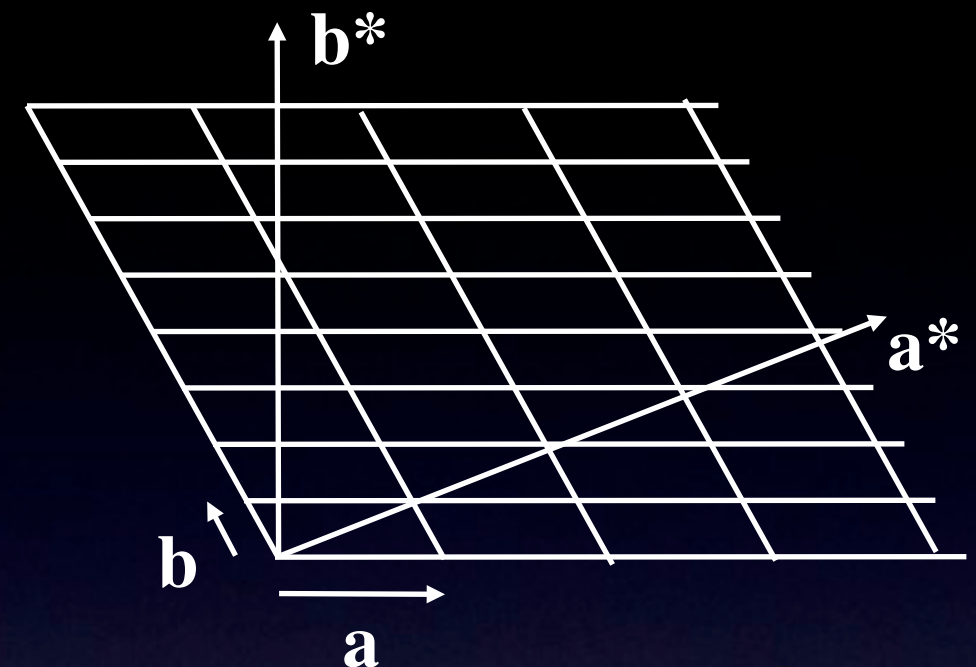
The Laue equations define a **reciprocal lattice** of allowed values of **S**, based on the “reciprocal” vectors **a***, **b***, **c***

$$\mathbf{S} = h \mathbf{a}^* + k \mathbf{b}^* + l \mathbf{c}^*$$

$$\mathbf{a} \cdot \mathbf{a}^* = 1 \quad \mathbf{a} \cdot \mathbf{b}^* = 0$$

$$\mathbf{b} \cdot \mathbf{b}^* = 1 \quad \mathbf{b} \cdot \mathbf{c}^* = 0$$

$$\mathbf{c} \cdot \mathbf{c}^* = 1 \quad \mathbf{c} \cdot \mathbf{a}^* = 0$$



The reciprocal lattice vectors are perpendicular to the *planes* of the real crystal lattice, since the scattering can be considered as coming from reflecting planes (the Bragg planes)

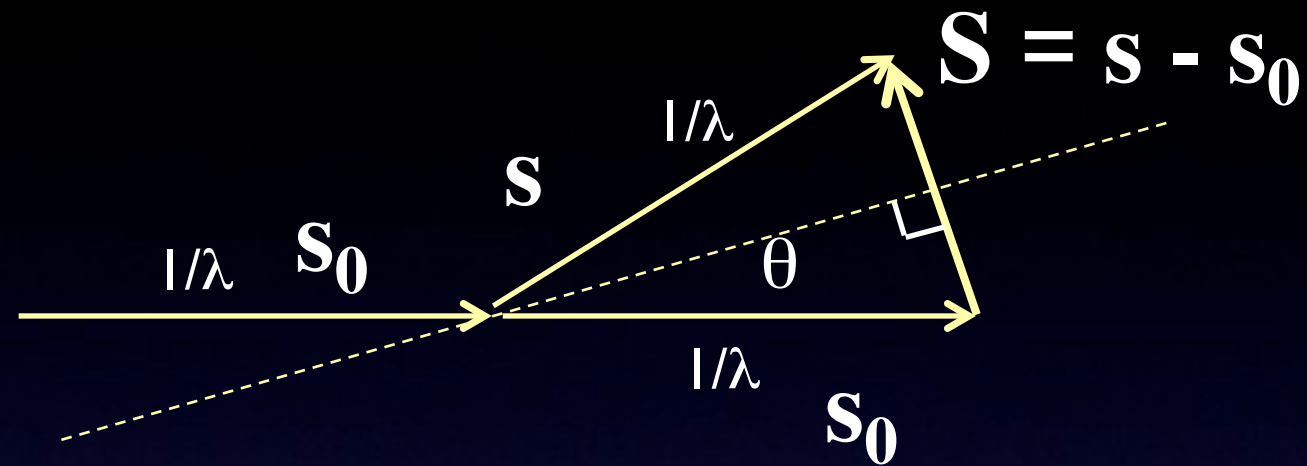
$$\mathbf{a}^* = (\mathbf{b} \times \mathbf{c})/V \quad \mathbf{b}^* = (\mathbf{c} \times \mathbf{a})/V \quad \mathbf{c}^* = (\mathbf{a} \times \mathbf{b})/V \quad V = \text{cell volume}$$

$|\mathbf{a}^*|$ is the spacing between the (bc) planes, $|\mathbf{b}^*|$ between the (ca) planes, $|\mathbf{c}^*|$ between the (ab) planes

For the special case of an orthogonal lattice (only),

$$|\mathbf{a}^*| = 1/|\mathbf{a}|, \quad |\mathbf{b}^*| = 1/|\mathbf{b}|, \quad |\mathbf{c}^*| = 1/|\mathbf{c}|$$

The Ewald Sphere Construction



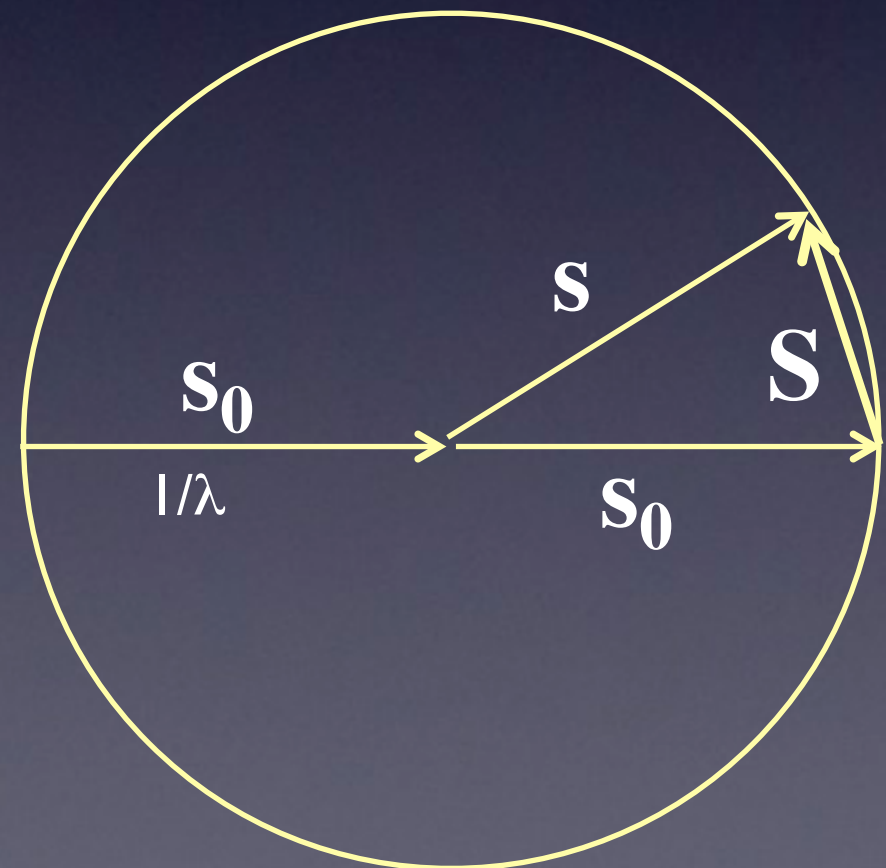
The general condition for diffraction is illustrated by the vector equation

$$\mathbf{S} = \mathbf{s} - \mathbf{s}_0$$

Because $\mathbf{s}_0$ and $\mathbf{s}$ have the same length ($1/\lambda$), we can generalise this diagram by drawing a sphere of radius $|\mathbf{s}_0| = |\mathbf{s}| = 1/\lambda$

$\mathbf{S}$ is the diffraction vector in *reciprocal space*

For a crystal, $\mathbf{S}$ may only take certain values,
 $\mathbf{S} = h \mathbf{a}^* + k \mathbf{b}^* + l \mathbf{c}^*$



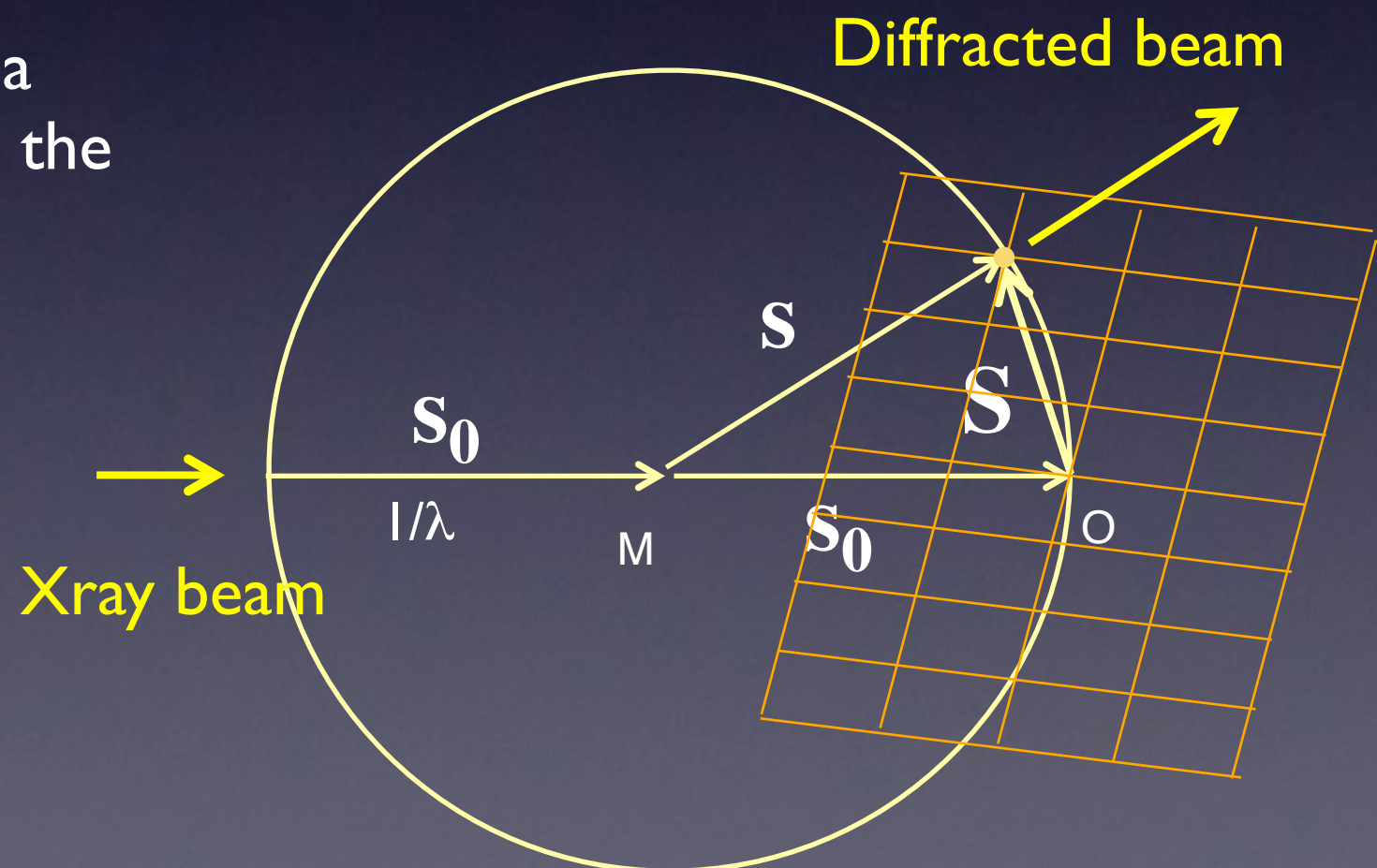
The Ewald sphere is only a construction but is very useful to understand the *geometry* of diffraction. Confusingly, it has two origins:-

M is the centre of the sphere, and may be considered as the position of the crystal, since this is the source of the secondary beam s

O is the origin of reciprocal space, the origin of the diffraction vector S , and the centre of the reciprocal lattice

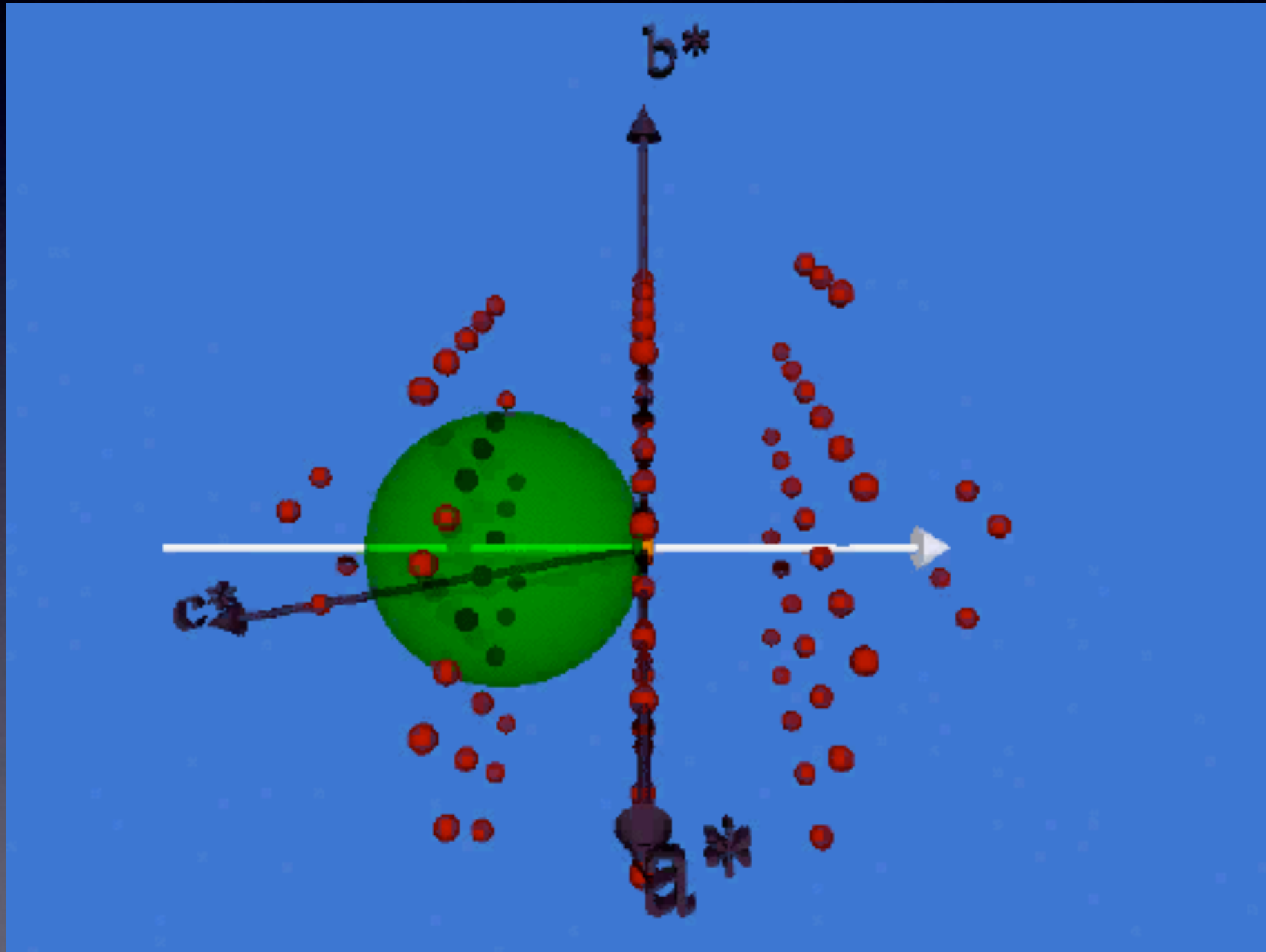
As the crystal rotates, the reciprocal lattices rotates in exactly the same way

Diffraction only occurs when a reciprocal lattice point lies on the sphere

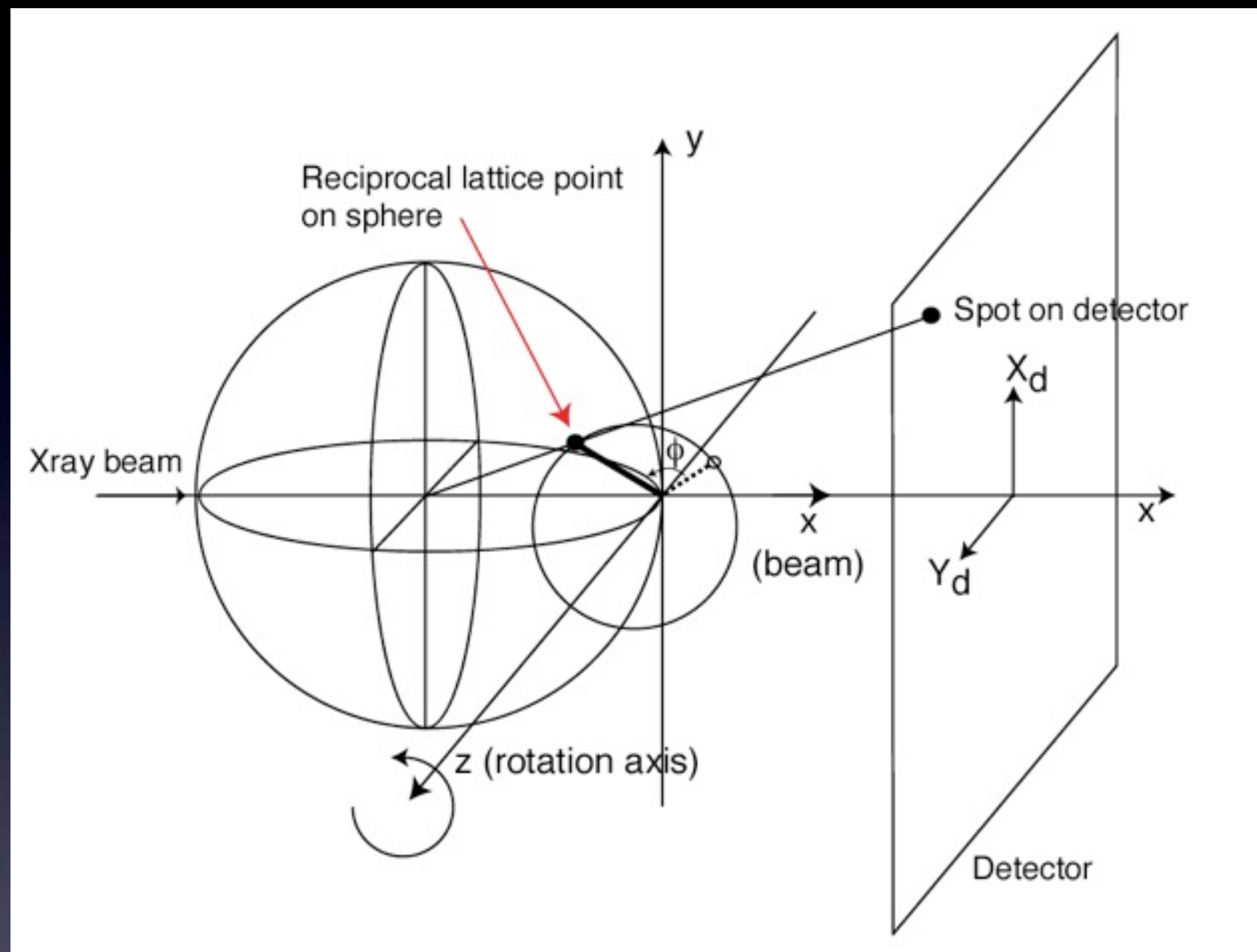


As the crystal rotates, so does the the reciprocal lattice

As a reciprocal lattice point passes through the Ewald sphere, a diffracted beam is observed along the line from the sphere centre to the reciprocal lattice point



The part of the reciprocal lattice which intersects the sphere is projected on to the detector



As the crystal rotates, each lattice point in turn passes through the sphere, and a spot is recorded on the detector

We can use the Ewald construction to understand

- what diffraction images look like
- how to collect a complete dataset without missing bits

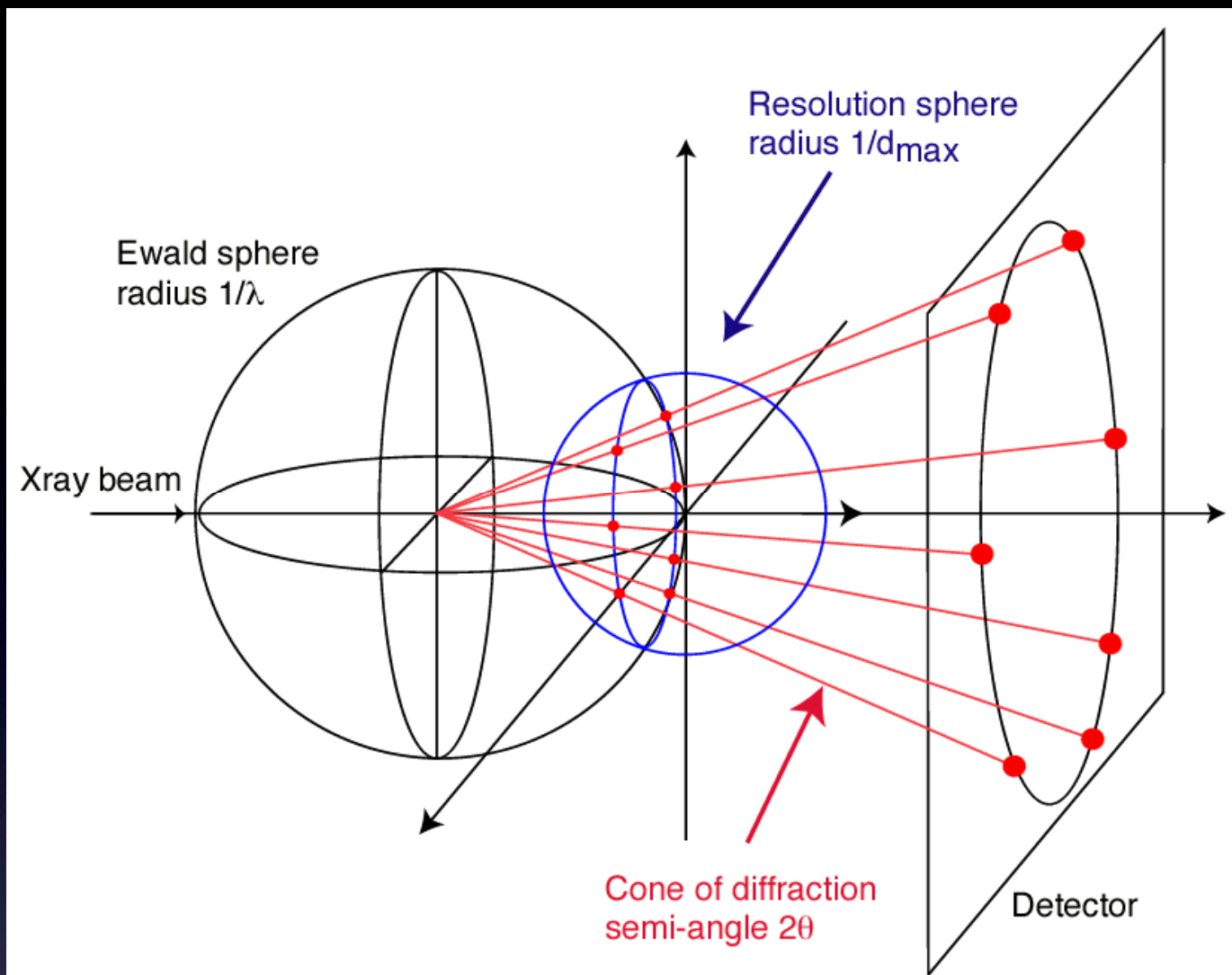
We can imagine the reciprocal lattice sitting on the crystal on the camera, and rotating as the crystal rotates

Detector position

For a maximum resolution of $d_{\max}$, all diffraction vectors S must lie within a resolution sphere of radius $1/d_{\max}$

As the crystal rotates, the diffracted beams all lie within a cone of semi-angle $2\theta_{\max}$

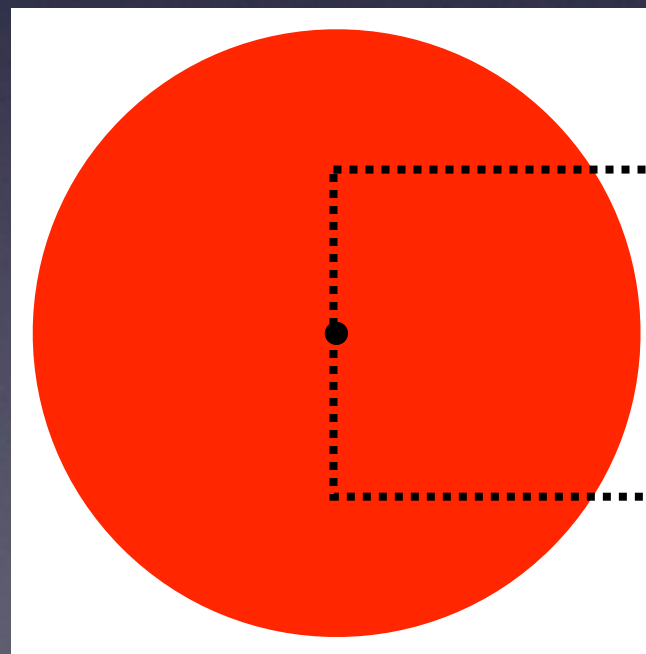
$$\lambda/d_{\max} = 2 \sin \theta_{\max}$$



A detector centered on the beam collects the whole cone

This gives optimum efficiency and simple strategy

The corners of a square detector collect incomplete data

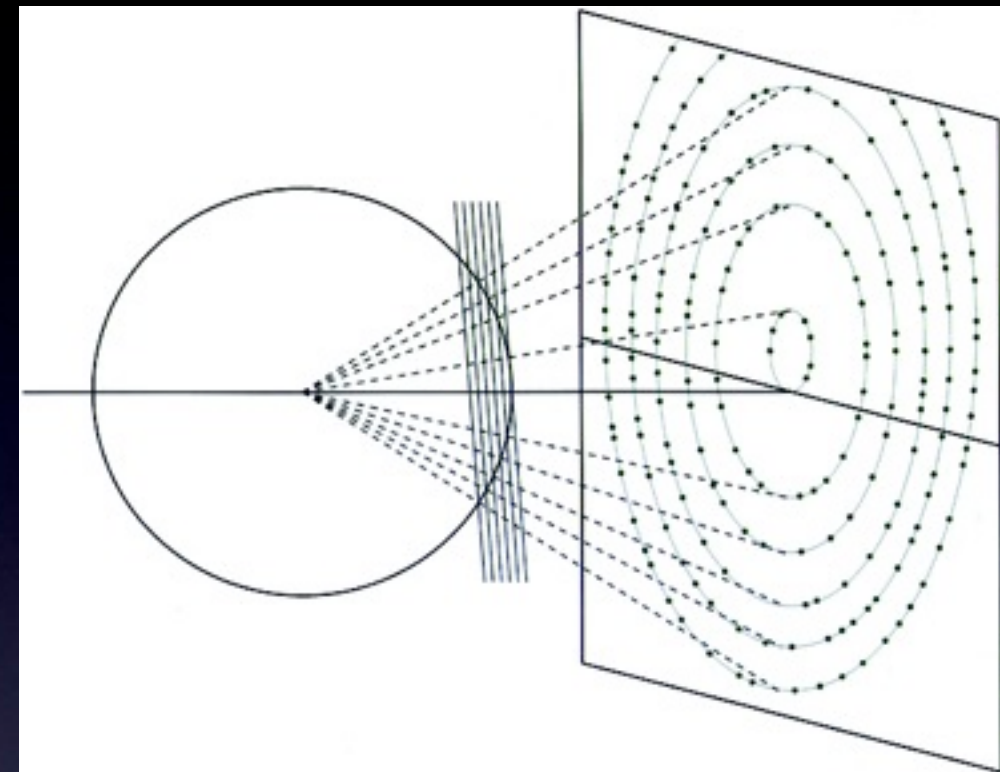


For long axes (close spot separation) it may be necessary to use a long detector distance and an offset detector

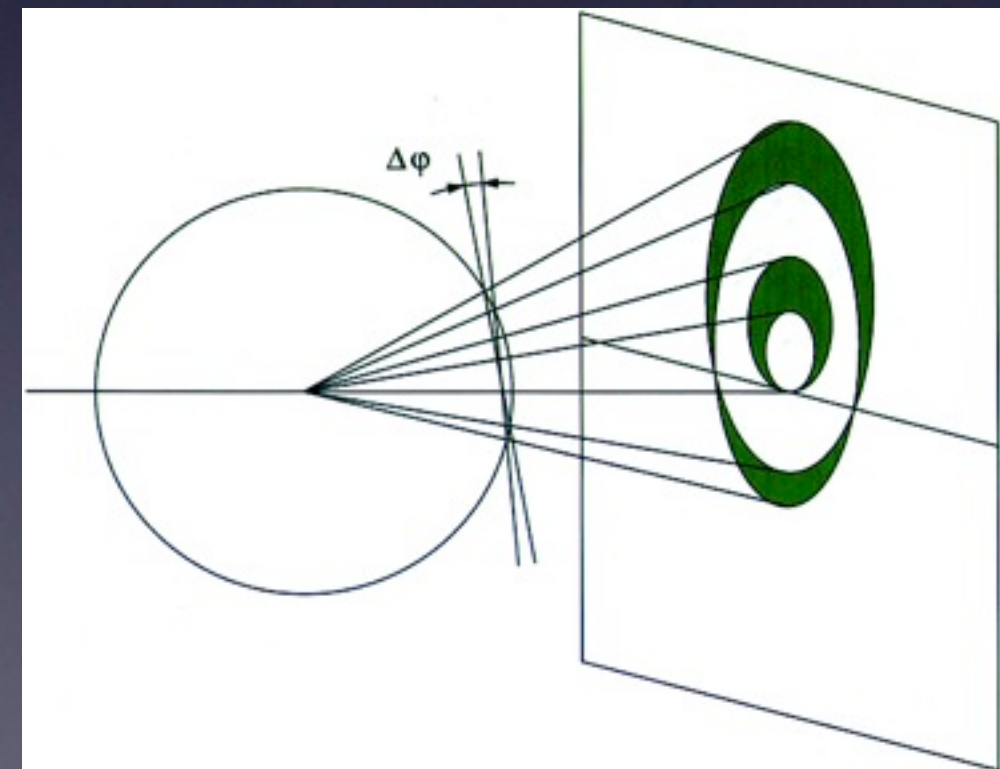
This gives a lower efficiency, and to get complete data requires a complicated strategy

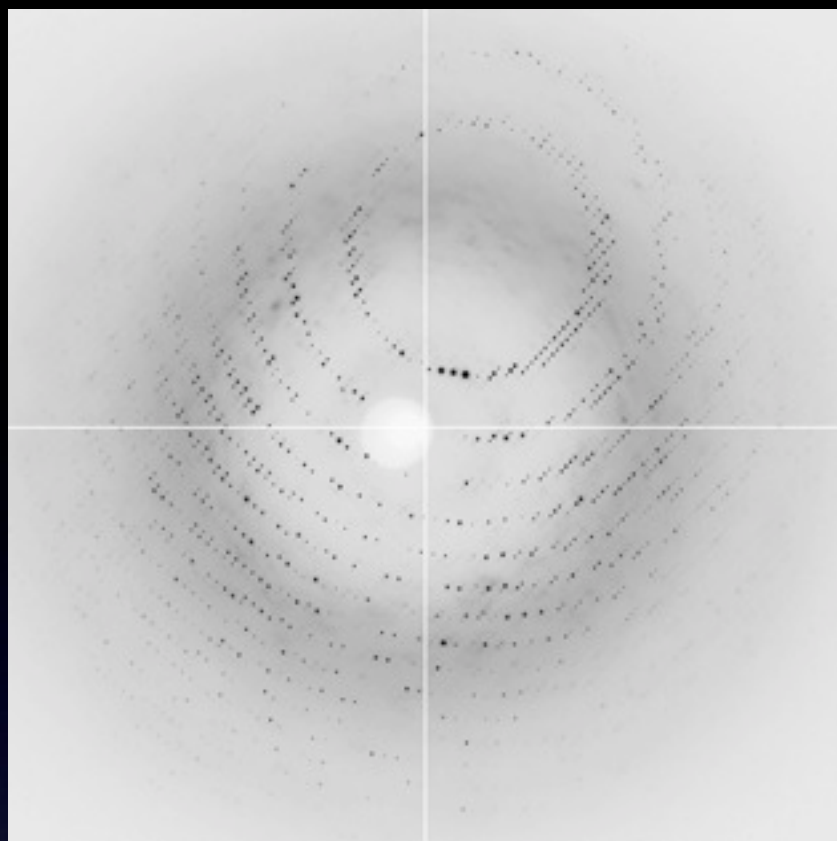
The appearance of diffraction images

Reciprocal lattice points lie in layers (planes). Each plane intersects the sphere in a circle, and the spots projected on the detector lie in ellipses

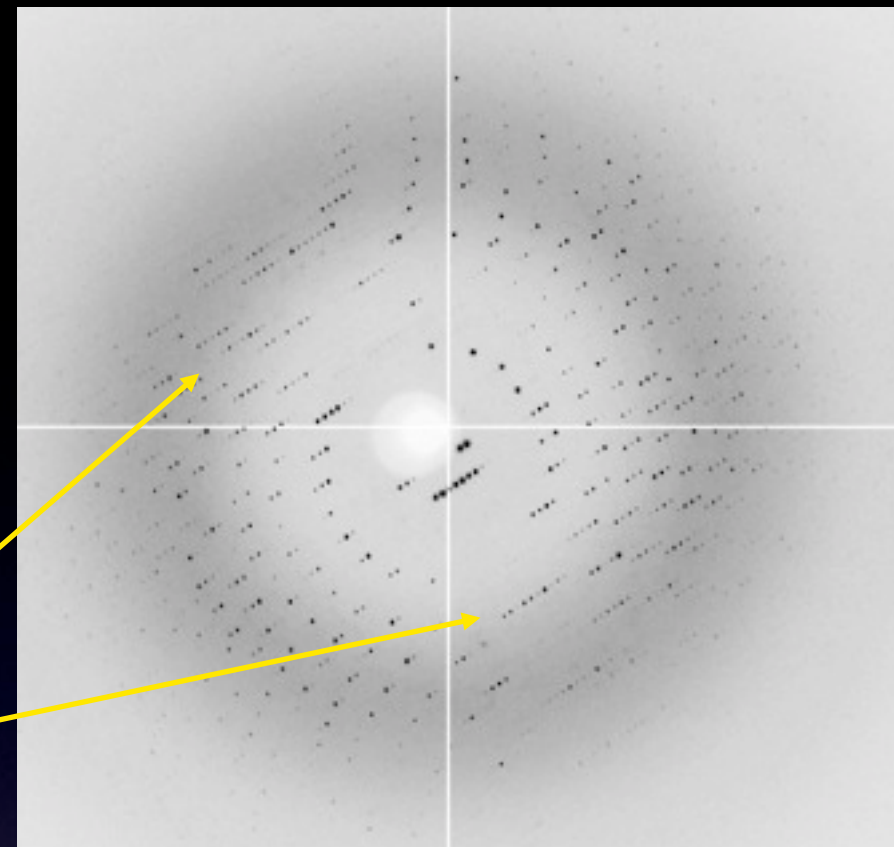


If the crystal is rotated through a small angle, each circle is broadened into a *lune*. All the spots in a lune belong to one plane of the reciprocal lattice (not necessarily a principal plane)



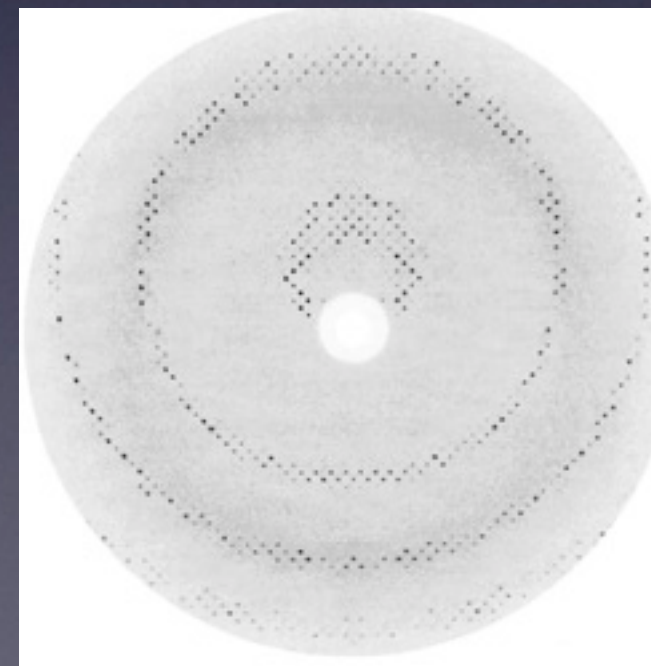
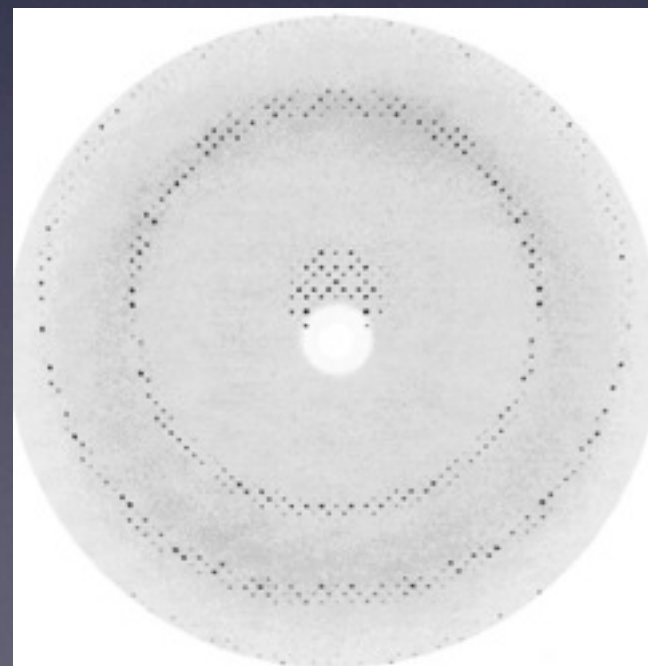
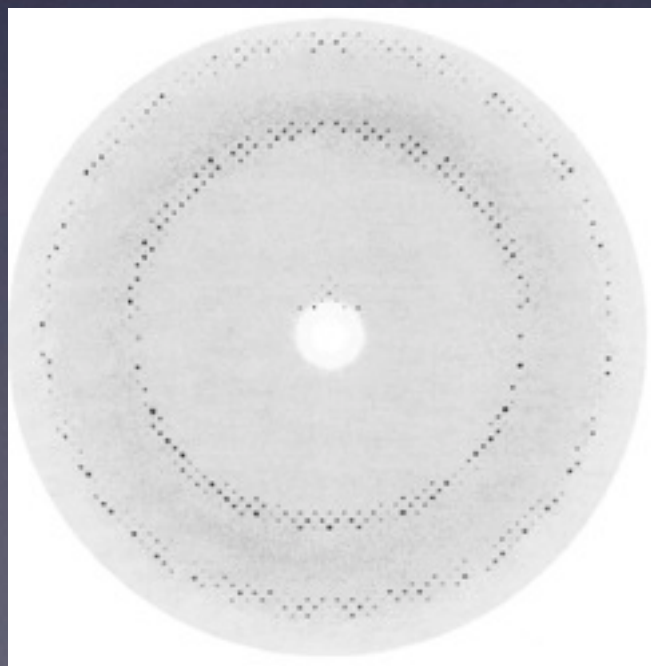
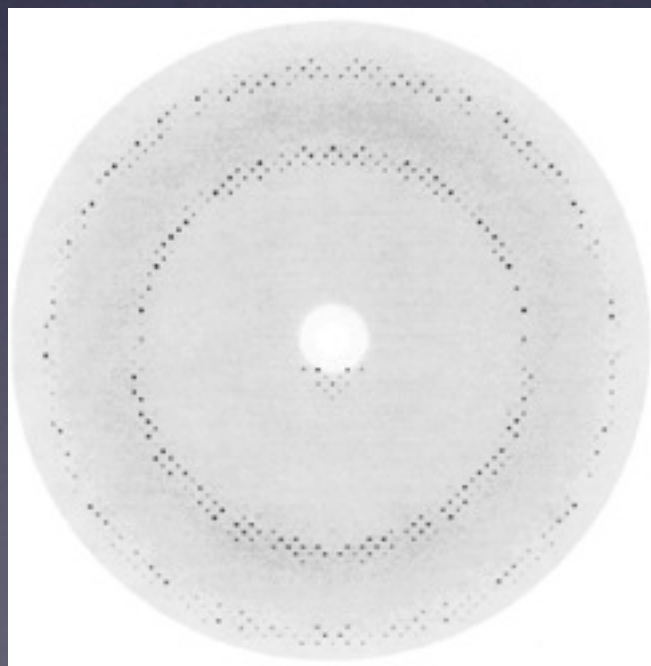


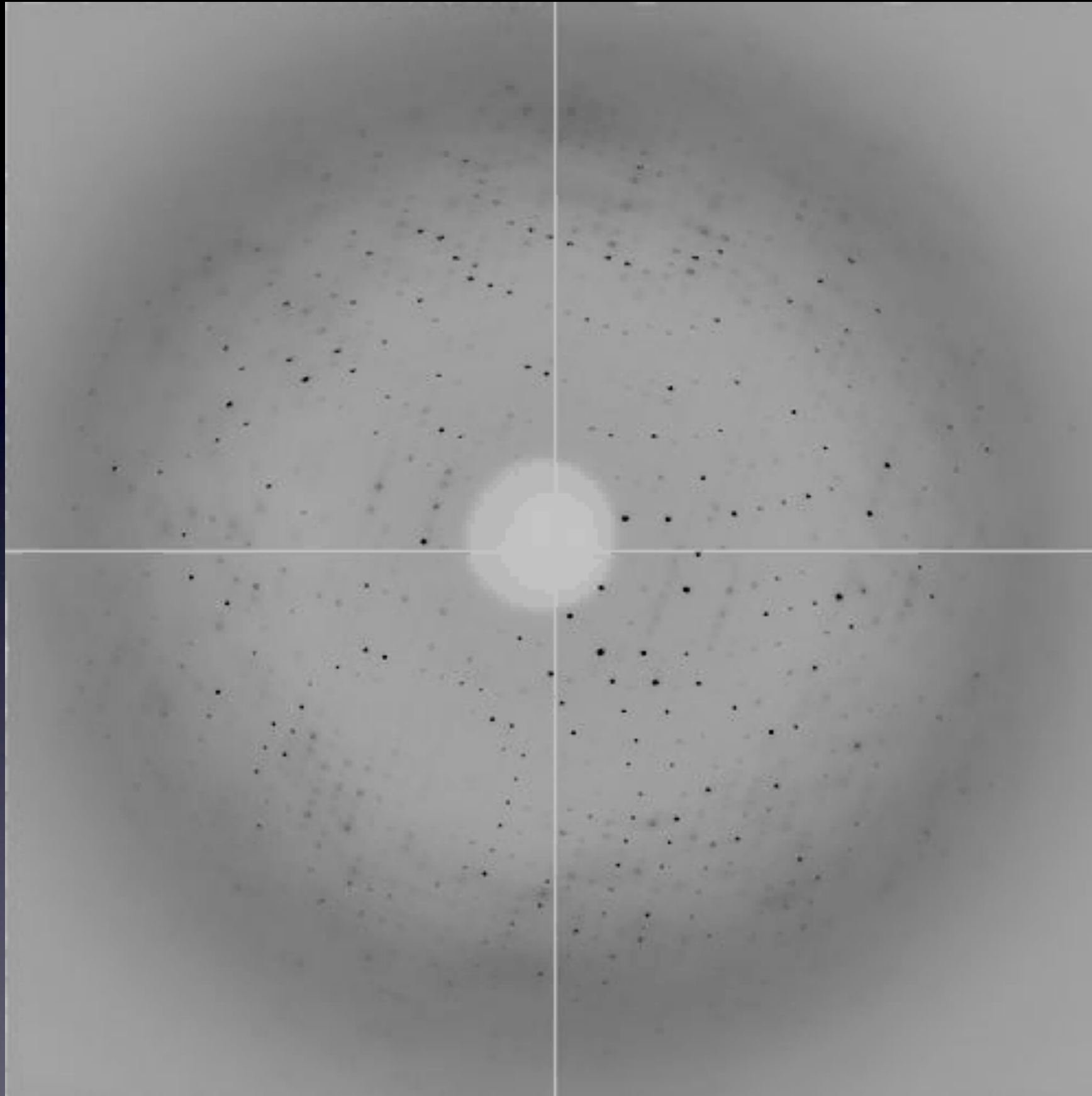
Examples of lunes in
rotation images



Lunes corresponding
to different sets of
planes

A series of successive rotation images showing the lunes moving up the image





The full diffraction pattern (ie the reciprocal lattice) is 3-dimensional, and we want to measure the whole sphere to the maximum resolution (radius) available.

The dataset should also be complete in dynamic range, including weak & strong spots, ie avoiding too many *overloads*, since the structure of the asymmetric unit is inferred from the measured intensities.

The size of spots in reciprocal space and on the detector

Real observed diffraction is complicated by the imperfections of real crystals and X-ray beams

The X-ray beam

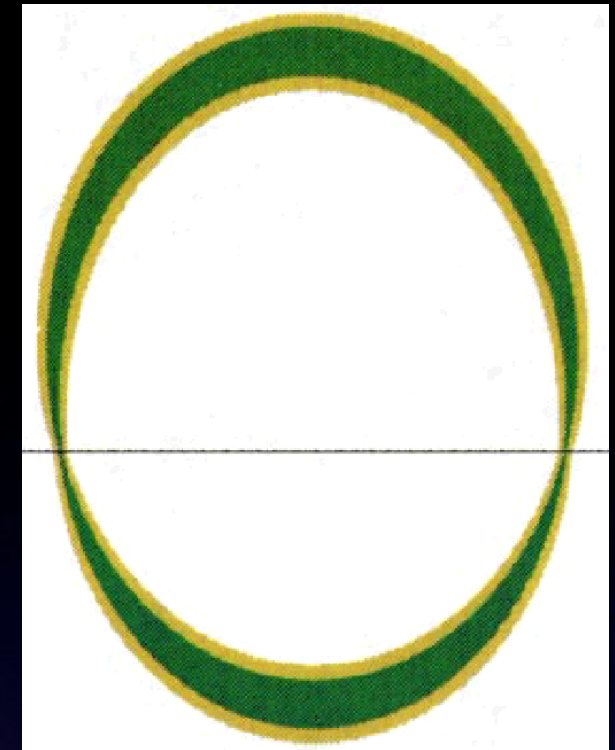
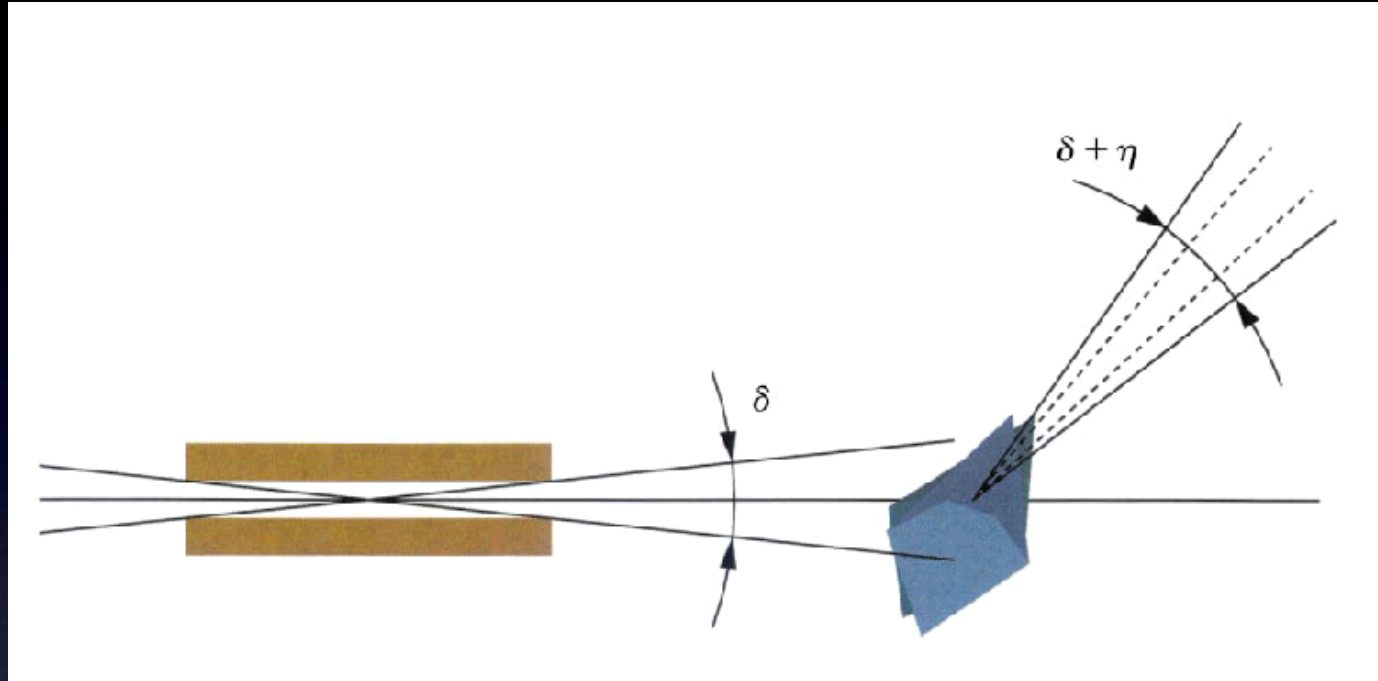
- the incident beam has a finite width and is not exactly parallel (**beam divergence**)
- the beam is not entirely monochromatic (**dispersion**)

The crystal

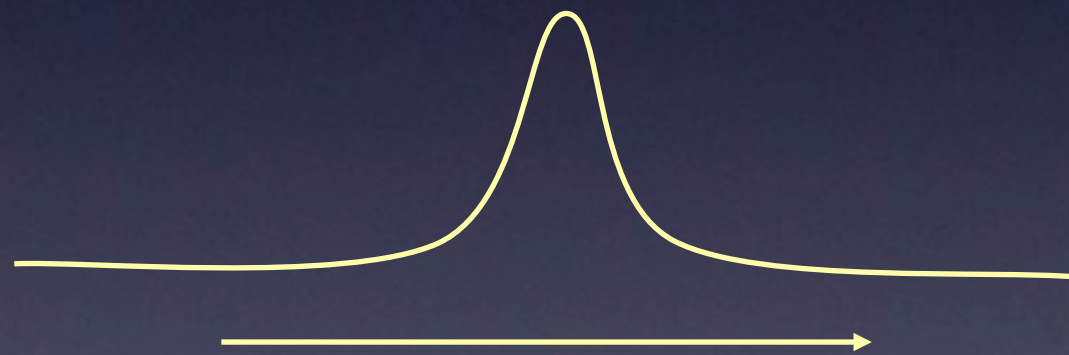
- the crystal has a finite size
- the crystal is not perfect, but may be considered a mosaic of blocks in slightly different orientations (**mosaicity**)

The effect of these factors can be considered as a broadening of the reciprocal lattice points, giving them a non-zero size

Beam divergence δ and mosaicity η add up to increase the angular width of the diffracted beam



High mosaicity causes broadening of the lunes
Most obvious along the rotation axis

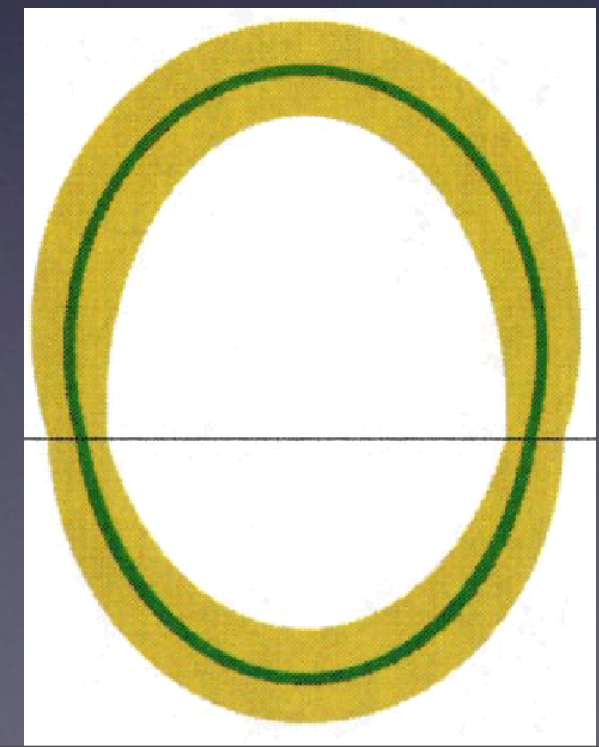


rotation angle ϕ

Reflection width in rotation

$$= \delta + \eta + \text{geometric factor}$$

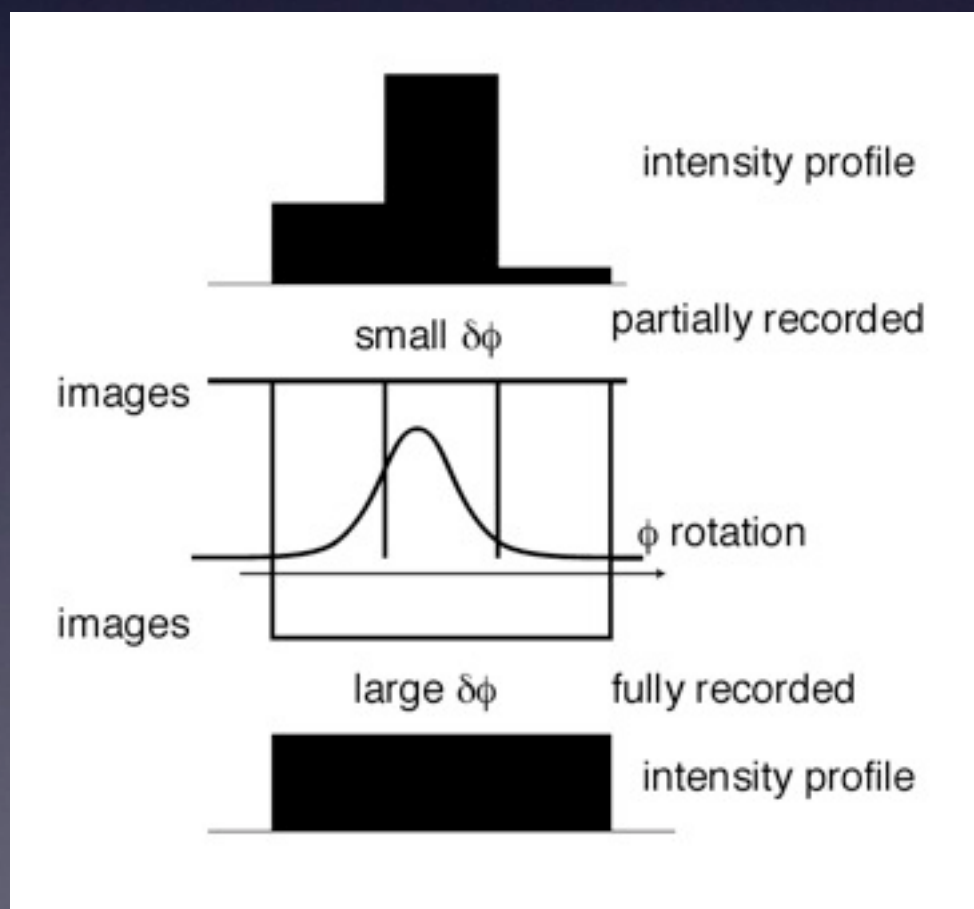
(geometric factor depends on angle between the rotation axis & S)



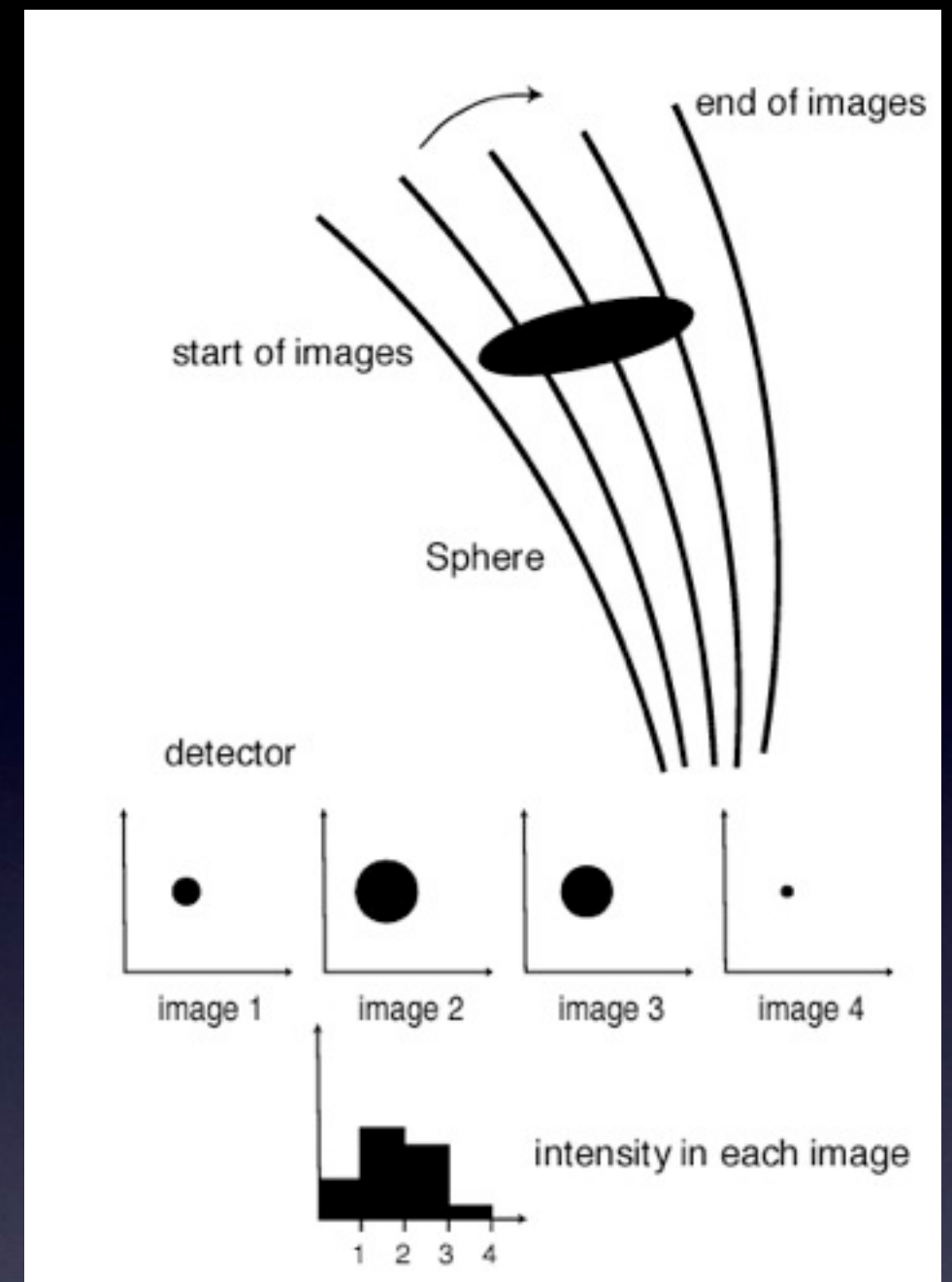
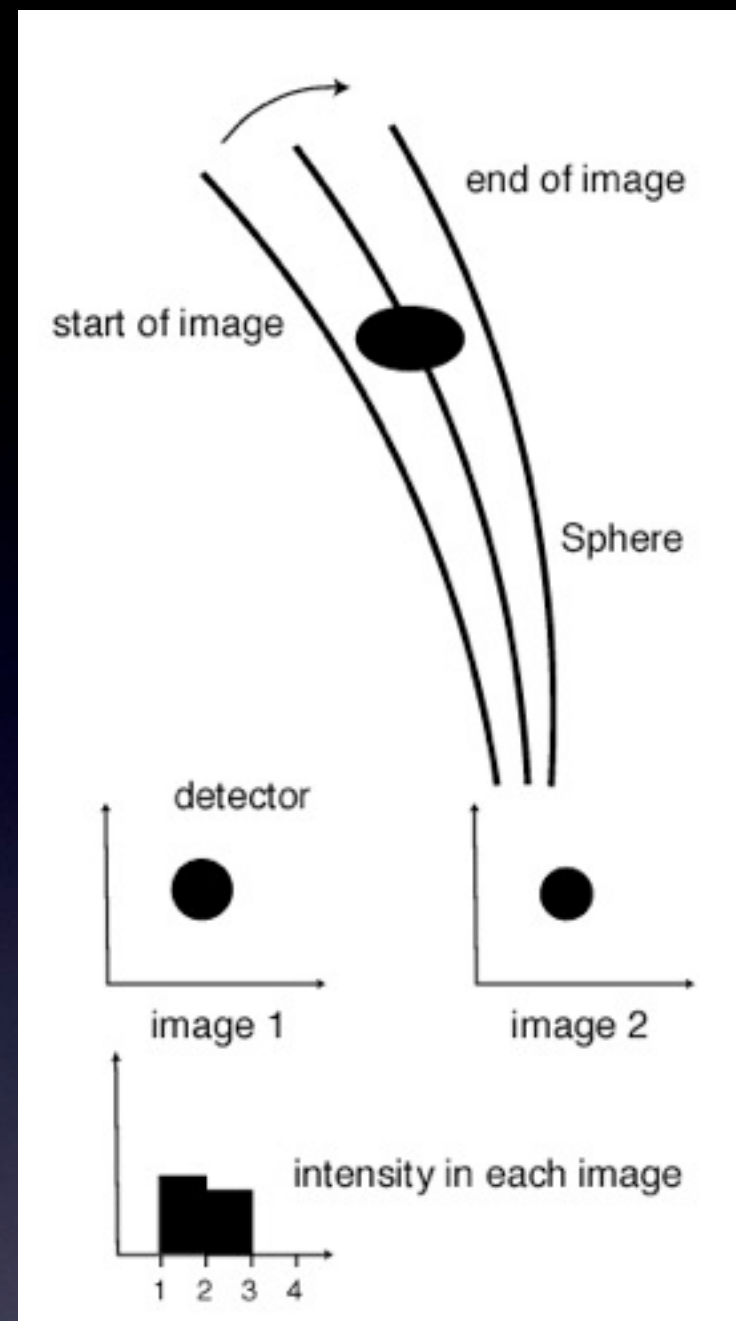
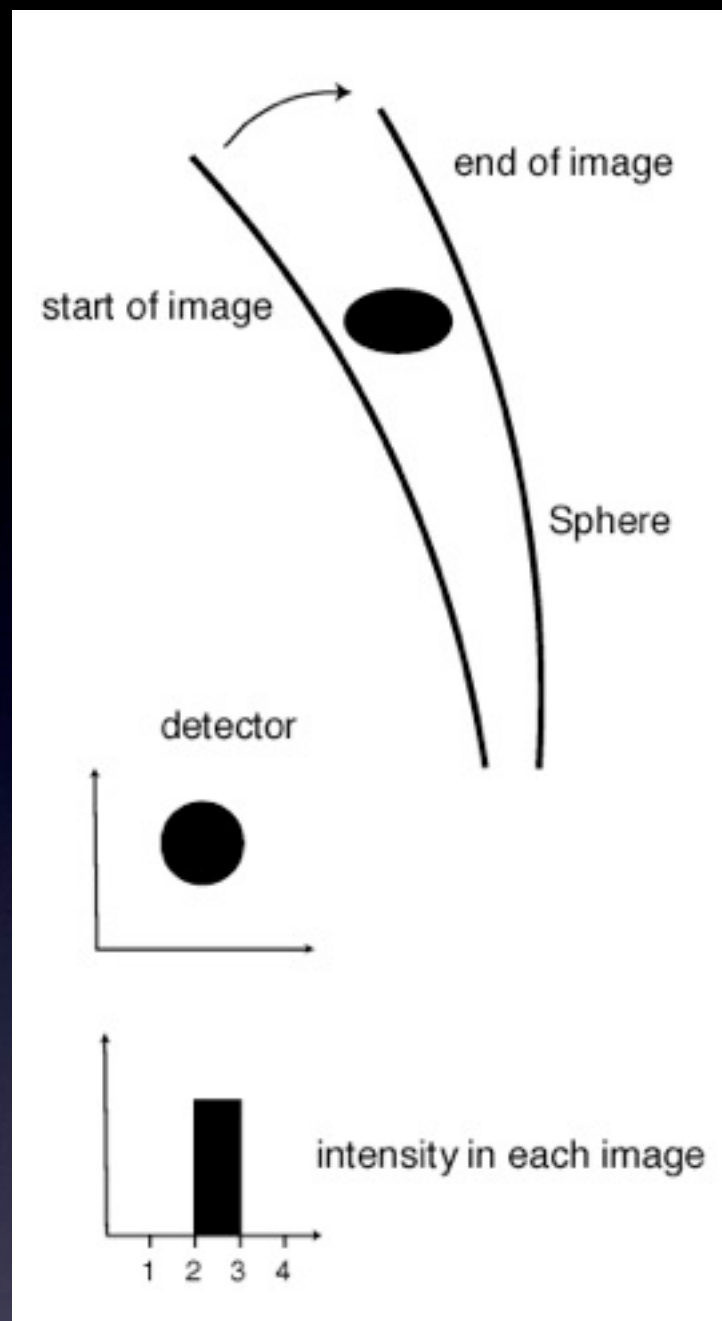
Images: fully recorded and partially recorded reflections

We want to determine the intensity of a reflection, integrated over its extent in reciprocal space by rotating the crystal so that the extended reciprocal lattice point passes through the sphere.

CCD and image plate detectors take a significant time to read out, so for these have to close the shutter & stop the rotation (simultaneously!). Pixel detectors (eg Pilatus) with very fast read-out can be used with continuous rotation with the shutter open. In both cases our sampling of the 3-dimensional reciprocal space is in consecutive slices, typically of between about 0.1° and 1°



Depending on the slice width and the reflection width a reflection may occur on one image (*full or fully recorded*) or on several (*partial or partially recorded*)



A fully-recorded spot is entirely recorded on one image

Partials are recorded on two or more images

“Fine-sliced” data has spots sampled in 3-dimensions

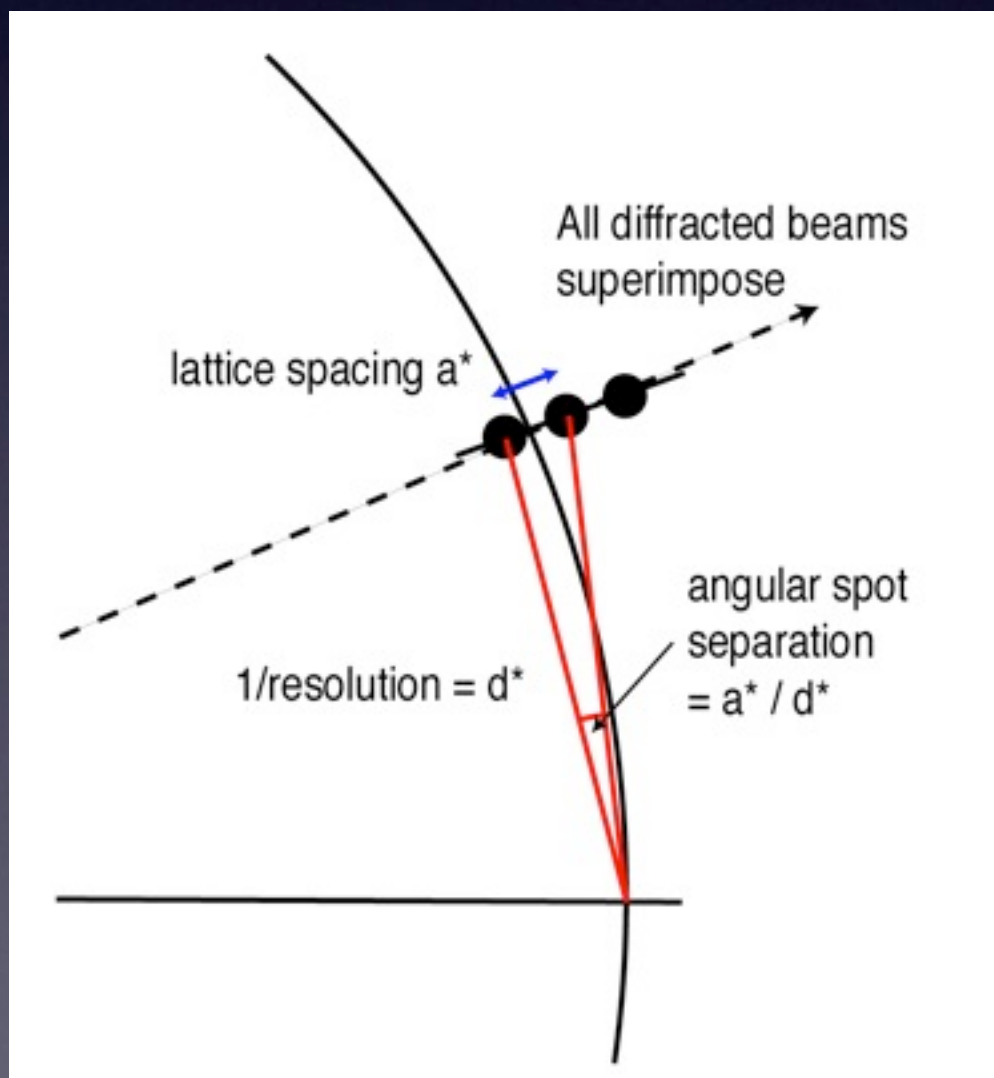
Perhaps best processed with a 3D program (eg d*trek, XDS)

Overlaps and rotation range

Current integration programs assume that spots are resolved, both on the detector and on rotation ϕ . This means that the intensity goes down to background all round the spot

Resolution is a problem for large unit cells, high mosaicity and high resolution

Overlap between spots on the detector is easy to see, but to understand overlap on ϕ we need to look in reciprocal space



When a closely-spaced row of spots (eg along a^*) is moving perpendicularly into the sphere, their diffracted beams almost coincide. The spots are on top of each other on the detector, and are only separated on ϕ

$$\text{Maximum slice width} = (a^*/d^*) - w$$

$$= d/a - w$$

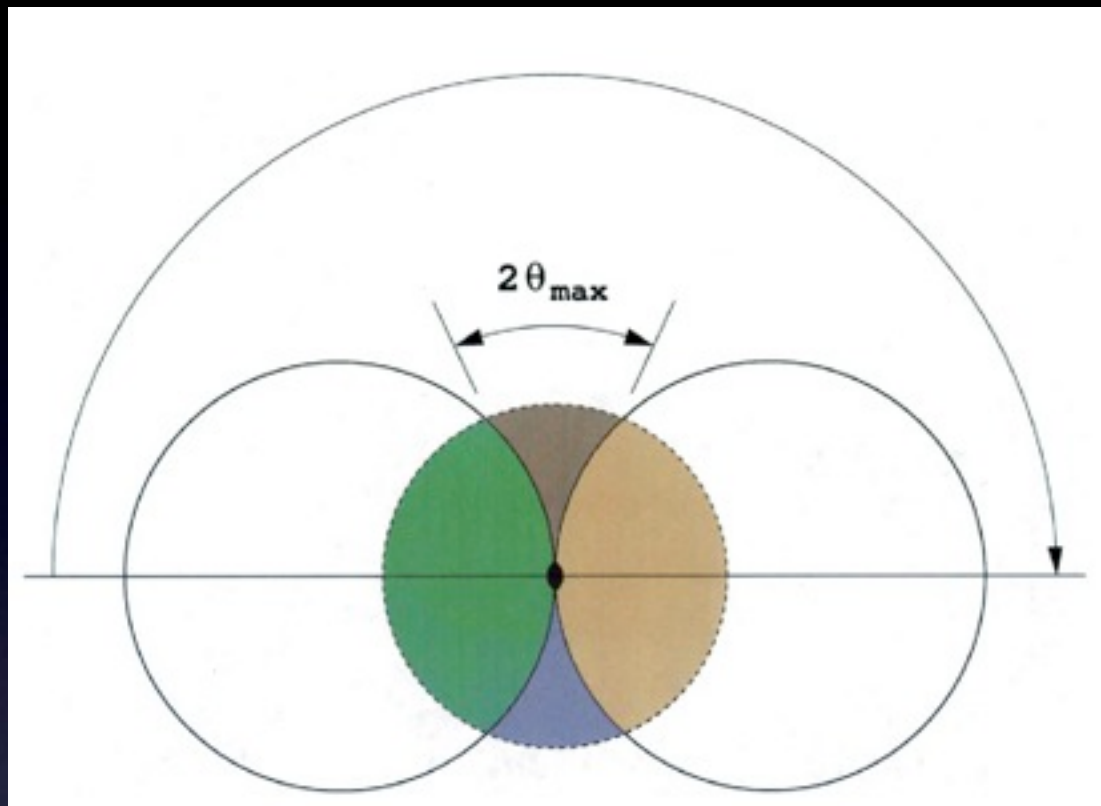
$$w = \text{reflection width} = \delta + \eta$$

$$\text{eg cell} = 200\text{\AA}, \text{ resolution} = 2\text{\AA}, \text{ width} = 0.3^\circ$$

$$\text{Maximum Slice} = 0.27^\circ$$

If possible, orient a long axis along the rotation axis to minimise overlap problems

Completeness: total rotation range and the blind region

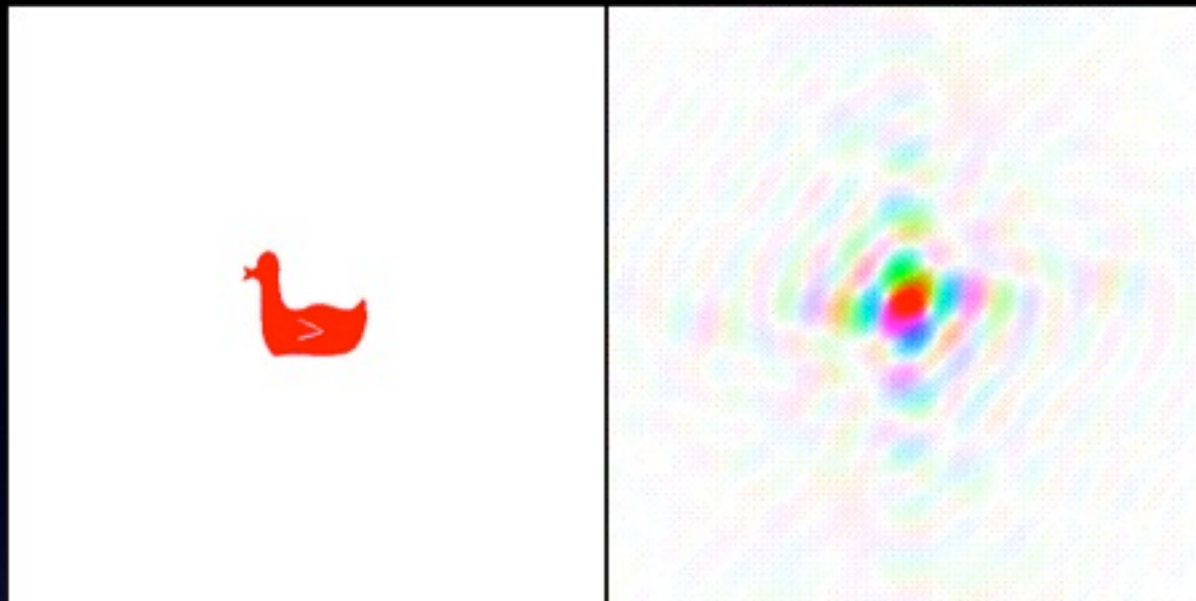


To use the Ewald sphere construction to understand which parts of reciprocal space are measured, it is easier to fix the “resolution sphere” of all reciprocal lattice points within a maximum resolution, and to rotate the Ewald sphere. The region collected is the volume swept out by the leading and trailing surfaces of the sphere

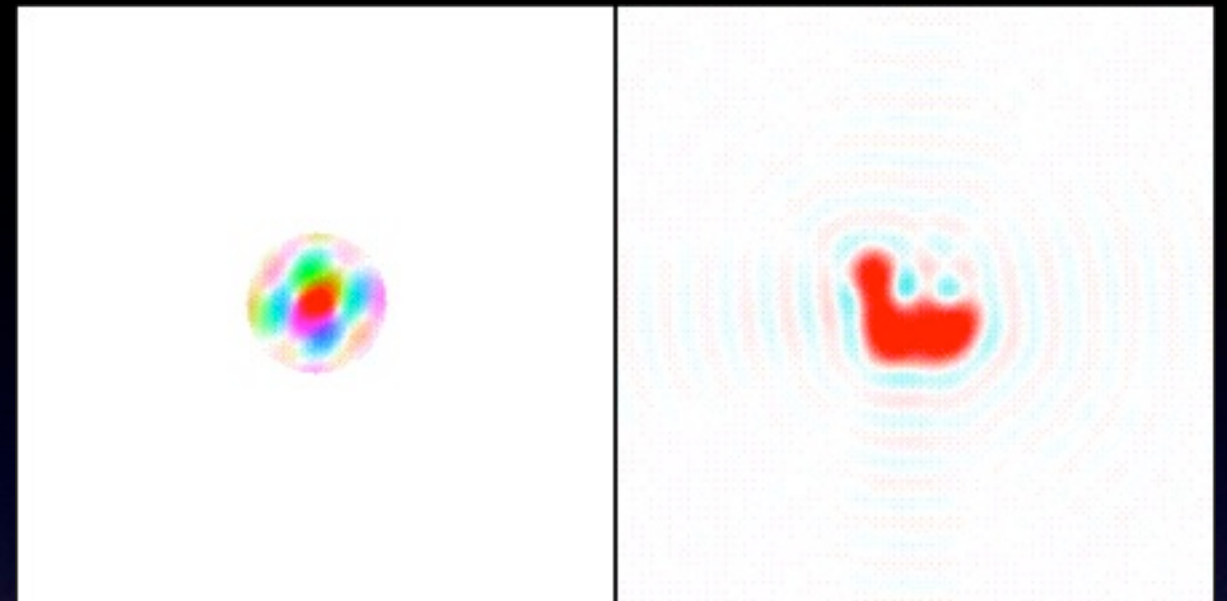
In a rotation of 180° above, the lower boundary of the initial sphere sweeps out the volume coloured green & the upper boundary the light brown part. The dark brown part is measured twice, and the blue part not at all

Because of Friedel’s law, this dataset is complete (apart from the *blind region*), but if complete anomalous differences are required, then $180^\circ + 2\theta_{\max}$ is required (unless there is symmetry)

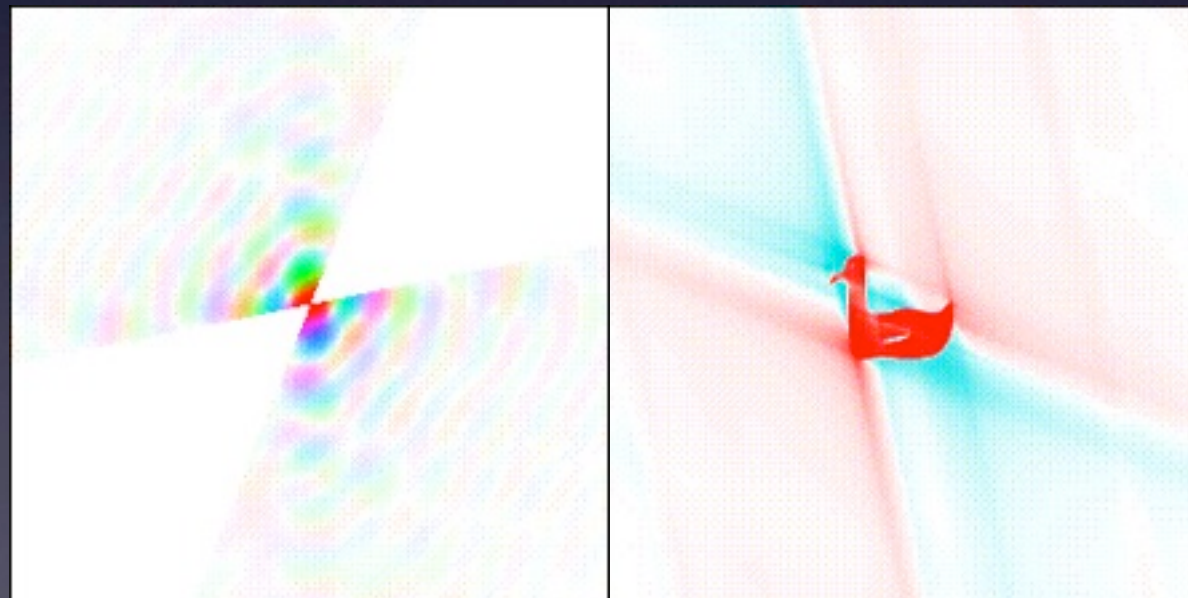
The importance of data completeness



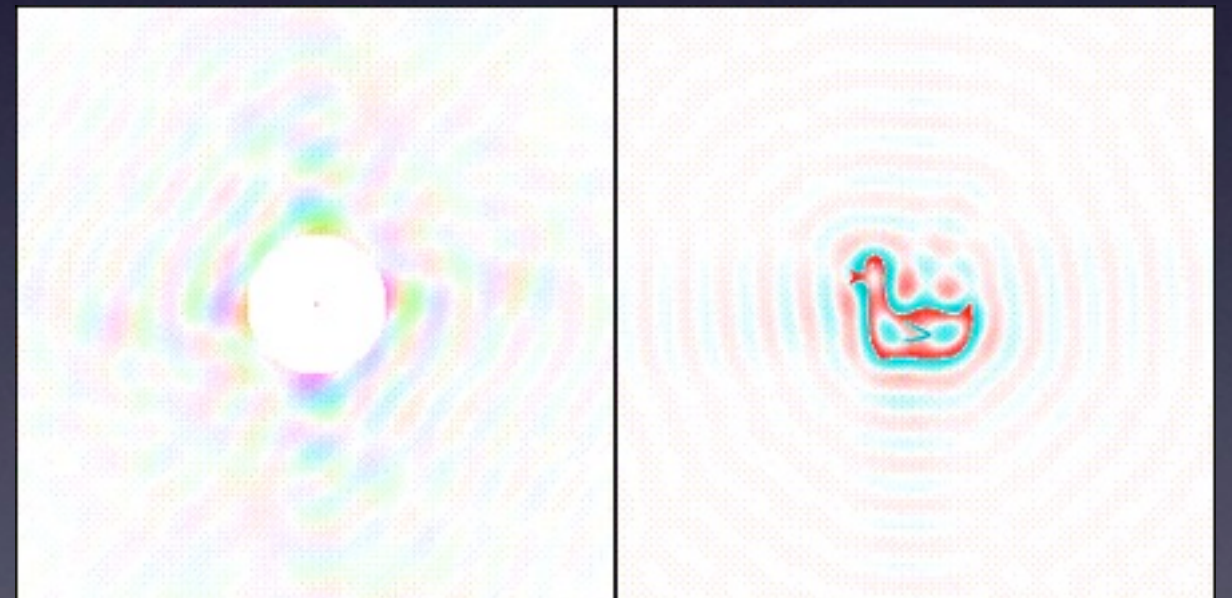
A duckand its Fourier transform



A low-resolution duck



Incomplete data: missing wedge

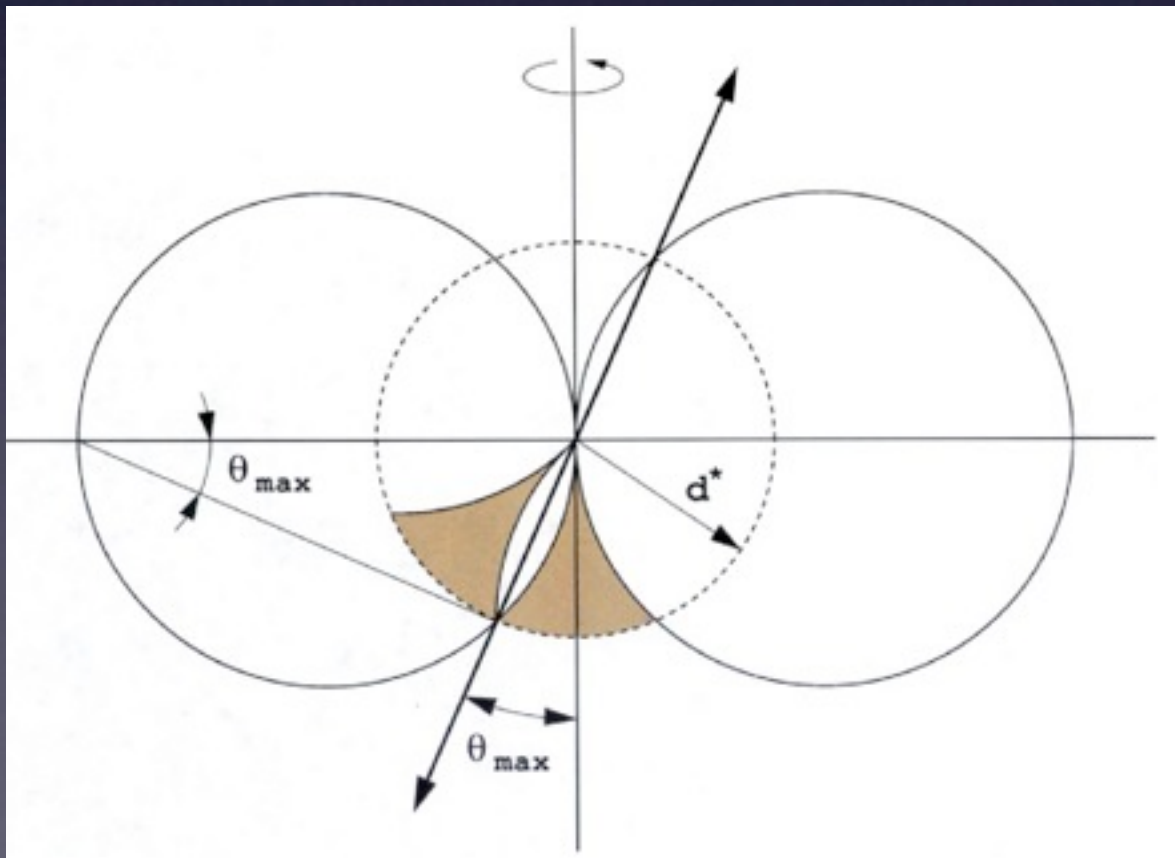
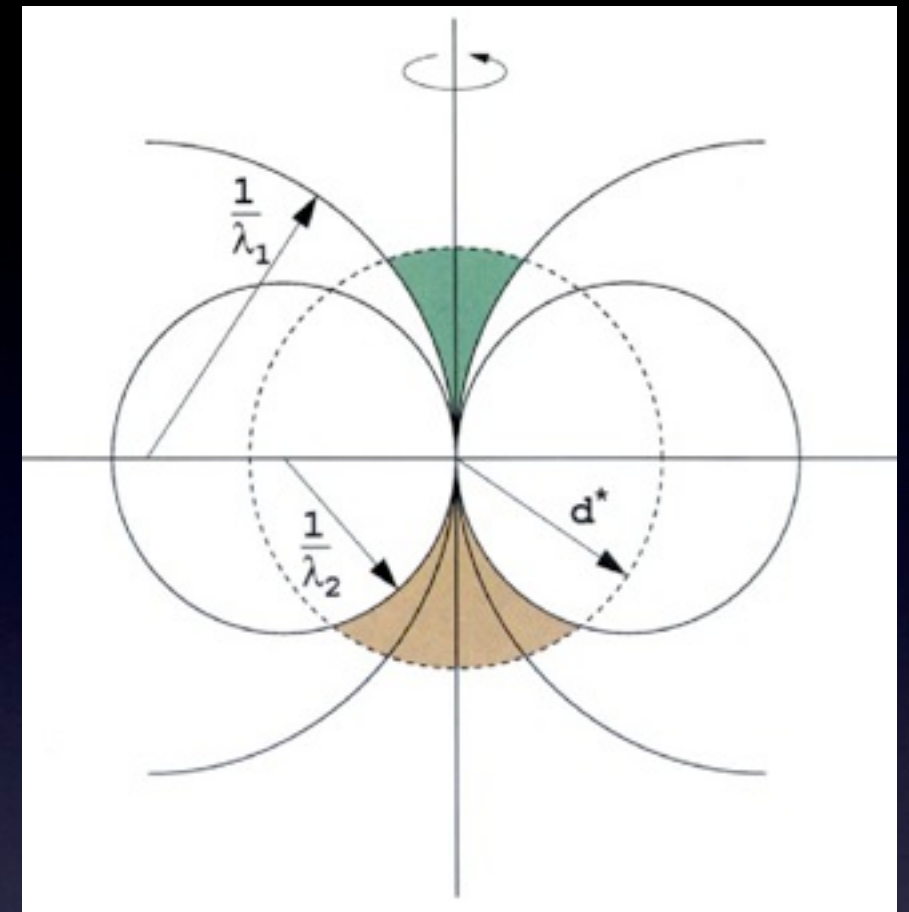


A duck without low-resolution reflections

The blind region

Diffraction vectors close to the rotation axis will never pass through the sphere, even in a 360° rotation

The blind region is smaller for short wavelengths, as the Ewald sphere is flatter

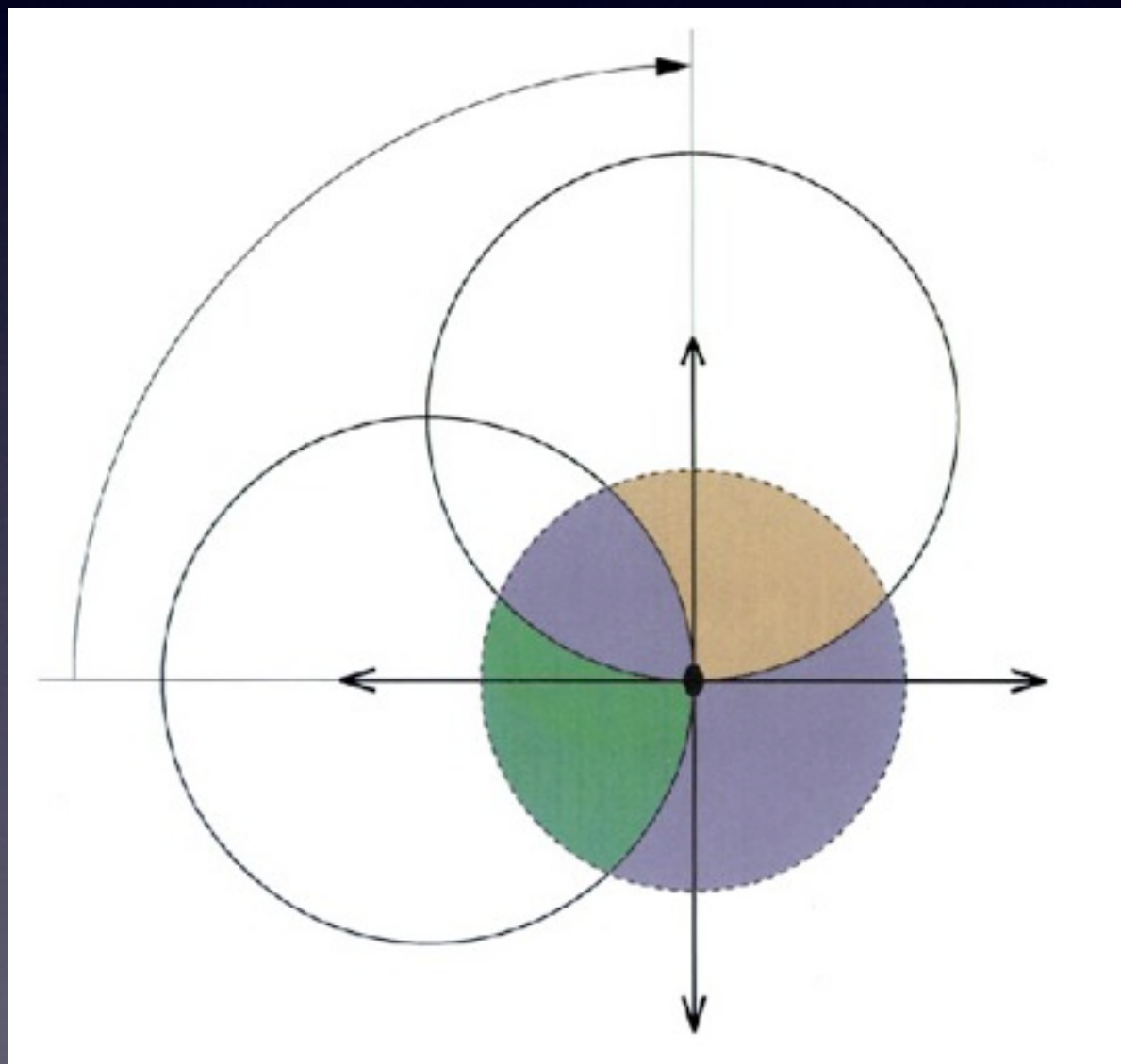


The blind region may be filled in by collecting a second set of data, offsetting the crystal by at least $\theta_{\max}$ or by symmetry (except in PI)

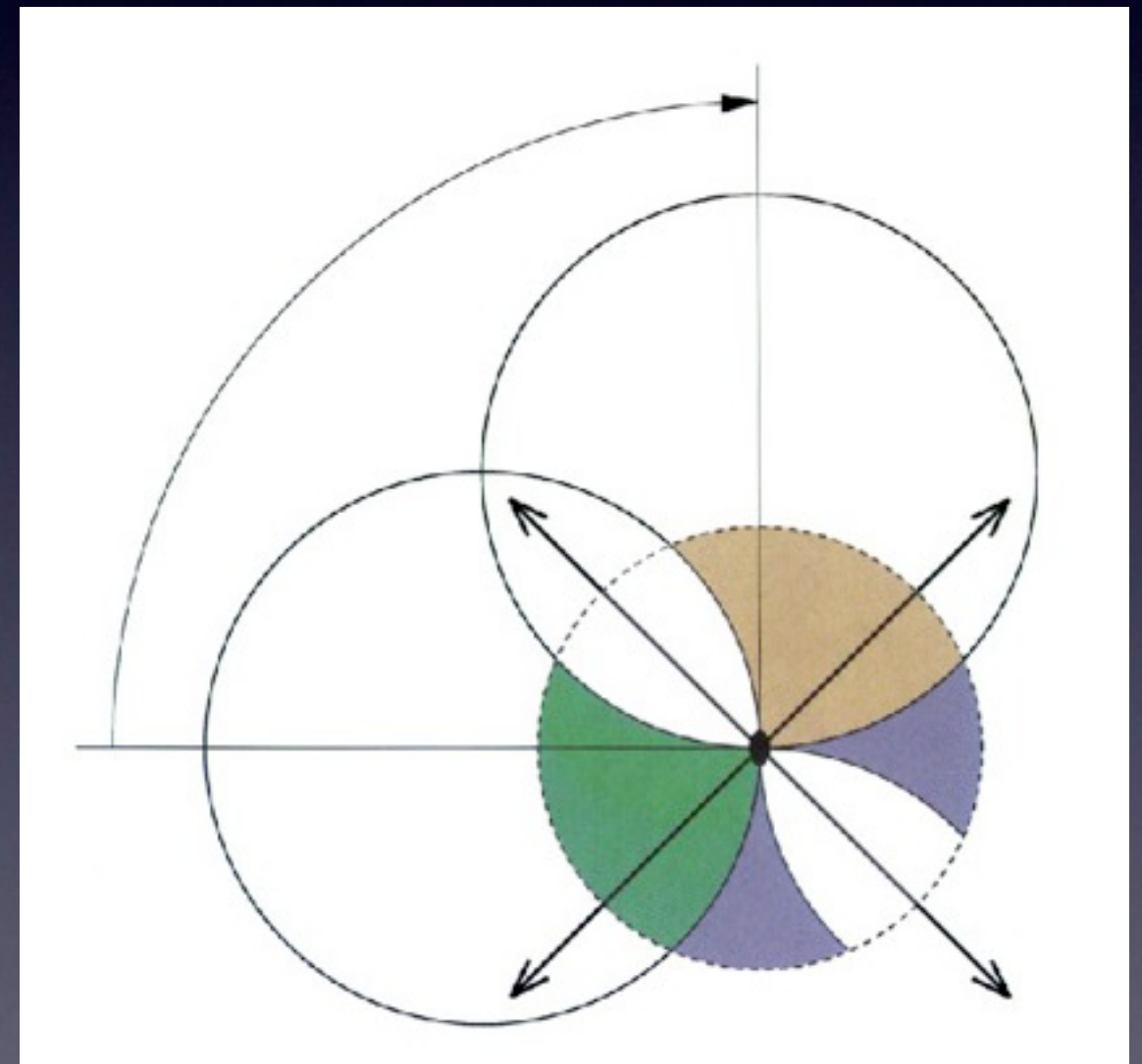
If there is symmetry, offsetting from an axis can remove or reduce the blind region for a single setting

Symmetry and total rotation range: an orthorhombic example

Rotation of an orthorhombic crystal by 90° starting from an axis gives a complete dataset (except for the blind region)



A 90° rotation starting at a diagonal collects the same 45° twice, and gives incomplete data



How to collect good data

Crystal



Data collection

*Diffraction
geometry
Strategy*

Images



Integration

Indexing

$h\ k\ l\ \quad I\ \quad \sigma(I)$



Scaling & merging (data reduction)

*Space group determination
Quality assessment*

$h\ k\ l\ \quad F\ \quad \sigma(F)$

Decisions

- **Select crystal**

Collect a few images to judge quality

Is this your best crystal? Mosaicity, resolution, size, ice

- **Decide strategy and collect all images**

Total rotation, rotation/image, exposure time, position of detector.

Programs: MOSFLM

DNA (EDNA), BEST

- **Integration**

- **Index**

choose lattice

- **Refine unit cell**

- **Integrate**

What is the correct lattice?

[Integration parameters: box size, overlap check]

- **Choose Laue group (point group)**

What Laue group, space group?

- **Scale & merge**

How good is the dataset? Any bad bits?

- **Convert I to F**

Is the crystal twinned?

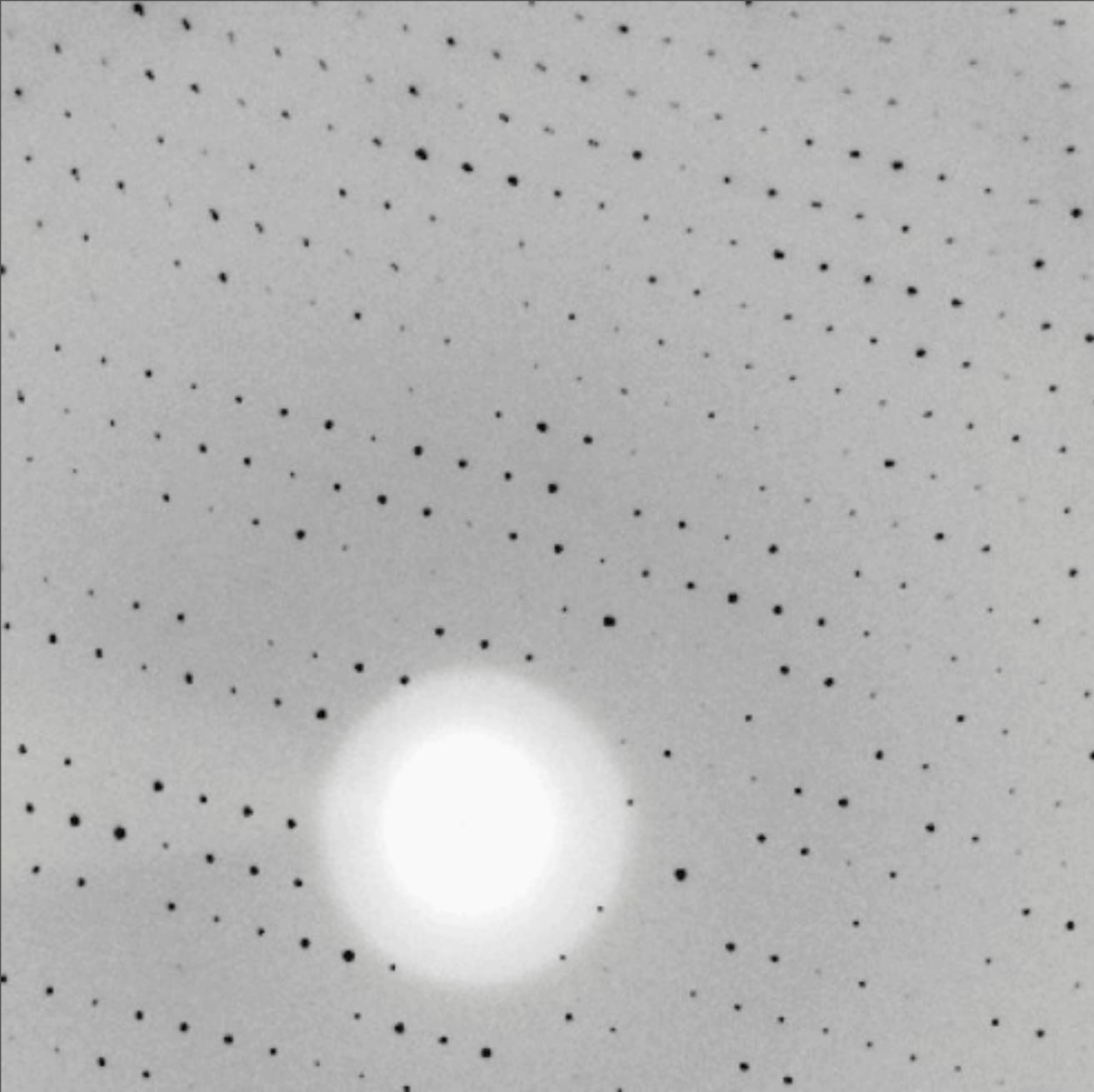
What is a good crystal?

- Single only one lattice
check by indexing pattern and looking for unpredicted spots
- Diffracts to high angle
- Low mosaicity
- Large *the diffracted intensity is proportional to the number of unit cells in the beam: not much gain for a crystal much larger than beam (100–200 μ m). Smaller crystals may freeze better (lower mosaicity)*
- Good freeze *no ice, minimum amount of liquid (low background)*
Optimise cryo procedure, and worry about crystal transfer procedures
- The best that you have! (the least worst)

Beware of pathological cases (twinning etc)

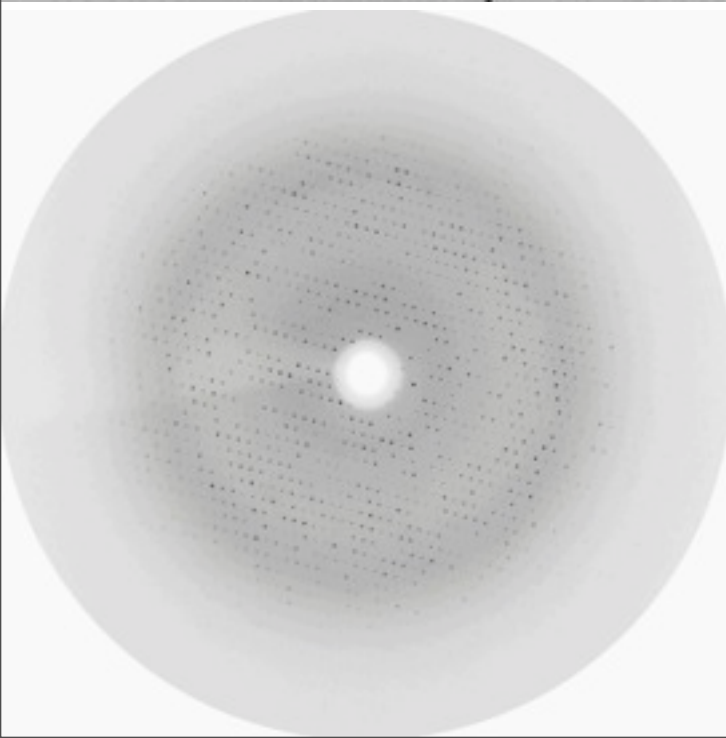
The quality of the crystal determines the quality of the dataset

You can get bad data from a good crystal,
but you can't get good data from a bad crystal

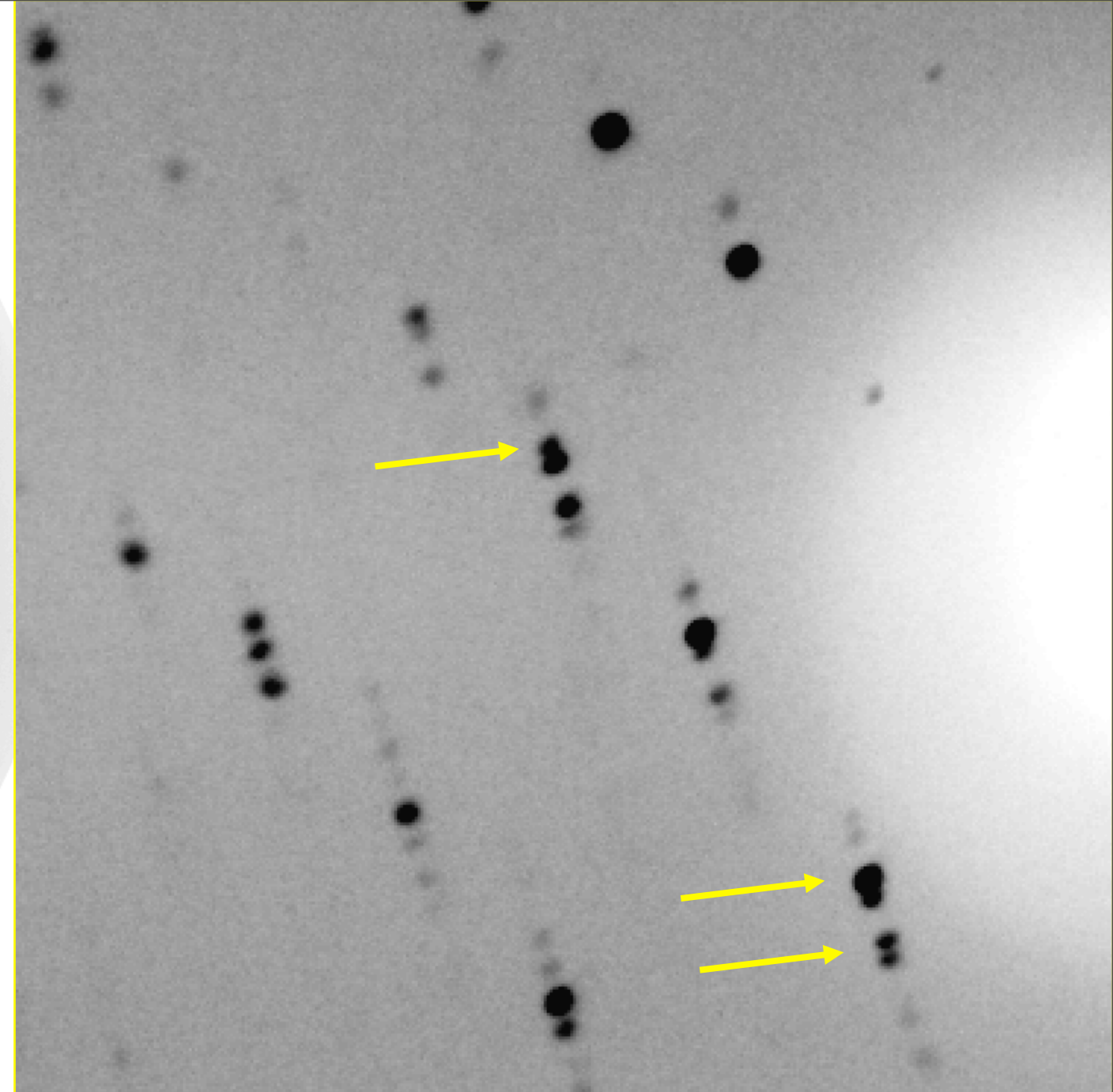
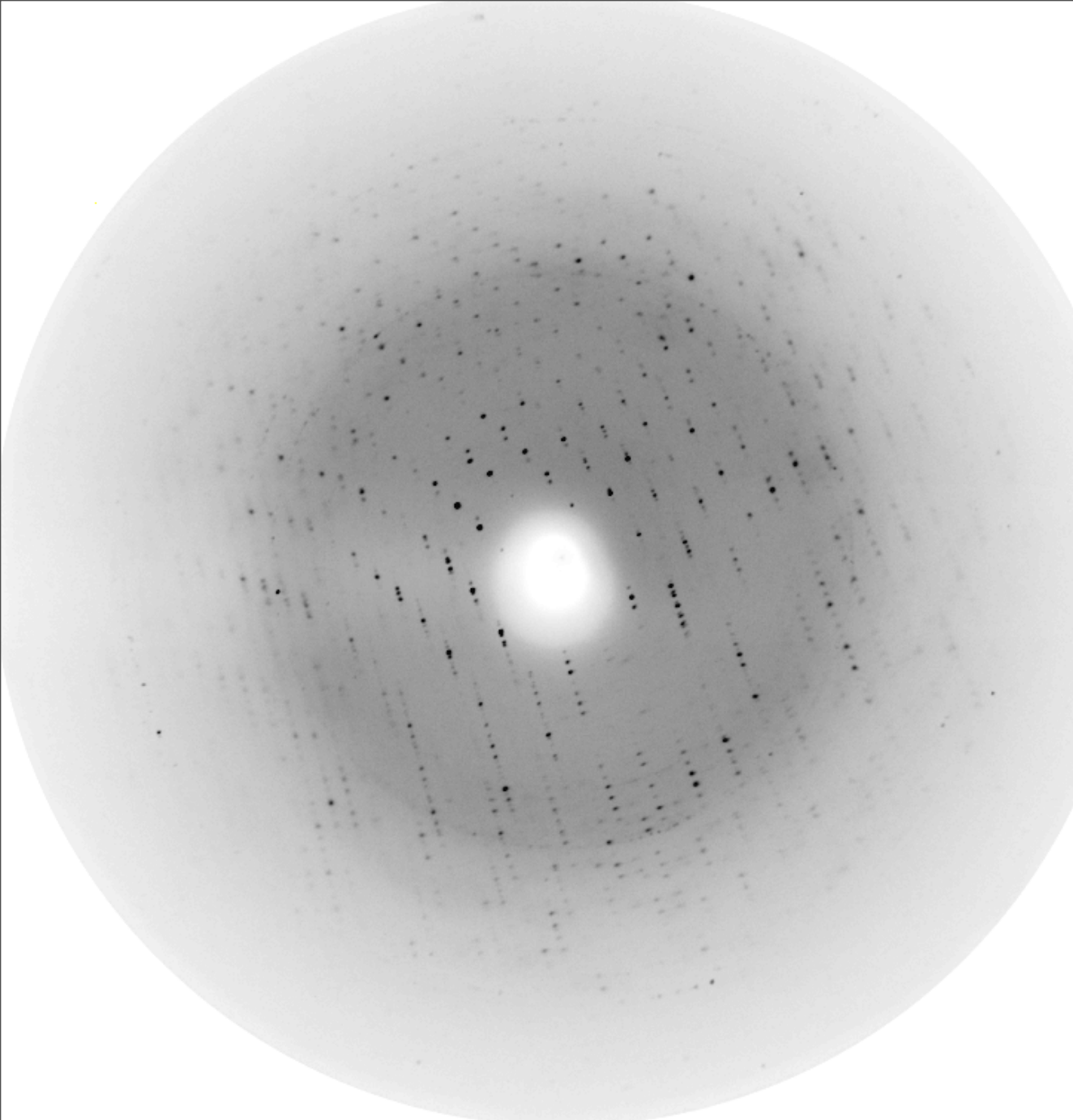


$\Phi = 0^\circ$

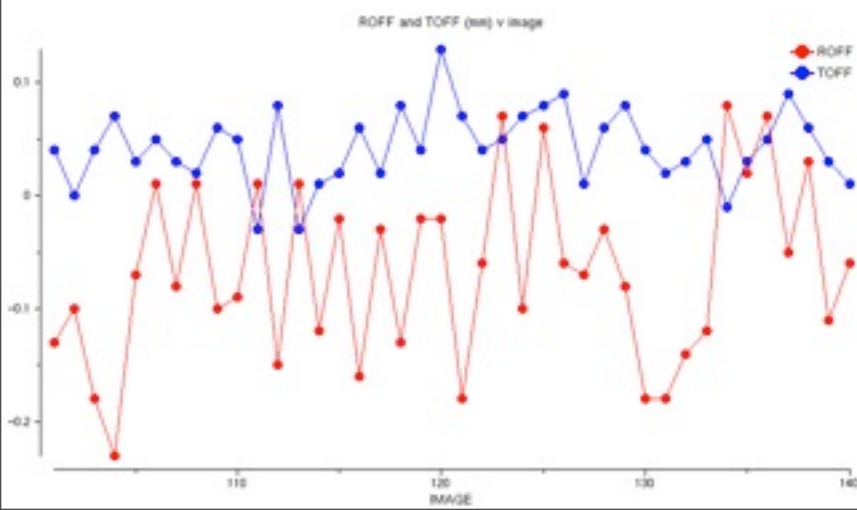
$\Phi = 90^\circ$



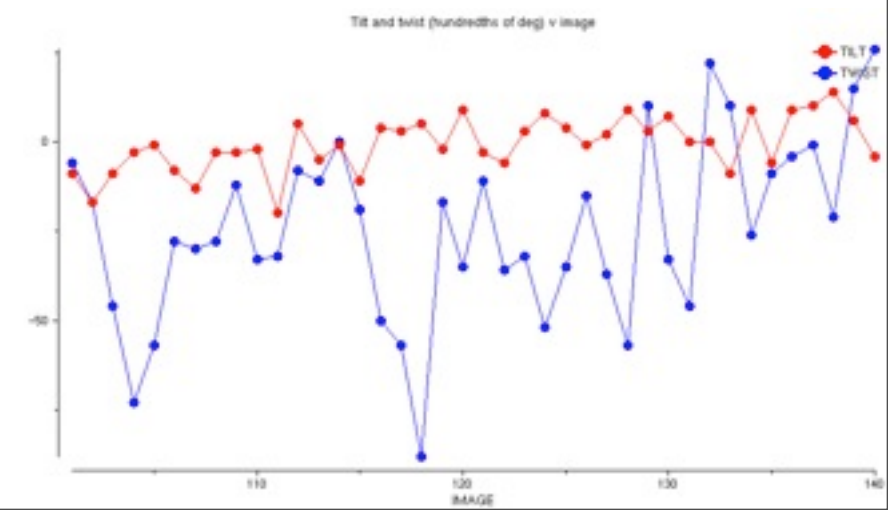
Always check diffraction in two
orthogonal images !

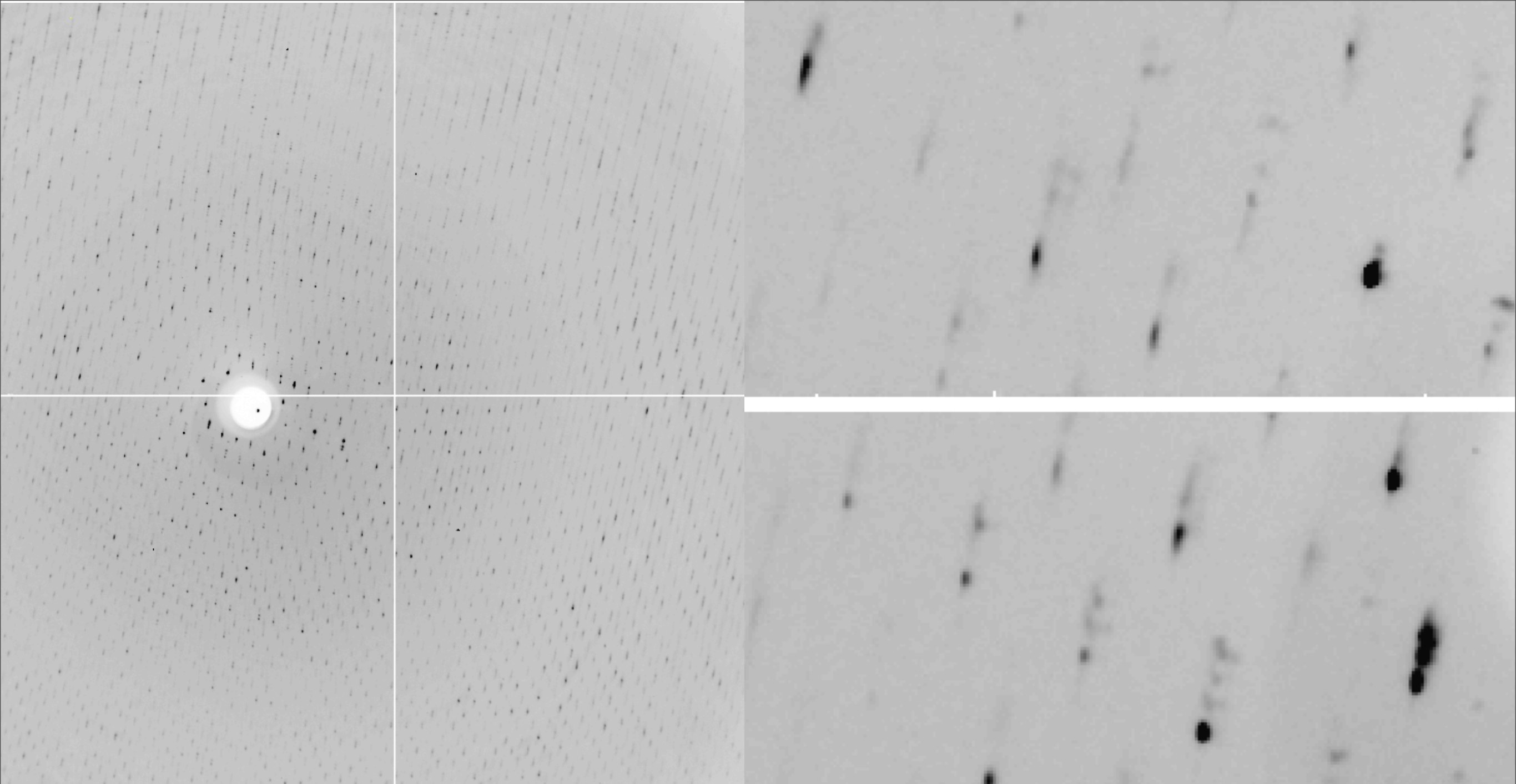


Additional spots present, not resolved.



Results in instability in refinement of detector parameters.





Spots not resolved, very poor spot shape and streaking

Data collection strategy

Compromise between statistics (enough photons/reflection, and multiplicity) and radiation damage. **Radiation damage is the big problem.**

Radiation damage controls the total time available for crystal exposure.

Data collection strategy

Compromise between statistics (enough photons/reflection, and multiplicity) and radiation damage. **On synchrotrons, radiation damage is the big problem.**

Radiation damage controls the total time available for crystal exposure (~1 to 3 minutes on a synchrotron). Radiation damage is worst at an absorption edge.

- Total rotation range

Ideally 180° (or 360° in PI to get full anomalous data)

Use programs (eg Mosflm) to give you the smallest required range (eg 90° for orthorhombic, or 2 x 30°) and the start point.

- Rotation/image: **not necessarily 1°!**

good values are often in range 0.25° - 0.5°, minimize overlap and background

- Time/image depends on total time available

- Detector position: *further away to reduce background and improve spot resolution*

Two Cases:

Anomalous scattering, MAD

High redundancy is better than long exposures (eliminates outliers)

Split time between all wavelengths, be cautious about radiation damage, reduce time & thus resolution if necessary

Collect Bijvoet pairs close(ish) together in time: align along dyad or collect inverse-beam images

Recollect first part of data at end to assess radiation damage

Data for refinement

Maximise resolution: longer exposure time (but still beware of radiation damage)

High multiplicity less important, but still useful

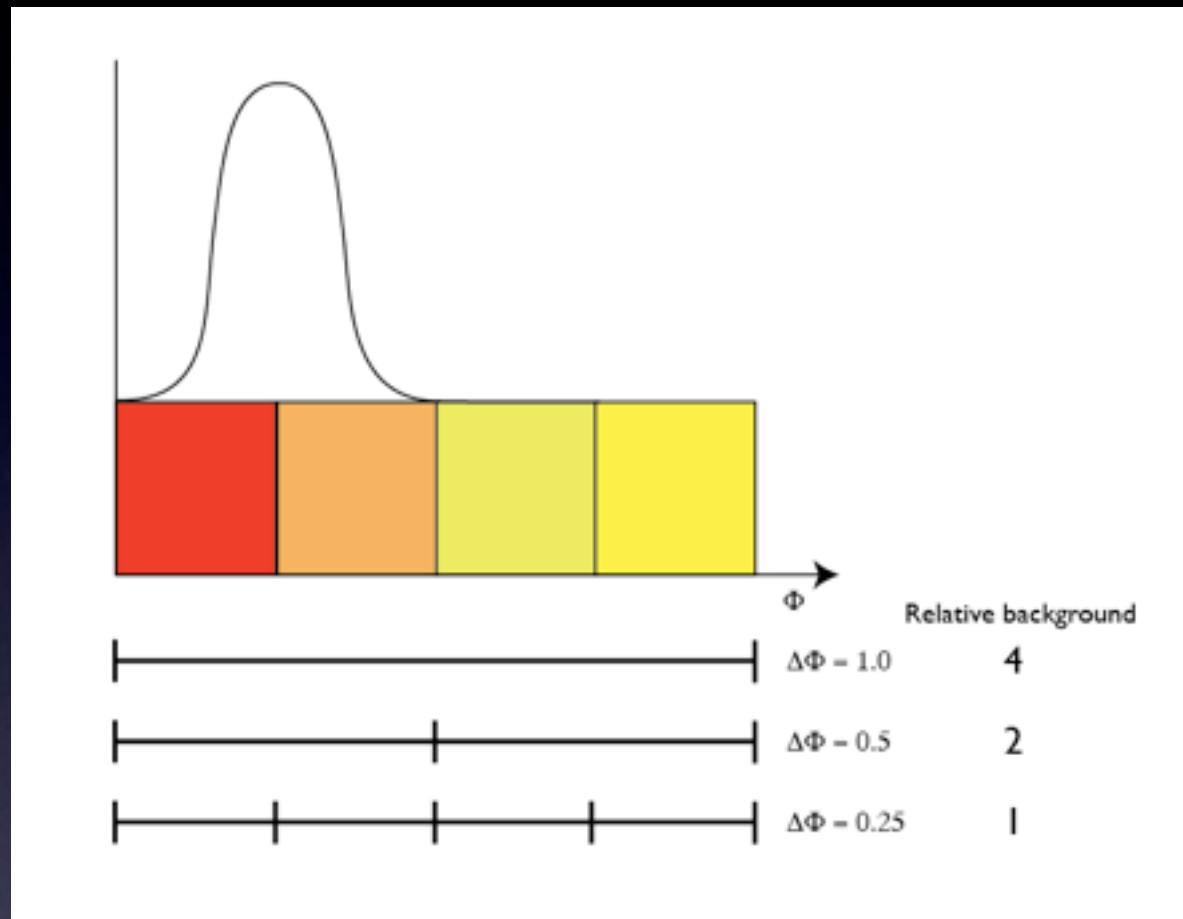
Use two (or more) passes with different exposure times (ratio ~ 10) if necessary to extend range of intensities (high & low resolution)

Short wavelength ($< 1 \text{ \AA}$) to minimise absorption

Collect symmetry mates at different times and in different geometries, to get best average (even with higher R_{merge} !). Rotate about different axes.

Advantages of fine phi slicing

Using an oscillation angle smaller than the reflection width (in phi) will improve signal to noise for weak reflections by minimising the background:



$$I_{\text{spot}} = I_{\text{tot}} - I_{\text{bck}}$$

$$\text{var}(I_{\text{spot}}) = \text{var}(I_{\text{tot}}) + \text{var}(I_{\text{bck}})$$

$$= I_{\text{tot}} + I_{\text{bck}}$$

$$I/\sigma(I) = (I_{\text{tot}} - I_{\text{bck}})/(I_{\text{tot}} + I_{\text{bck}})^{1/2}$$

For weak reflections, the background will dominate $I/\sigma(I)$.

Fine phi slicing *should* give better data but:

- 1) Assumes no errors in shutter synchronisation
this is demanding for very short (<0.5 sec) exposures although fast detectors now allow shutterless collection
- 2) There will be detector readout noise in each image
- 3) There is not much advantage in slice widths less than $\sim 1/4$ reflection width

(see J. Pflugrath, *Acta Cryst D55*, 1718-1725, 1999)

Summary of strategy choices

Detector position

- Place detector far enough away to resolve spots (or reduce beam size)
- Use the whole detector area (don't have blank region around edge)
- Don't use an offset detector unless desperate for spot resolution. If you have to offset the detector, be **very careful** in strategy planning

Total rotation range

- If possible, collect 180° (360° in PI with anomalous). High redundancy is *Good*, provided that radiation damage is not serious
- When rotating around (or close to) a symmetry axis of order n , the minimum rotation is about $180^\circ/n$ for 2- & 4-folds, $360^\circ/n$ for 3- & 6-folds (more complicated in dihedral or cubic symmetry)
- With an offset detector, a larger rotation range is needed, as only one surface of the Ewald sphere is active rather than two

Crystal orientation and rotation start point

- To remove the blind region, avoid rotating exactly around a symmetry axis
- To optimise anomalous differences with respect to absorption, rotate exactly around a symmetry axis (even-fold only)
- Use a strategy program (eg MOSFLM) to determine range and start point
- Collect 180° or 360° and start anywhere

Exposure time/image

- Compromise between high resolution (good) and radiation damage (bad)
- Process & assess first data collection, then revise strategy
- Use estimates from eg EDNA/BEST

Image rotation range (slicing)

- Use a strategy program to determine optimum width
- Set width $< (\text{maximum resolution})/(\text{longest axis not along spindle}) - \text{spotwidth}$
- Process data & check for overlaps
- Fine-slicing is more sensitive to errors in synchronisation of shutter opening and rotation (this potentially adds an error for each image)

Integration of diffraction images

Integration

Images $\rightarrow$ hkl I $\sigma(I)$

Two distinct methods:

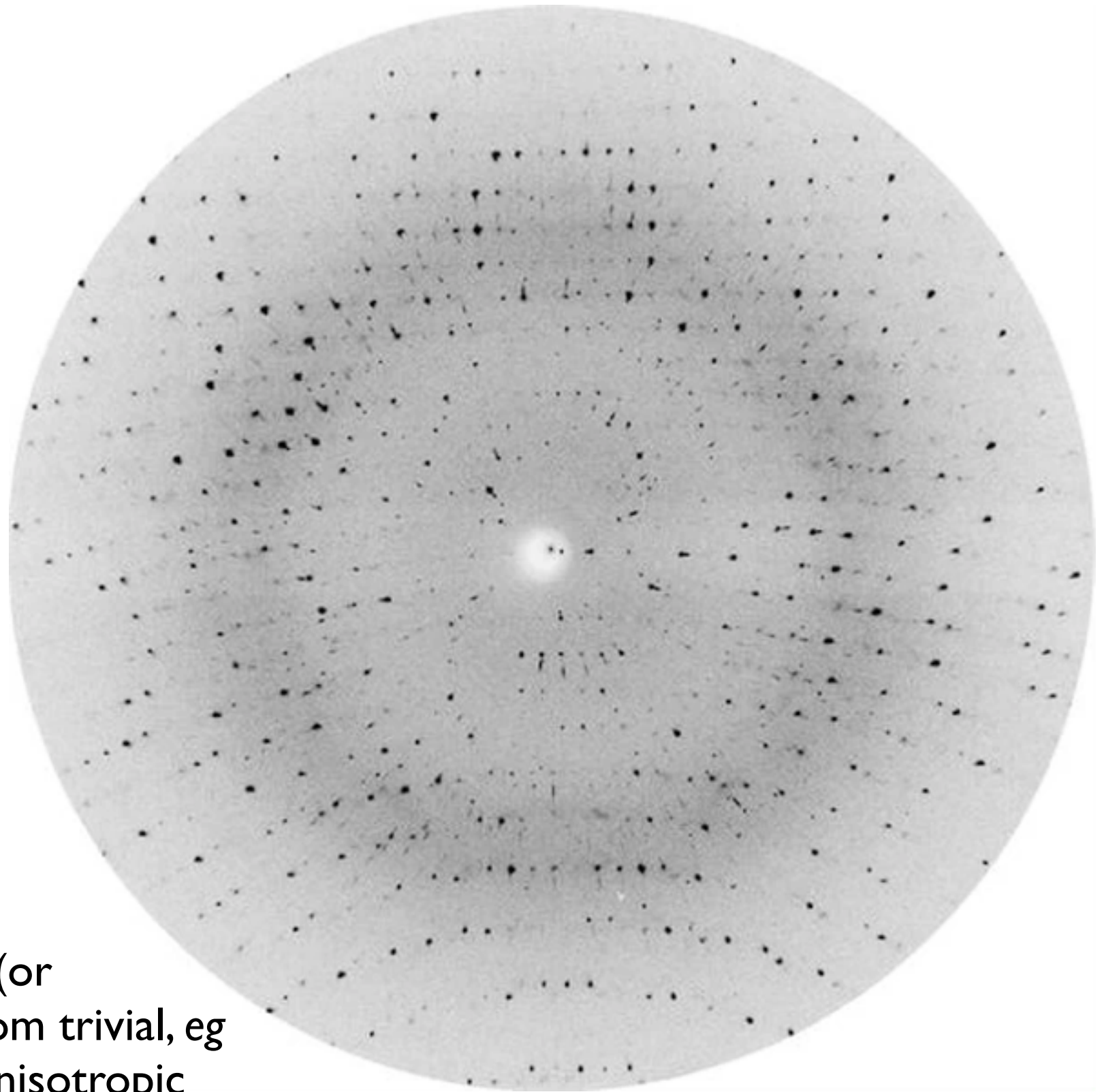
- 2-D: integrate spots on each image, add together partially recorded observations in the scaling program. MOSFLM, DENZO, HKL2000, etc
- 3-D: integrate 3-dimensional box around each spot, from a series of images. XDS, D*TREK, SAINT etc

For today: MOSFLM

Starting Point: A series of diffraction images, each recorded on a 2D area detector while rotating the crystal through a small angle (typically 0.2 - 1.0° per image) about a fixed axis (the Rotation/Oscillation Method).

Outcome: A dataset consisting of the indices (h,k,l) of all reflections recorded on the images with an estimate of their intensities and the standard uncertainties of the intensities: $h, k, l, I(hkl), \sigma(I)$

Note that a series of images samples the full 3-dimensional reciprocal space, Bragg diffraction and any other phenomena, all scattering from crystal and its environment.



In practice, defects in the crystals (or detectors) make integration far from trivial, eg weak diffraction, crystal splitting, anisotropic diffraction, diffuse scattering, ice rings/spots, high mosaicity, unresolved spots, overloaded spots, zingers/cosmic rays, etc, etc.

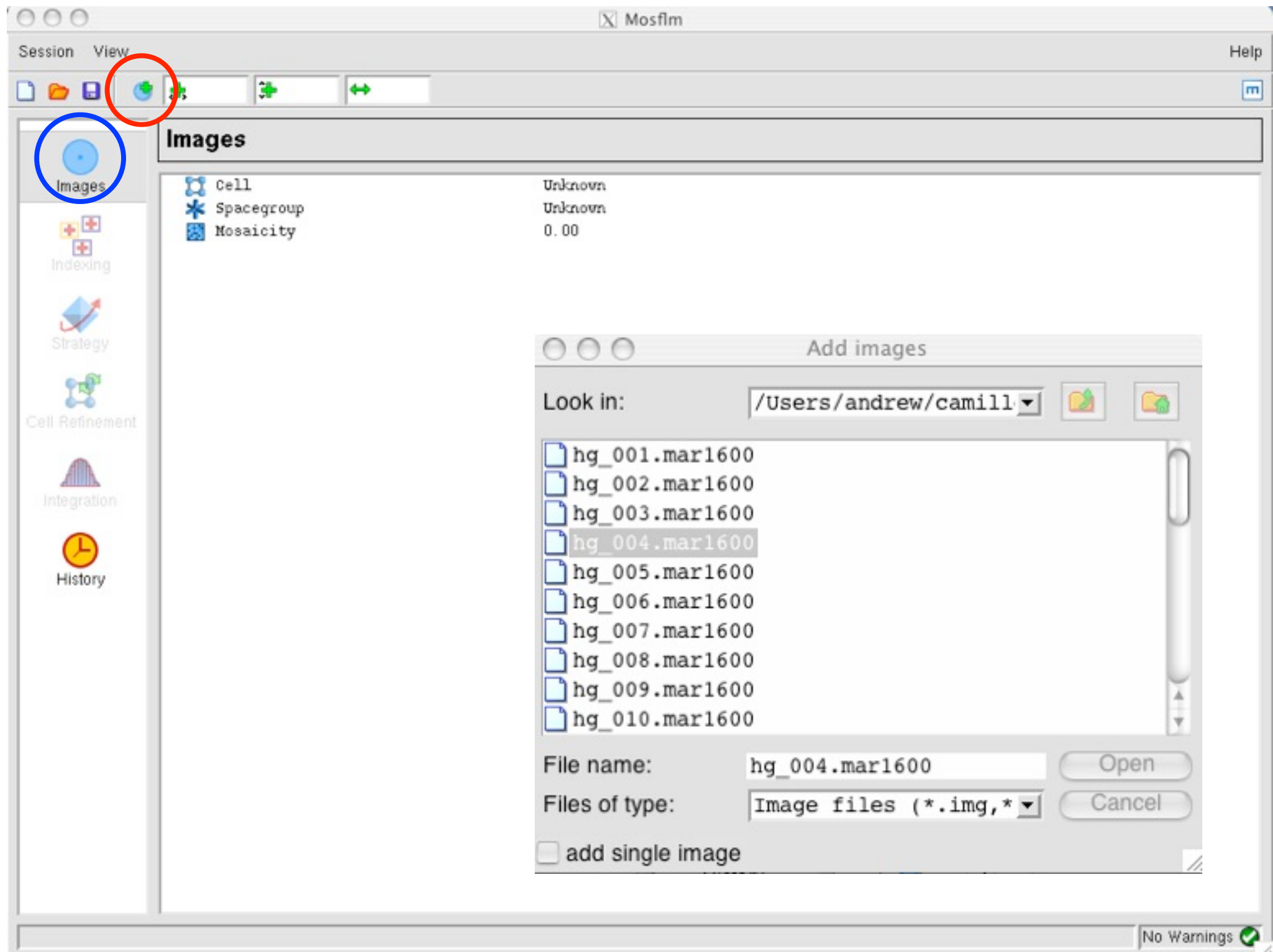
Integration

We want to calculate the intensity of each spot: then working backwards –

- The simplest method is draw a box around each spot, add up all the numbers inside, & subtract the background (or better, fit profile)
- To do this, we must know **where** the spot is: this needs
 - the unit cell of the crystal
 - the orientation of the crystal relative to the camera
 - the exact position of the detector
- To find the unit cell and crystal orientation, we must index the diffraction pattern
 - this can be done by finding spots on one or more images

Tools: the new iMosflm interface

Images window: select & load images (all images with a common template)



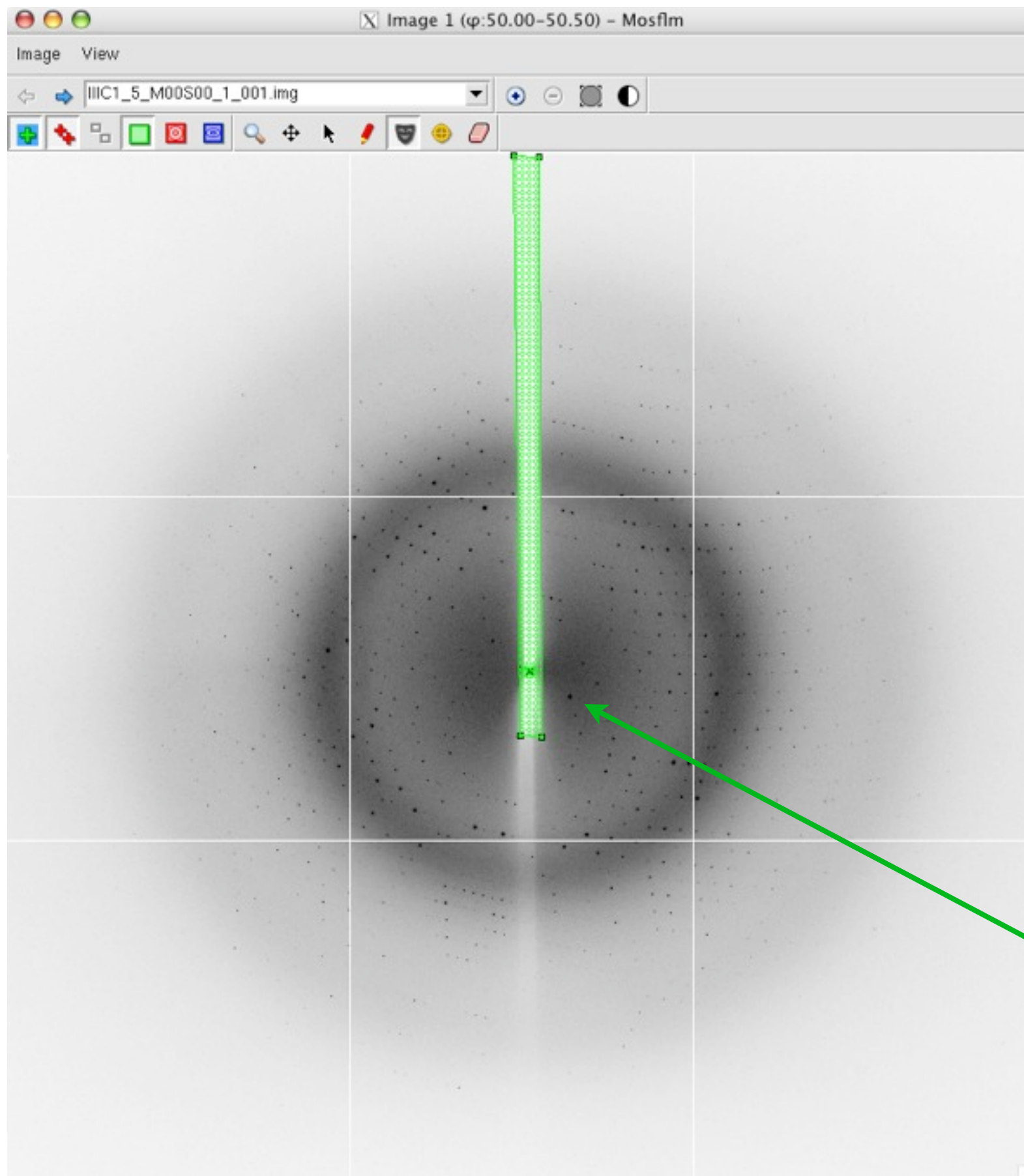


Image Display

Simple control over:

Found spots

Predicted pattern

Direct beam position

Resolution limits

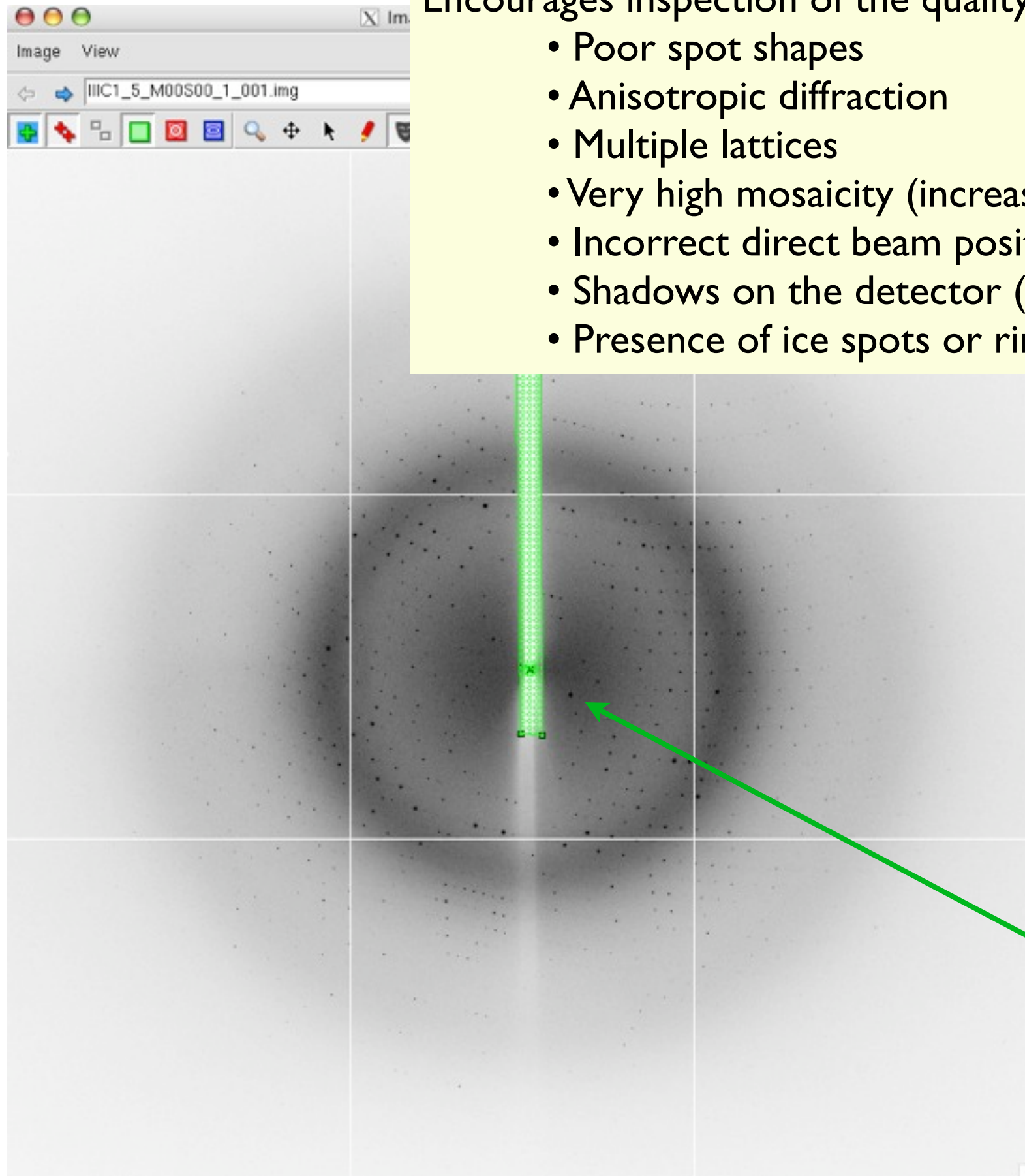
Masking function

Panning and Zooming

Note manually drawn
mask for beam-stop
shadow

Encourages inspection of the quality of the images (always a good thing) !

- Poor spot shapes
- Anisotropic diffraction
- Multiple lattices
- Very high mosaicity (increase threshold in indexing)
- Incorrect direct beam position (move it, try direct beam search)
- Shadows on the detector (mask them)
- Presence of ice spots or rings (exclude the resolution shells)



Note manually drawn
mask for beam-stop
shadow

Integration procedure in iMosflm

1. Find spots

what is a spot? should have uniform shape, not streak

2. Index

find *lattice* which fits spots

3. Estimate mosaicity

improve estimate later

4. Check prediction, on images remote in φ (90° away)

is the indexing correct?

5. Refine cell

use two wedges at 90°, or more in low symmetry

6. Mask backstop shadow

not (yet) done automatically by program

7. Integrate one (or few) image

to check resolution etc

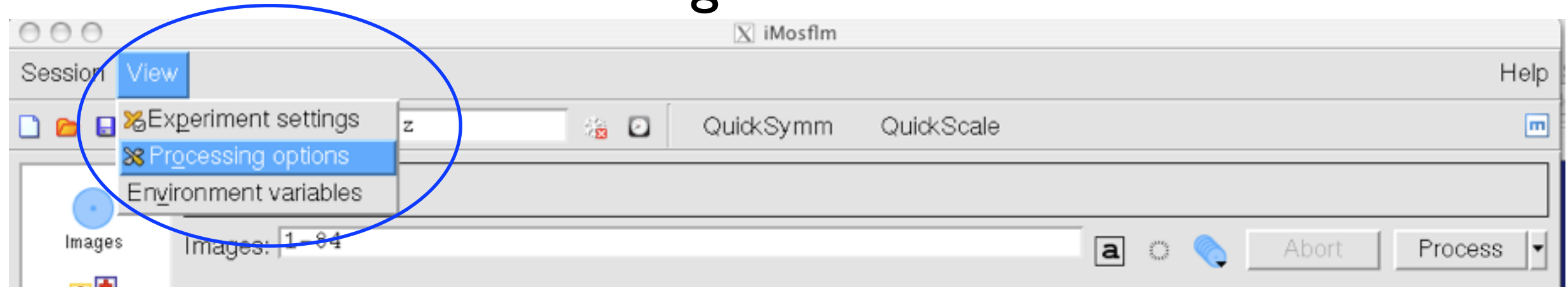
8. Integrate all images

may be run in background for speed

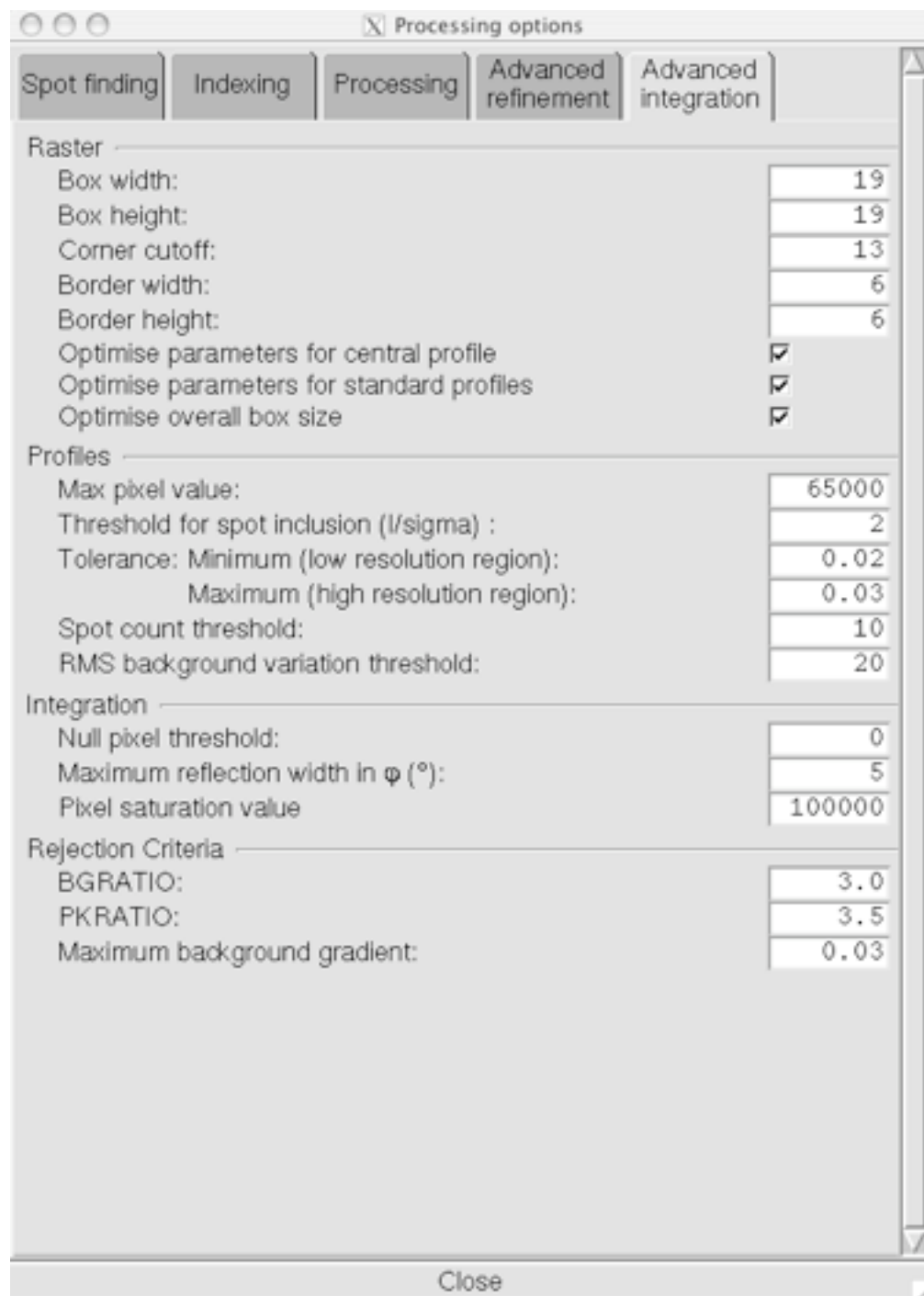
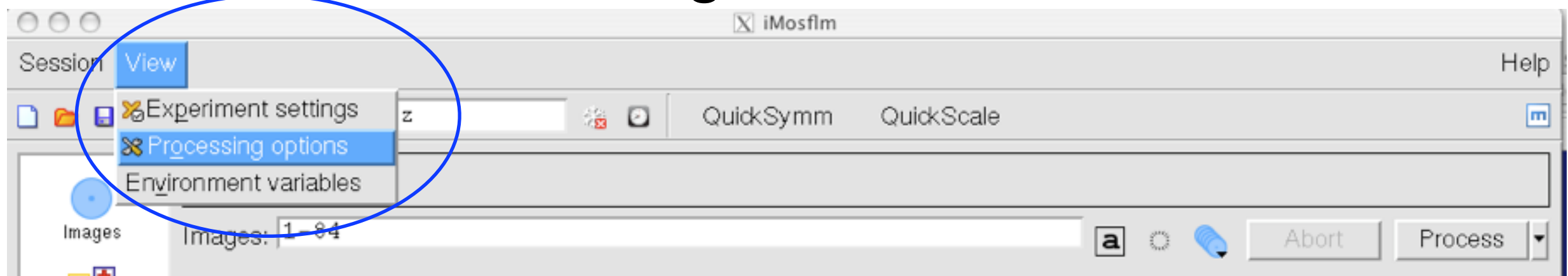


Strategy option, for use before data collection

Setting Parameters



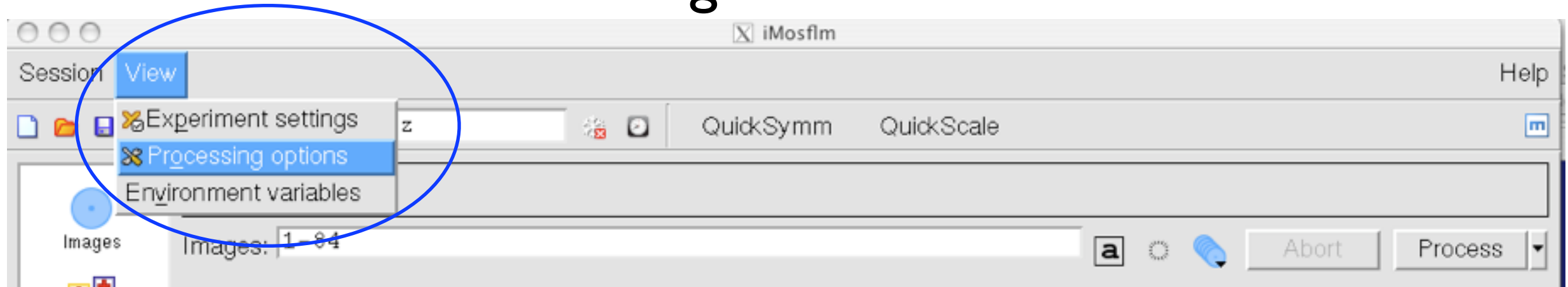
Setting Parameters



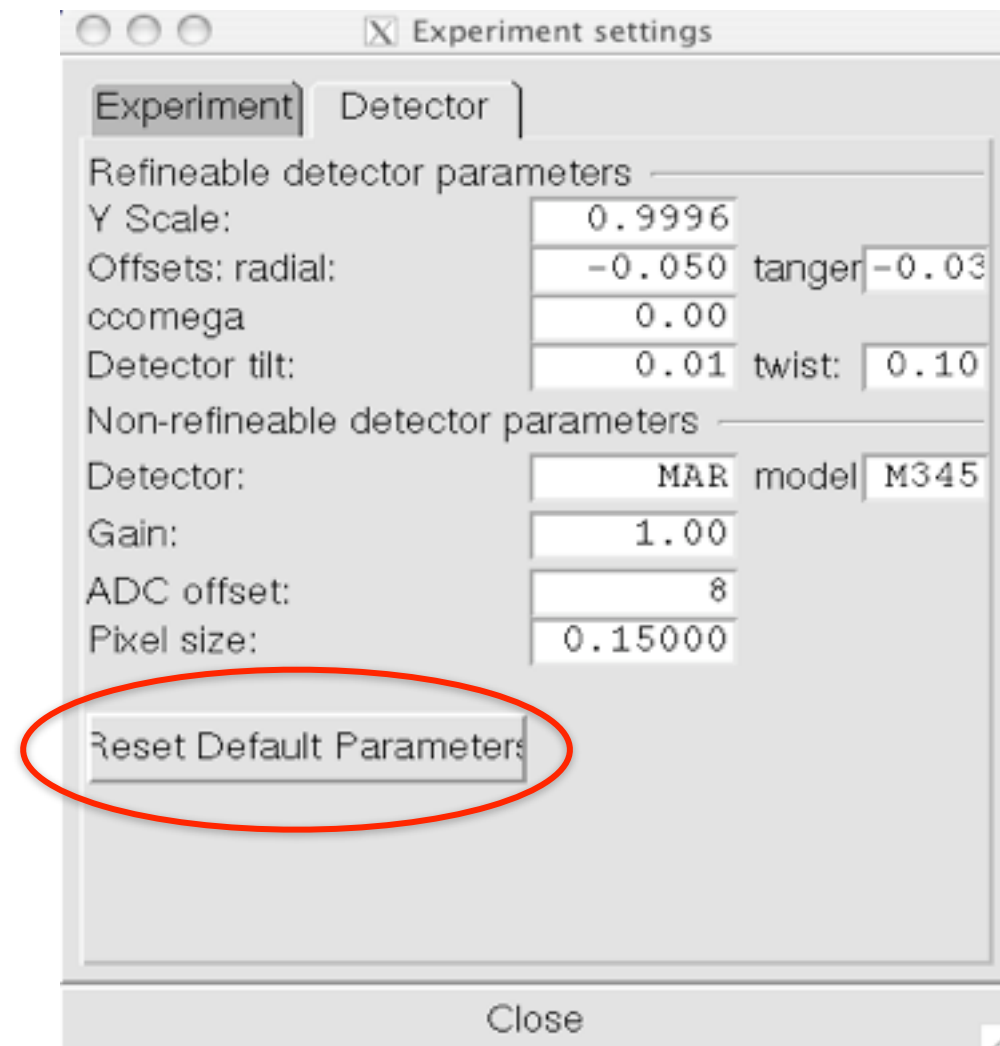
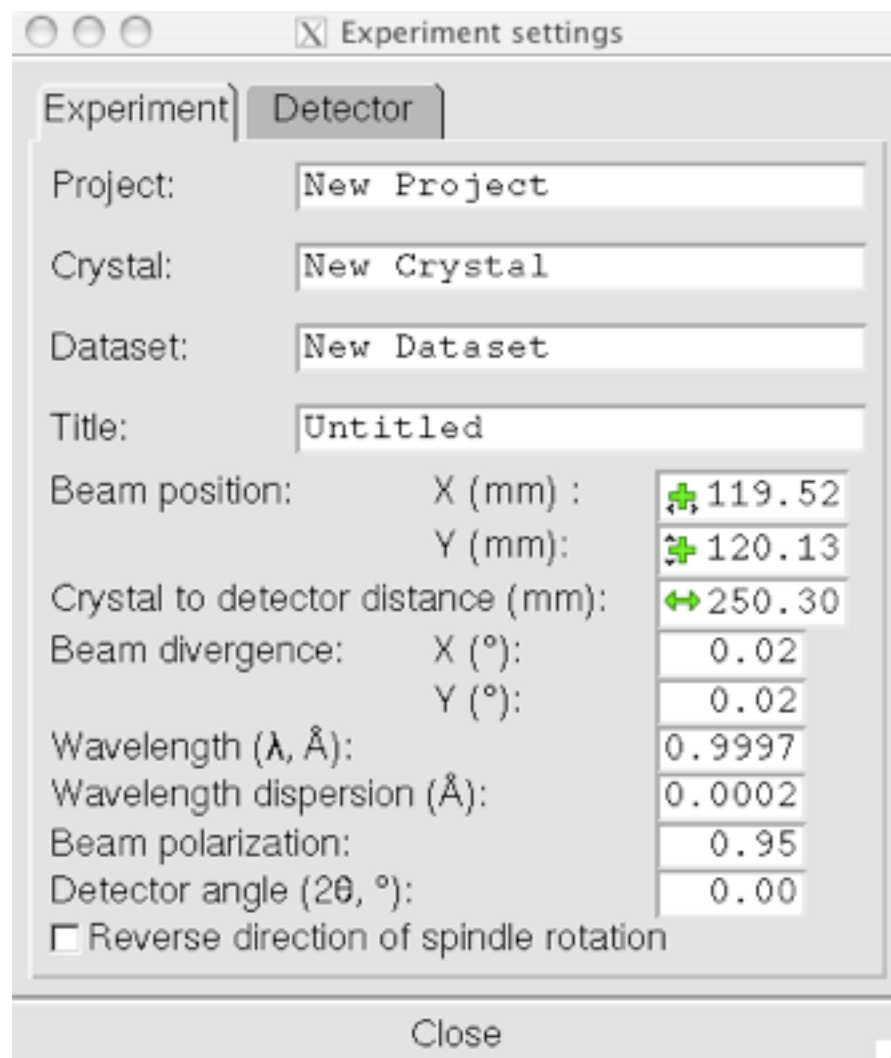
Processing options

Select the appropriate tab, all the settable parameters are listed.

Setting Parameters

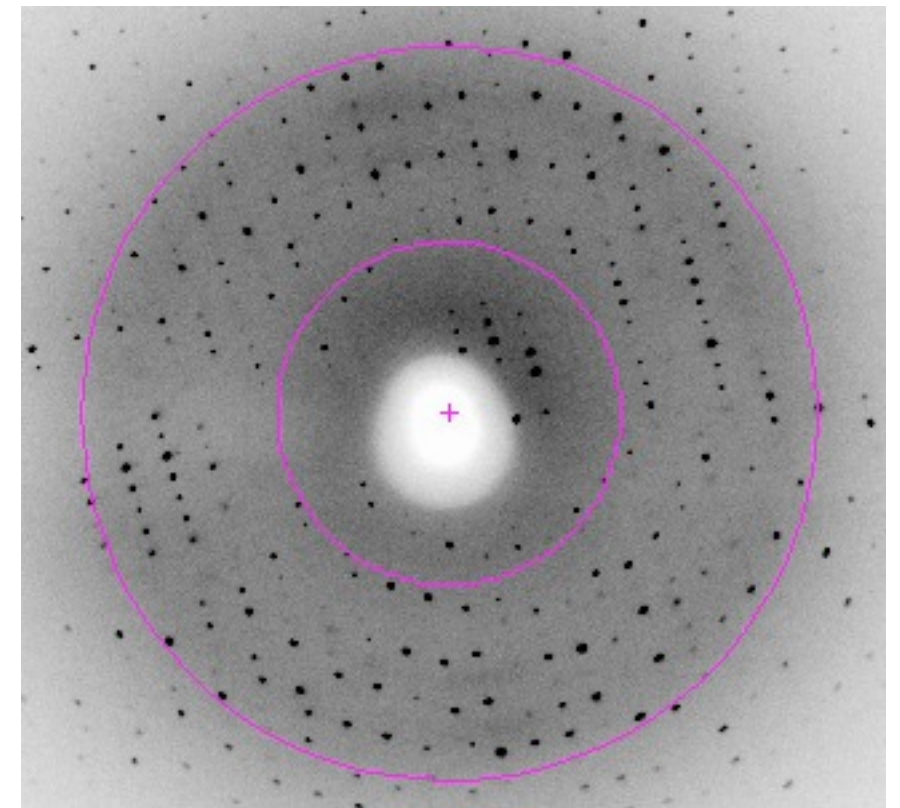
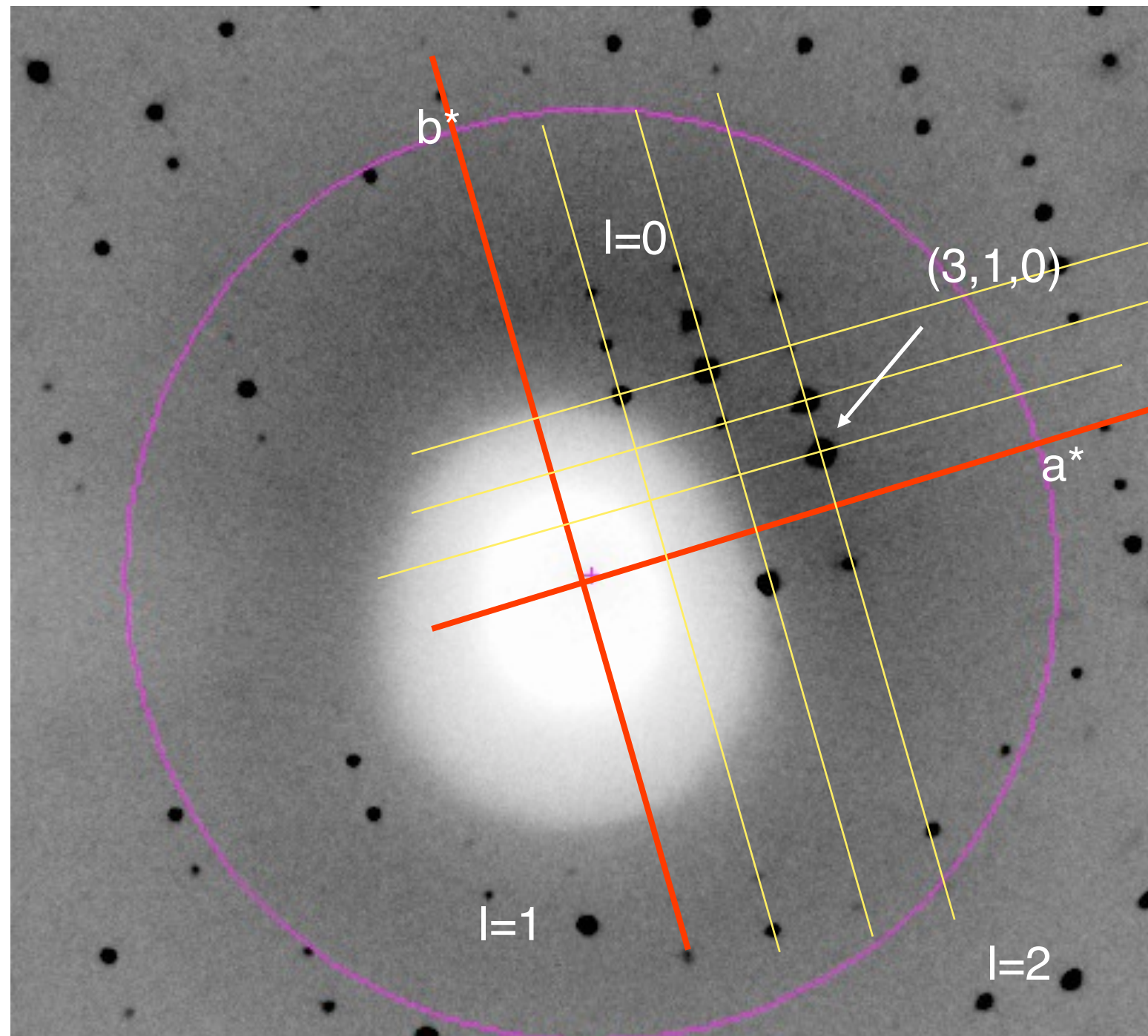


Experiment Settings



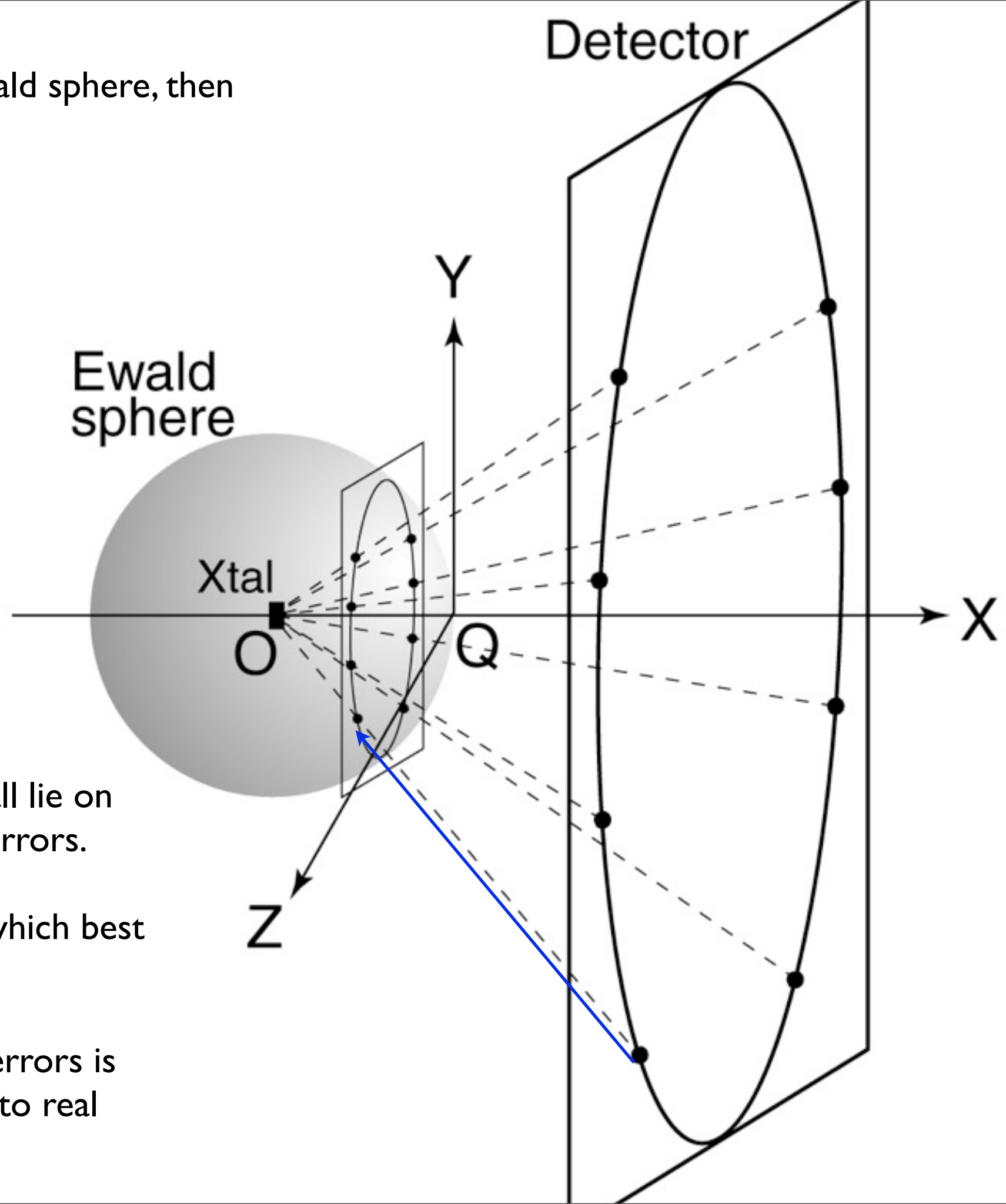
Indexing

If we know the main beam position on the image, we can count spots from the centre



To do it properly, we need to put the spots into 3 dimensions, knowing the rotation of the crystal for this image

Back-project each spot on to Ewald sphere, then rotate back into zero- φ frame



This gives a list of vectors which all lie on the reciprocal lattice, with some errors.

We then want to find a **lattice** which best fits these vectors.

The best way to average out the errors is to use a **Fourier transform** into real space

Autoindexing

Objective: to determine the unit cell, likely symmetry and orientation. (Note that intensities are required to find the true symmetry, see later).

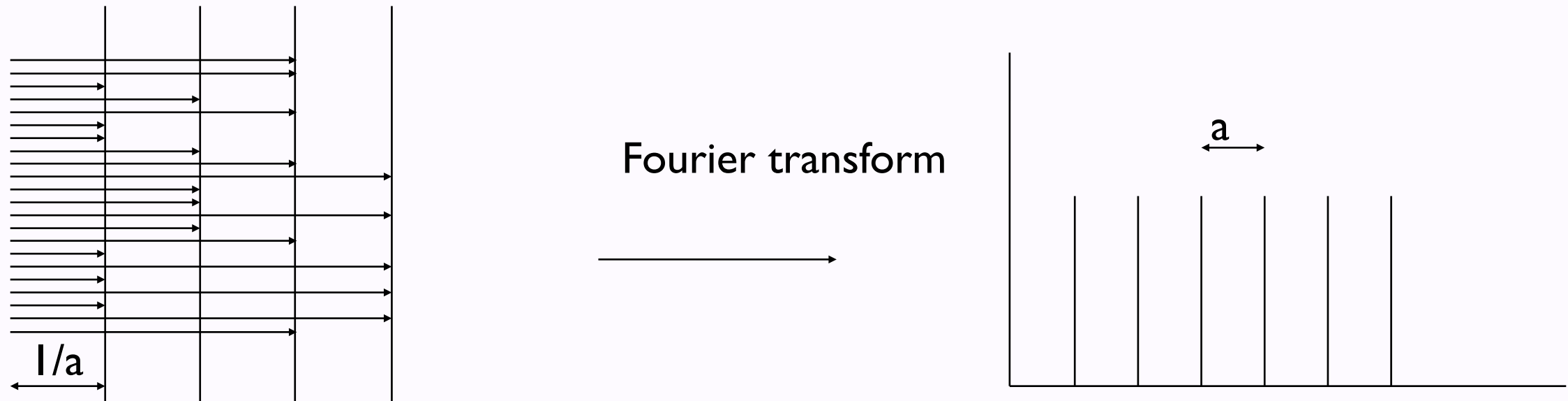
The spot positions in a diffraction image are a distorted projection of the reciprocal lattice. Using the Ewald sphere construction, the observed reflections (X_d, Y_d, Φ) can be mapped back into reciprocal space giving a set of scattering vectors $\mathbf{s}_i$.

$$\mathbf{s} = \begin{pmatrix} D/r - 1 \\ X_d/r \\ Y_d/r \end{pmatrix}$$

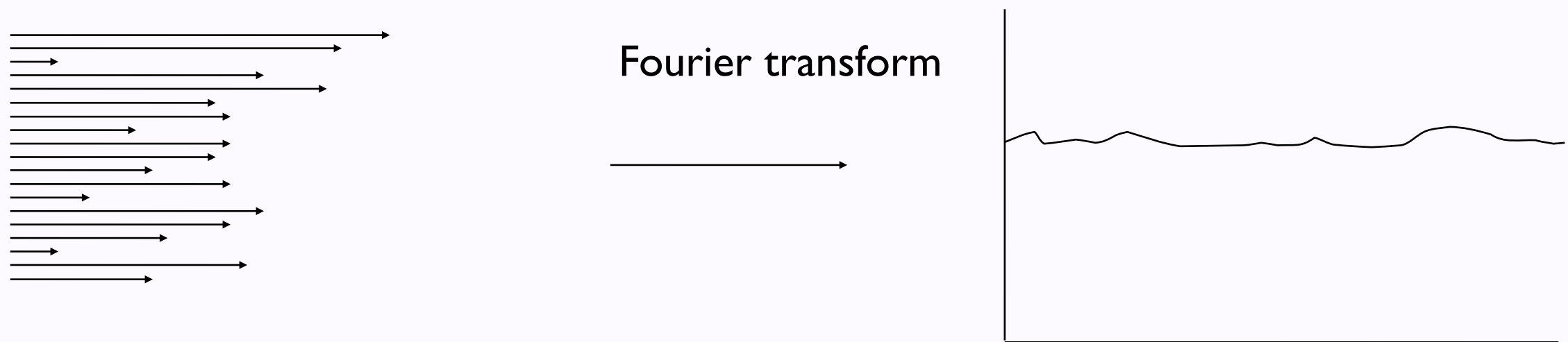
$$r = \sqrt{X_d^2 + Y_d^2 + D^2}$$

D is crystal to detector distance. Uncertainty in Φ leads to errors in $\mathbf{s}$

Consider every possible direction in turn as a possible **real-space** axis, ie perpendicular to a reciprocal lattice plane. Project all observed vectors on to this axis

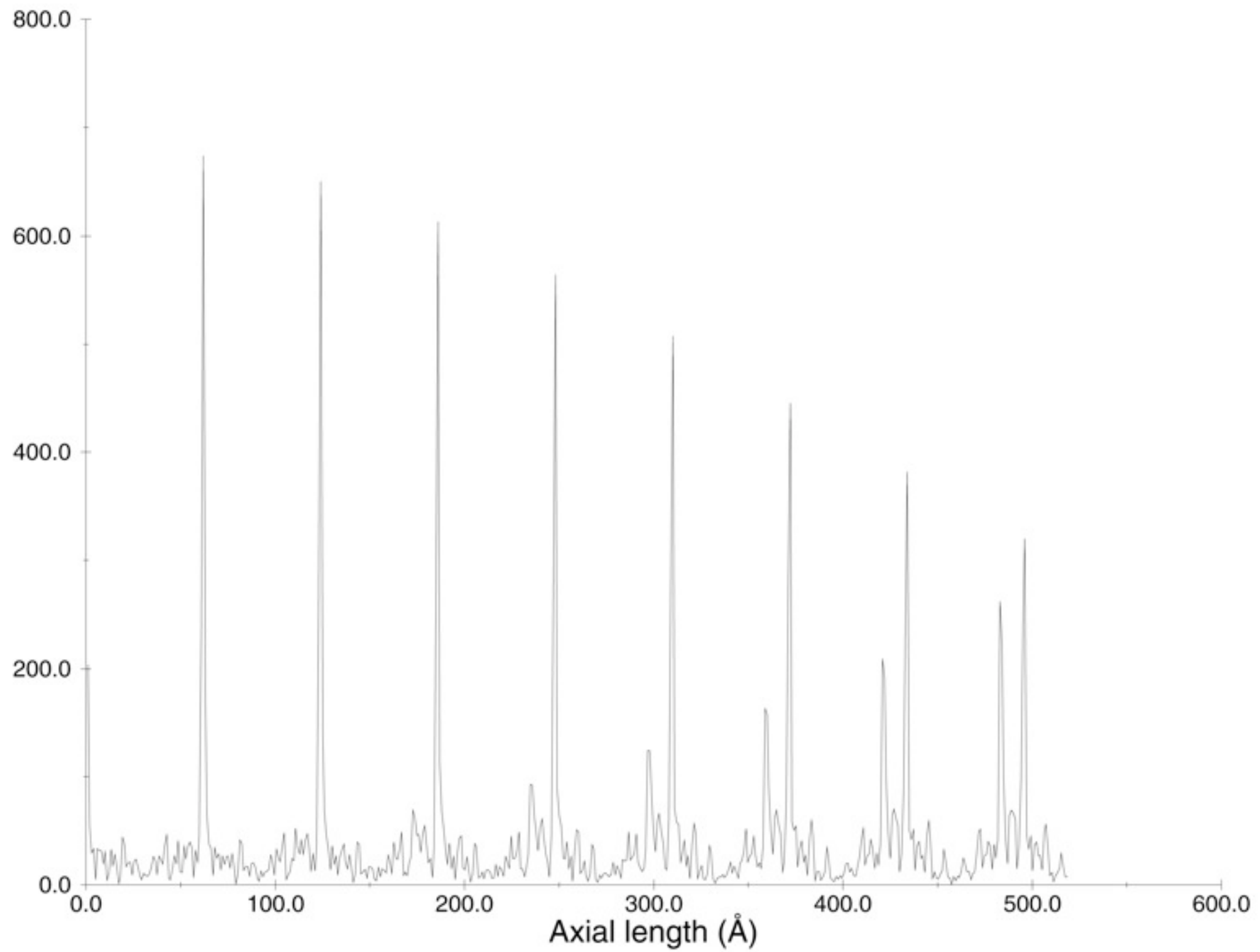


Lattice plane normal to lattice plane: vectors cluster at lengths which are multiples of the lattice spacing. Fourier transform shows sharp peaks



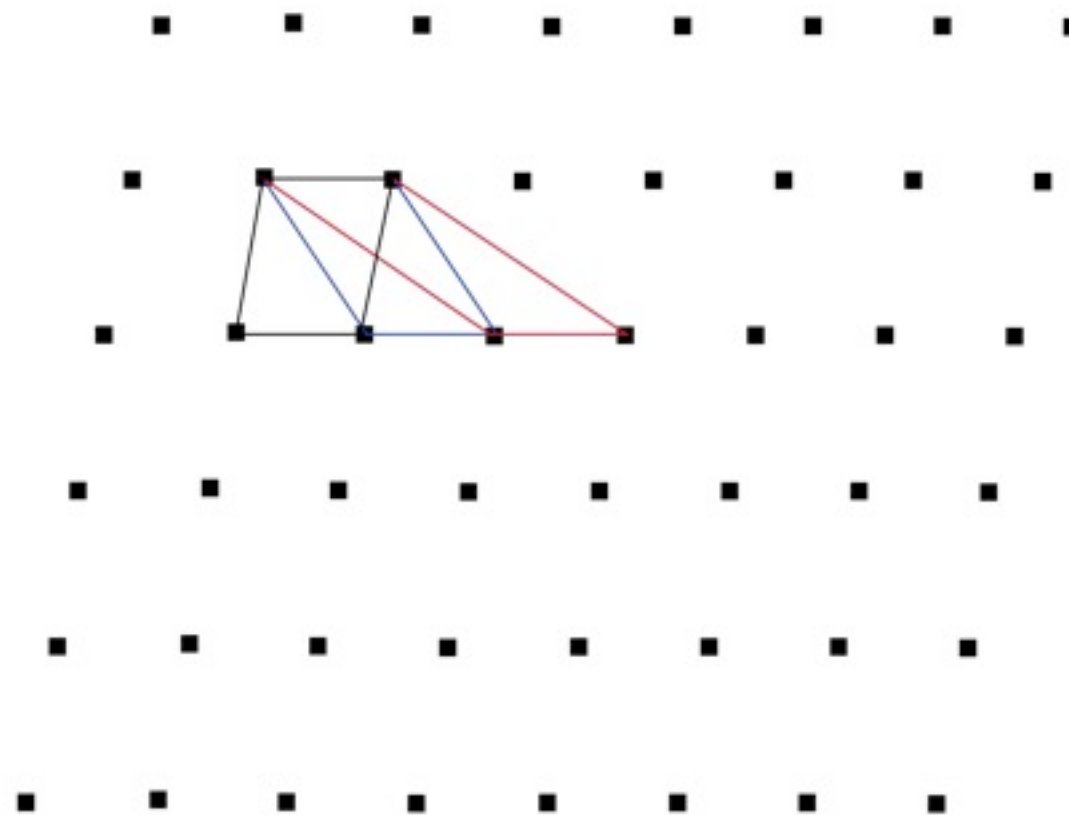
Non-lattice direction, random length. No peaks in Fourier transform

1D Fourier transform of projected scattering vectors



Pick three non-coplanar directions which have the largest peaks in the Fourier transforms to define a lattice.

This is not necessarily the simplest lattice (the “reduced cell”)



In the 2D example shown, the black cell corresponds to the reduced cell, while the red or blue cells may have been found in the autoindexing.

Indexing

Session View

119.55 120.09 250.00 5.00 10.0 1.05 1.05 0.00 20 25

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.0 - 1.0	294	0	0	148	☒	☒
84	83.0 - 84.0	222	0	0	105	☒	☒
Total		516	0	0	253		

Solutions:

Solution	Lat.	Pen.	a	b	c	α	β	γ	$\sigma(x,y)$	$\sigma(\varphi)$	δ beam
1 (ref)	aP	0	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.44 (0.1)
2 (ref)	aP	0	58.5	58.6	62.1	61.9	62.0	60.0	0.20	0.35	0.44 (0.1)
3 (ref)	mC	1	101.3	58.6	62.2	90.0	123.0	90.0	0.21	0.42	0.44 (0.1)
4 (ref)	mC	1	101.4	58.5	62.1	90.0	122.9	90.0	0.20	0.39	0.45 (0.2)
5 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45 (0.2)
6 (ref)	hR	2	58.6	58.6	156.4	90.0	90.0	120.0	0.21	0.54	0.46 (0.3)
7 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45 (0.2)
8 (reg)	hR	60	60.4	60.4	144.8	90.0	90.0	120.0	-	-	-
9 (reg)	mC	60	103.5	62.2	58.5	90.0	124.4	90.0	-	-	-
10 (reg)	mC	60	85.3	85.4	58.5	90.0	133.2	90.0	-	-	-
11 (reg)	oI	60	58.6	62.2	85.3	90.0	90.0	90.0	-	-	-
12 (reg)	mC	61	101.4	58.6	62.1	90.0	122.9	90.0	-	-	-
13 (reg)	tI	61	60.4	60.4	85.3	90.0	90.0	90.0	-	-	-
14 (reg)	oI	61	58.5	62.2	85.4	90.0	90.0	90.0	-	-	-
15 (reg)	mC	61	101.5	58.5	62.2	90.0	122.9	90.0	-	-	-

Spacegroup: h3

Mosaicity: 0.00 Estimate

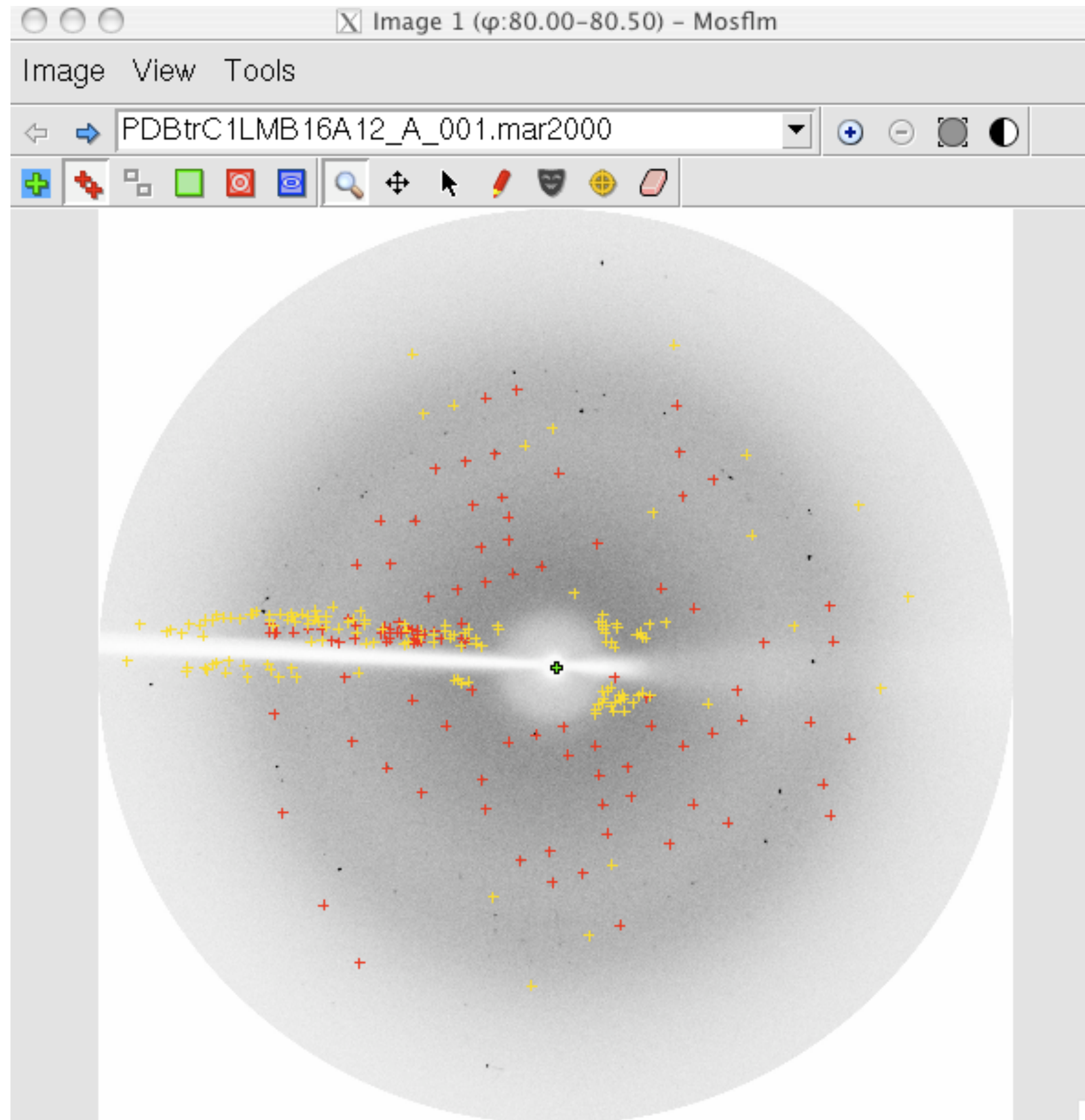
No Warnings

- Selects two images 90 degrees apart (if possible).
- Finds spots on these images
- Selecting “Index” attempts to index using these two images.
- Produces a list of solutions.
- Highlights the “best” solution. (Highest symmetry with a low penalty).

We only have information about the lattice shape at this stage, so assignment of symmetry is an assumption.

Indexing – Spot Finding

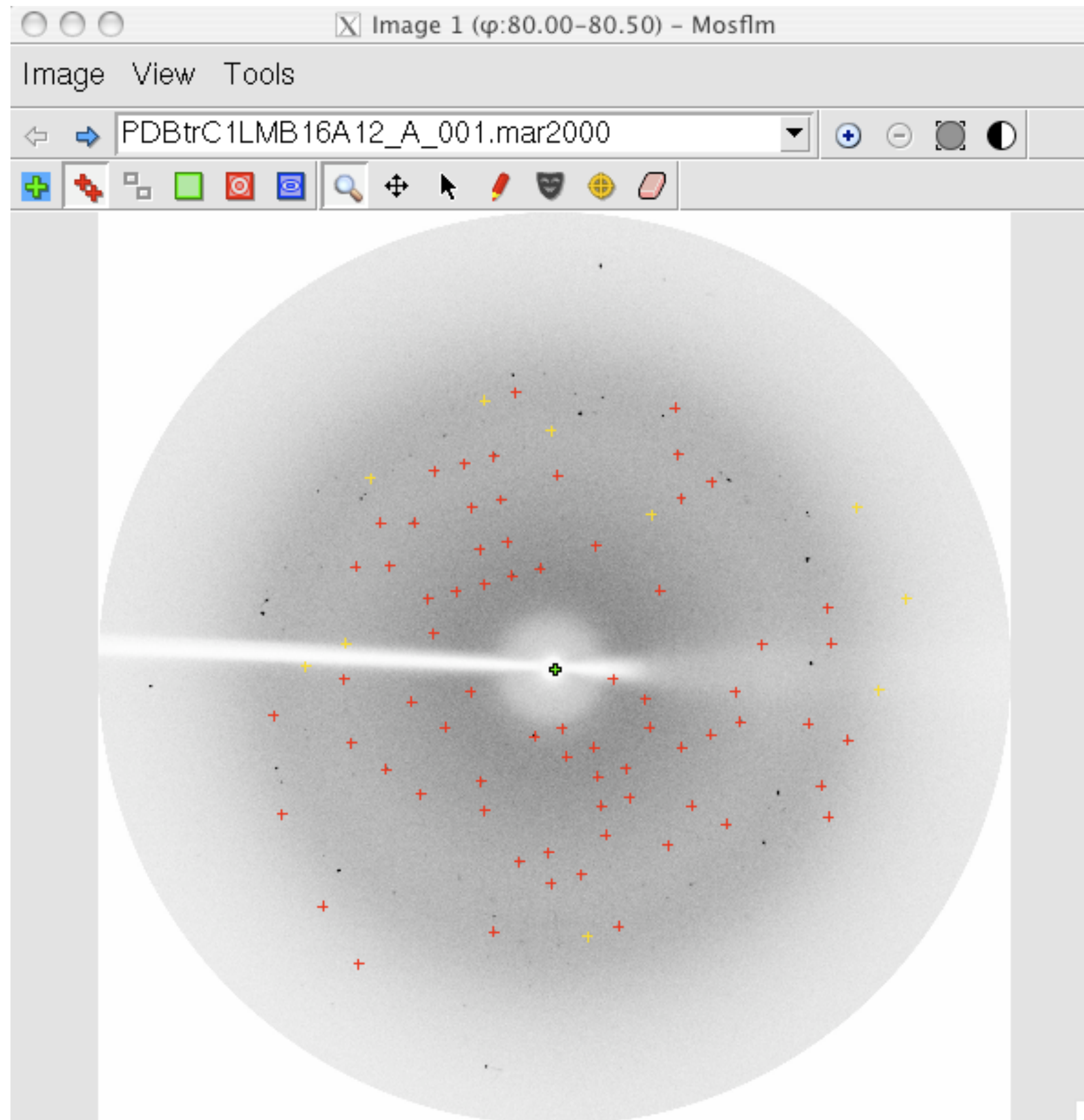
To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)



Indexing – Spot Finding

To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)

eg to 20,20 (pixels)

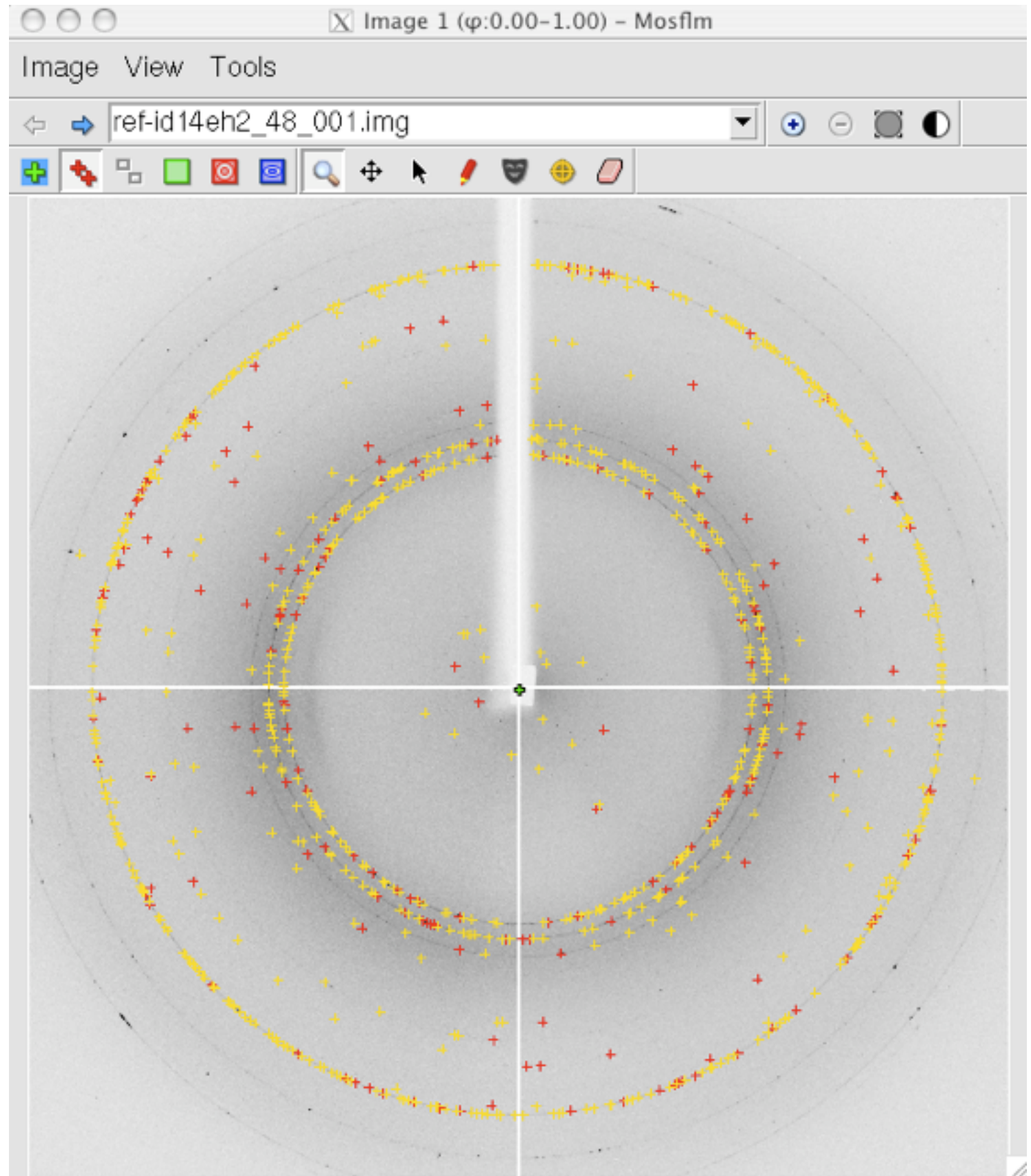


Indexing – Spot Finding

To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)

eg to 20,20 (pixels)

Ice rings will cause problems



Indexing – Spot Finding

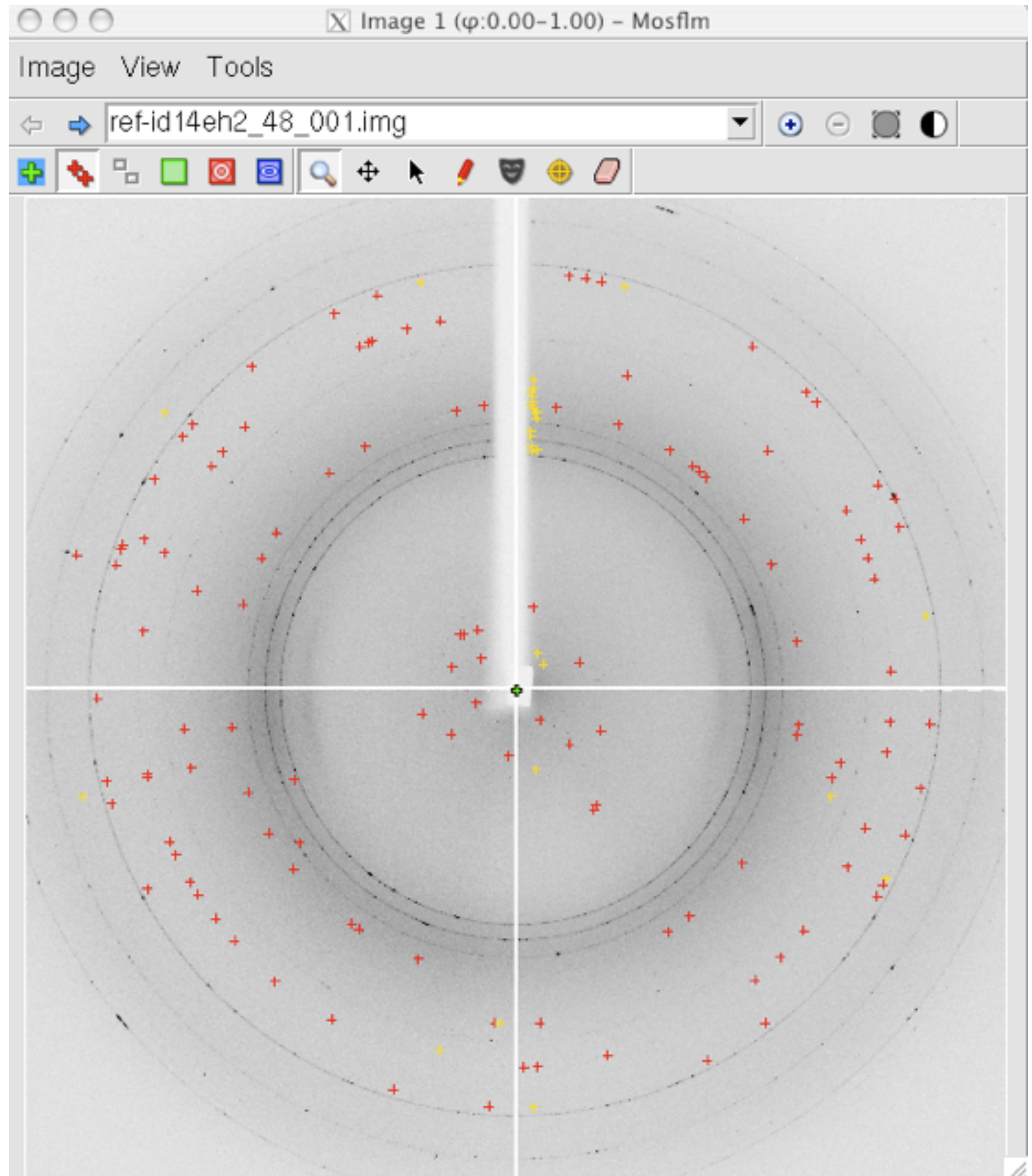
To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)

eg to 20,20 (pixels)

Ice rings will cause problems

So mosflm rejects all spots at the resolutions corresponding to ice.

Additional rings still give problems in this case.



Indexing – Spot Finding

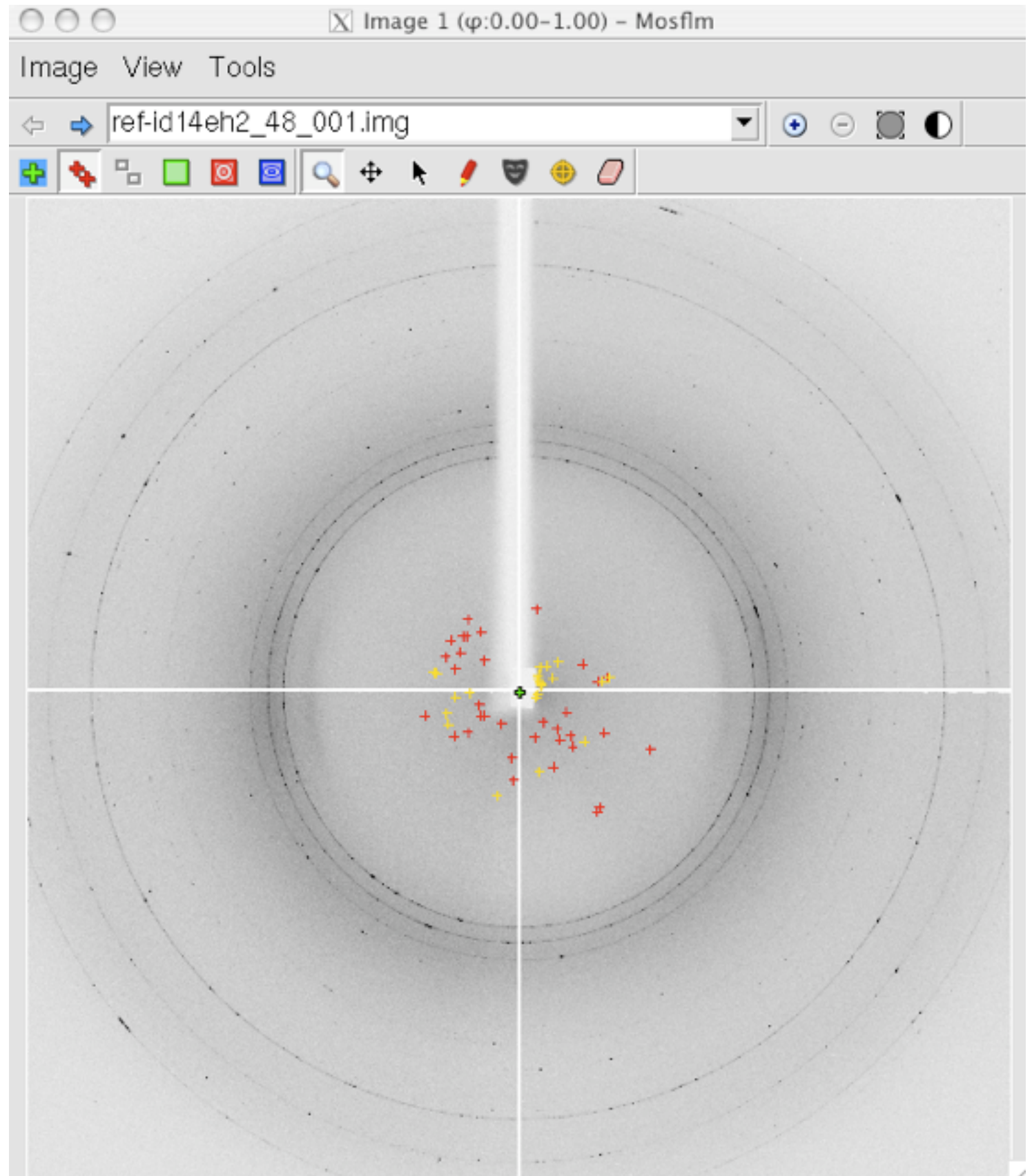
To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)

eg to 20,20 (pixels)

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So mosflm rejects all spots at the resolutions corresponding to ice.
Additional rings still give problems in this case.

Because the diffraction is very weak in this case, mosflm rejects all spots beyond 4.5Å



Indexing – Spot Finding

To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)

eg to 20,20 (pixels)

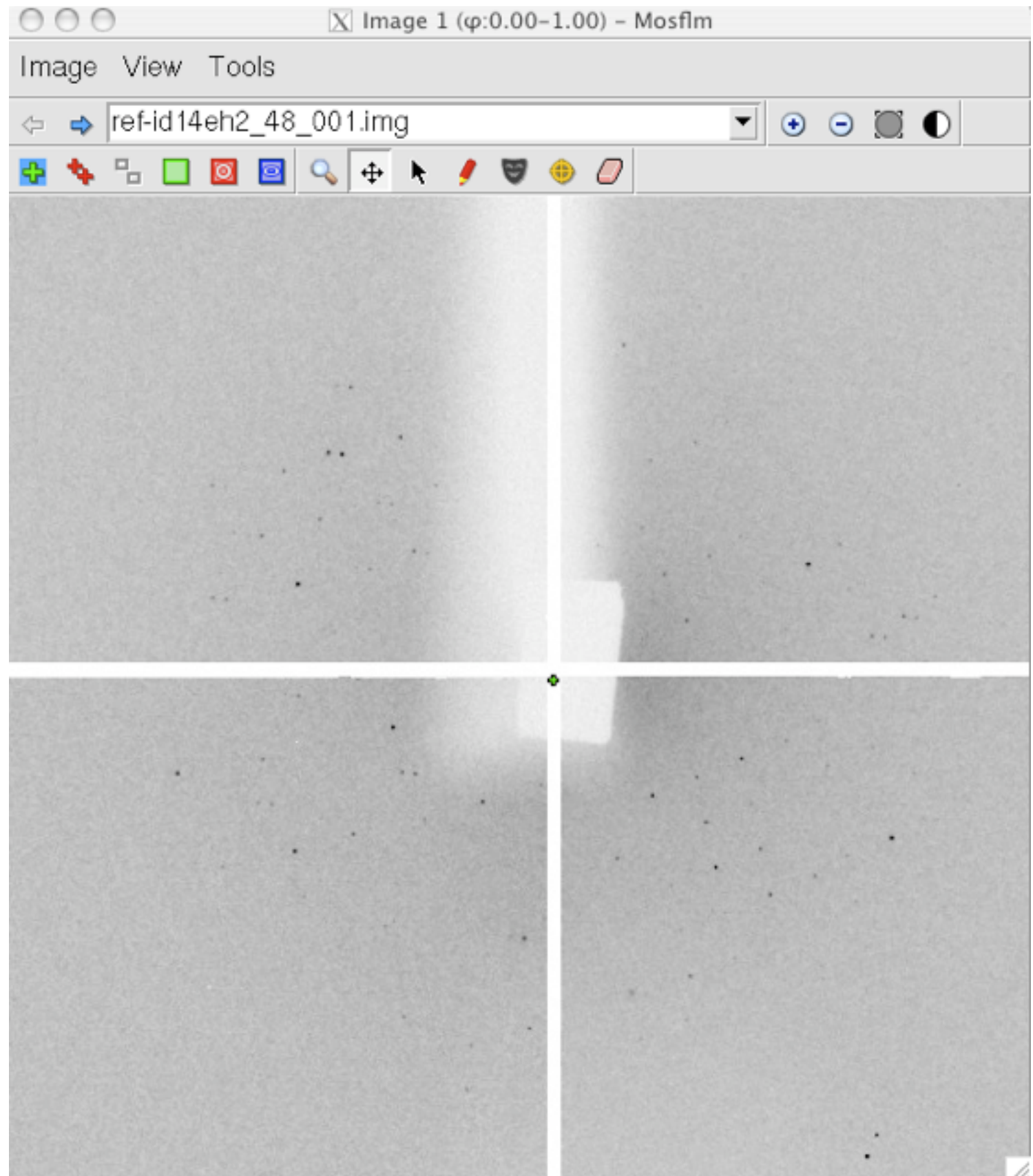
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Additional rings still give problems in this case.

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In addition, mosflm lowers the threshold for finding spots and the minimum spots size (in pixels)



Indexing – Spot Finding

To eliminate “false” spots near shadows, reduce the size of the local background box (100x100)

eg to 20,20 (pixels)

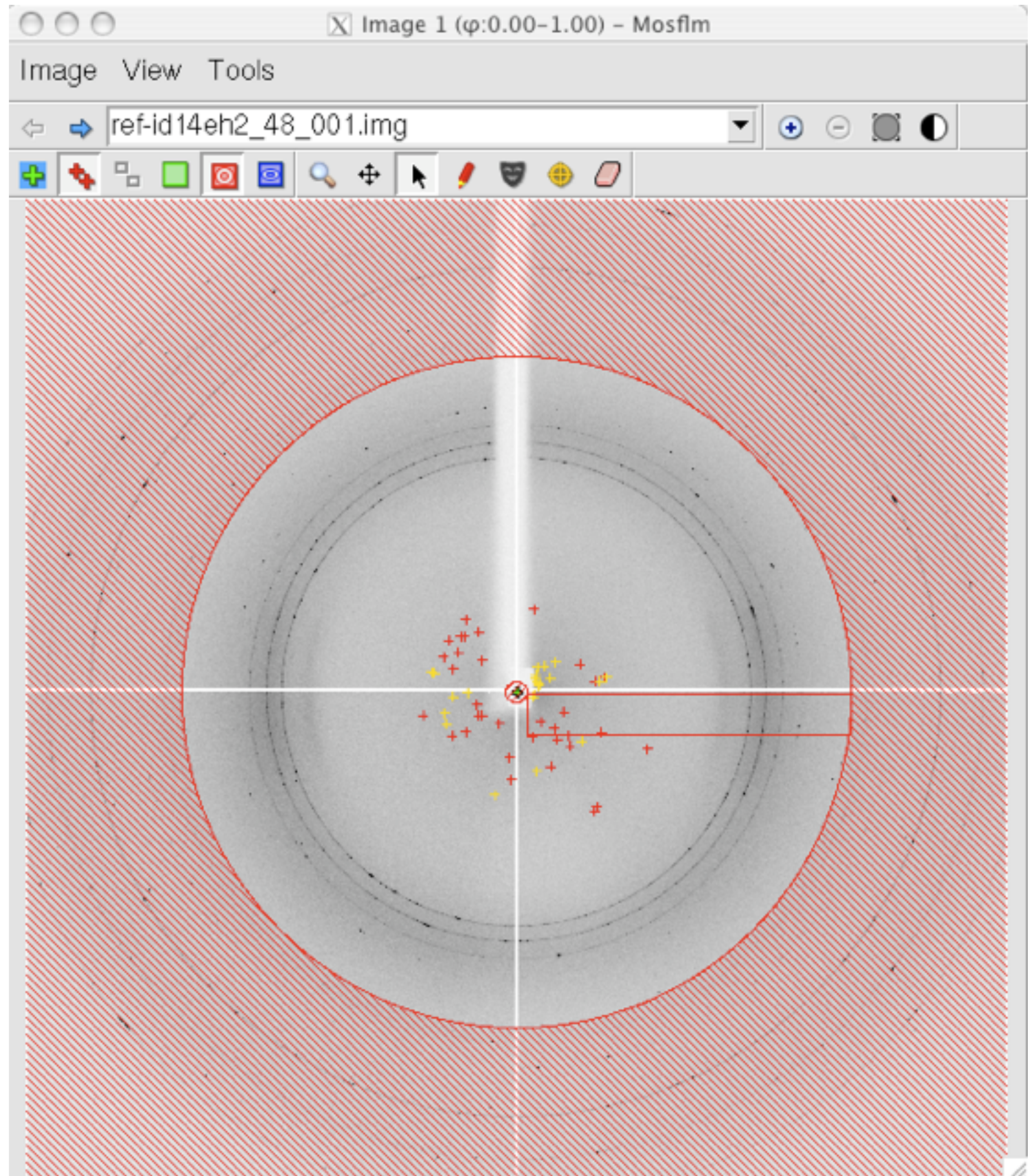
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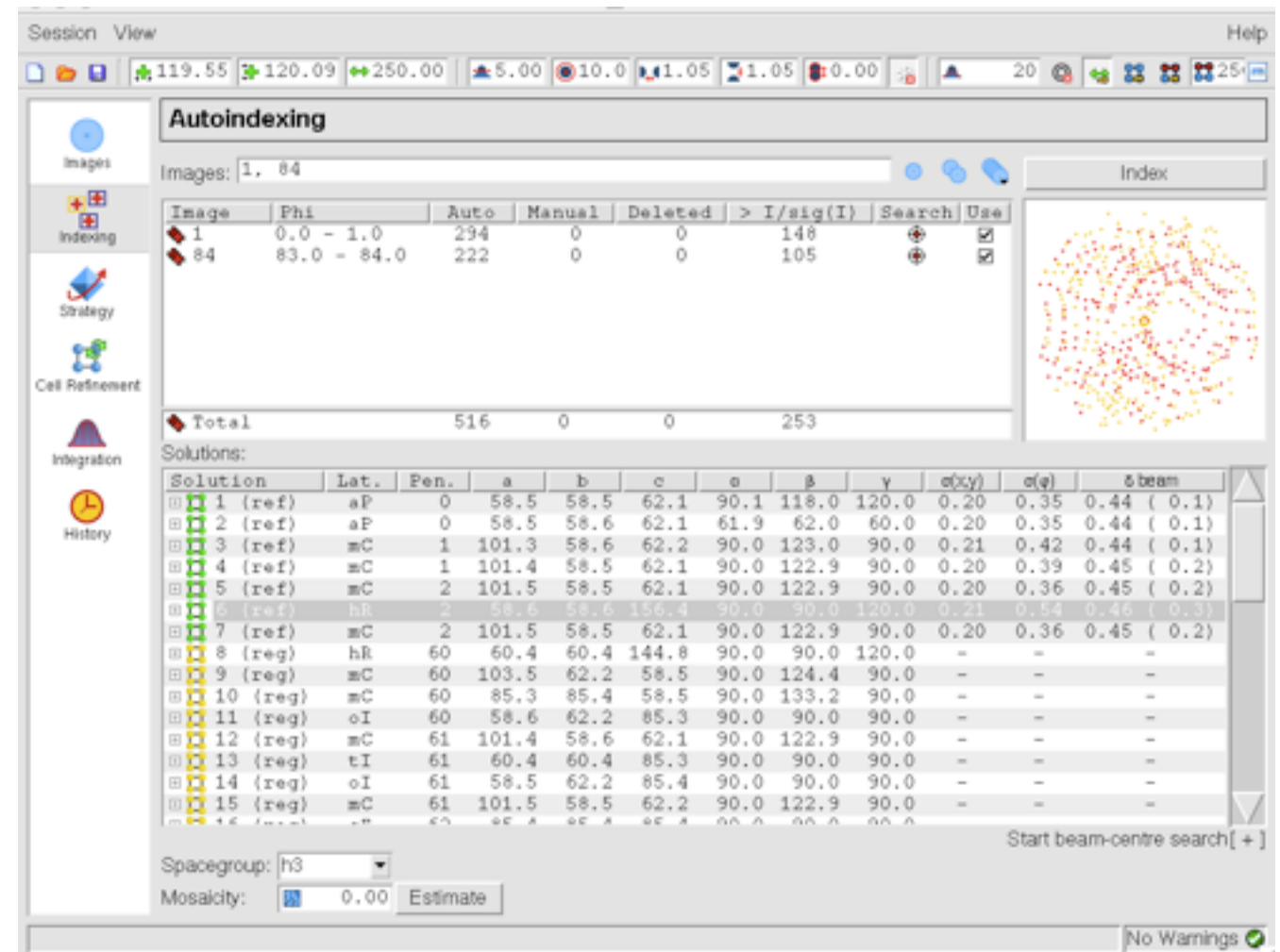
Because the diffraction is very weak in this case, mosflm rejects all spots beyond 4.5Å

In addition, mosflm lowers the threshold for finding spots and the minimum spots size (in pixels)

The spot finding radii can be set, and regions masked out for difficult cases



Indexing



How to tell if the solution is correct ...

Look at the image !

- Do the predicted spot positions agree with the real spot positions ?
- Is the overall appearance of the lunes correct ?
- Is the positional error $\sigma(xy)$ small ? (typically 0.1-0.3mm, but can be up to 1mm if spots are split)

Note that the list of solutions given by Mosflm are in fact all the **same** solution, with different lattice symmetries imposed, so that if the triclinic solution (number 1) is wrong, then all the others are too

What can be done if indexing fails ?

What can be done if indexing fails ?

The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a "Session View" menu. The "Autoindexing" panel is active, showing a table of indexed images. The "Images" field contains "1, 84". The table has columns: Image, Phi, Auto, Manual, Deleted, > I/sig(I), Search, and Use. The "Total" row shows 516 total reflections, 0 manual, 0 deleted, and 253 above the noise level. A dialog box with a yellow warning icon is overlaid on the main window, stating: "The indexing process has failed. It might be worthwhile trying again with:" followed by a list of four suggestions. The "Dismiss" button is at the bottom of the dialog. The bottom of the main window shows "Spacegroup: P1" and "Mosaicity: 0.00" with an "Estimate" button. A status bar at the bottom right indicates "1 Warning".

Session View

Help

120.00 120.00 250.00 5.00 10.0 1.05 1.05 0.00 20

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution

Spacegroup: P1

Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

What can be done if indexing fails ?

Check the direct beam (shown as a green cross on the image), if uncertain try a direct beam search (works best with 2 images)

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.0 - 1.0	294	0	0	148		☒
84	83.0 - 84.0	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution	Lat.	Pen.	a	b	c	α	β	γ	$\sigma(x,y)$	$\sigma(\varphi)$	δ beam
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5 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45 (0.2)
6 (ref)	hR	2	58.6	58.6	156.4	90.0	90.0	120.0	0.21	0.54	0.46 (0.3)
7 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45 (0.2)

Start Beam-centre search [-]

Beam x	Beam y	Beam x ref	Beam y ref	a	b	c	α	β	γ	$\sigma(x,y)$	$\sigma(\varphi)$	δ beam
118.5	119.1	119.57	120.09	58.5	58.5	62.1	90.1	118.0	119.9	0.22	0.34	1.40
118.5	119.6	119.57	120.09	58.5	58.6	62.1	90.1	118.0	120.0	0.19	0.54	1.10
118.5	120.1	119.57	120.09	58.5	58.6	62.1	90.1	118.0	120.0	0.19	0.54	1.00
118.5	120.6	119.57	120.09	58.5	58.6	62.1	90.1	118.0	120.0	0.19	0.54	1.10
118.5	121.1	119.56	120.09	58.6	58.5	62.1	118.0	90.1	120.0	0.21	0.54	1.40
119.0	119.1	119.57	120.08	58.5	58.5	62.1	118.0	90.1	119.9	0.21	0.35	1.10
119.0	119.6	119.57	120.09	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.72
119.0	120.1	119.57	120.09	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.52
119.0	120.6	119.57	120.08	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.72
119.0	121.1	119.57	120.08	58.5	58.5	62.1	118.0	90.1	119.9	0.21	0.35	1.10
119.5	119.1	119.57	120.08	58.5	58.5	62.1	90.1	118.0	119.9	0.21	0.35	0.99
119.5	119.6	119.57	120.09	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.50

Spacegroup: h3
Mosaicity: 0.00 Estimate

No Warnings

What can be done if indexing fails ?

Try only using one image, especially if disorder/multiple lattices are only present in one of the images or if the crystal has “died” by the last image.

The screenshot shows the iMosfilm software interface. The main window has a menu bar (Session, View, Help) and a toolbar with various icons. The left sidebar contains icons for Images, Indexing, Strategy, Cell Refinement, Integration, and History. The main area is titled "Autoindexing" and displays a table of indexed images. A dialog box with a yellow warning icon is overlaid on the main window, indicating that the indexing process has failed. The dialog box lists four suggestions for troubleshooting: 1. A large or smaller longest cell edge, 2. Using more or fewer reflections (200 - 1000 is best), 3. Using more and/or different images, and 4. Checking your direct beam position carefully. The dialog box has a "Dismiss" button. The main window also shows a "Total" row with values 516, 0, 0, and 253. The "Solutions:" section is empty. The "Spacegroup:" is set to P1 and the "Mosaicity:" is 0.00. The "Index" button is visible in the top right of the main window. The status bar at the bottom right shows "1 Warning".

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

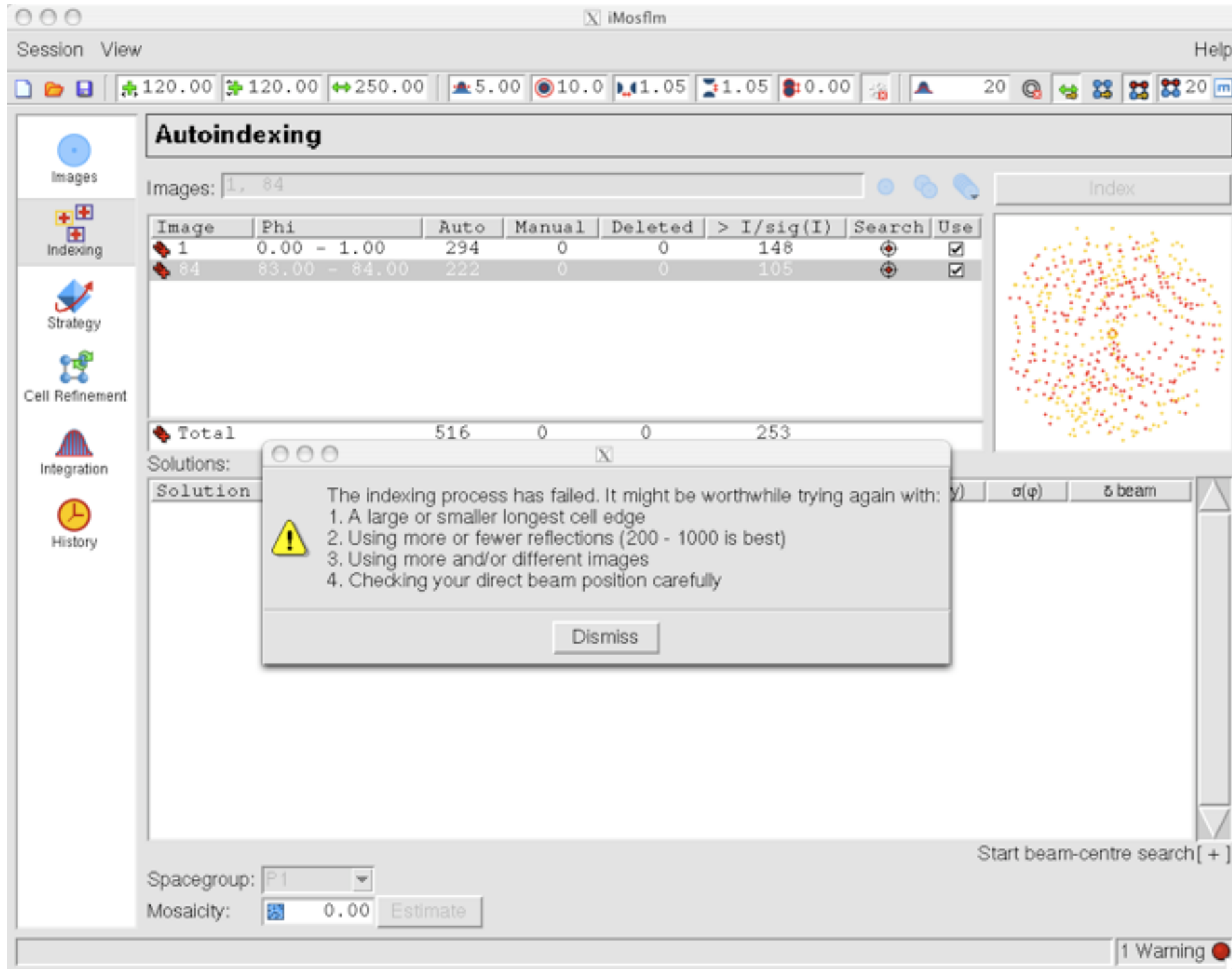
Spacegroup: P1
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

If very mosaic, or there are multiple lattices, increase the threshold for spots to be used up to ~100 (this is set automatically to 5, 10 or 20 by mosflm depending on strength of the image).



The screenshot shows the iMosflm software interface. The main window is titled "iMosflm" and has a menu bar with "Session", "View", and "Help". Below the menu bar is a toolbar with various icons. The left sidebar contains icons for "Images", "Indexing", "Strategy", "Cell Refinement", "Integration", and "History". The main area is titled "Autoindexing" and contains a table of indexed images. The table has columns: "Image", "Phi", "Auto", "Manual", "Deleted", "> I/sig(I)", "Search", and "Use". The table shows two images: "1" and "84". Image "1" has a Phi range of 0.00 - 1.00, 294 Auto spots, 0 Manual spots, 0 Deleted spots, and a threshold of 148. Image "84" has a Phi range of 83.00 - 84.00, 222 Auto spots, 0 Manual spots, 0 Deleted spots, and a threshold of 105. The "Total" row shows 516 Auto spots, 0 Manual spots, 0 Deleted spots, and a threshold of 253. A dialog box is open in the center of the screen, titled "The indexing process has failed. It might be worthwhile trying again with:". The dialog box contains a list of four suggestions: 1. A large or smaller longest cell edge, 2. Using more or fewer reflections (200 - 1000 is best), 3. Using more and/or different images, and 4. Checking your direct beam position carefully. The dialog box has a "Dismiss" button. The bottom of the iMosflm window shows "Spacegroup: P1" and "Mosaicity: 0.00" with an "Estimate" button. The status bar at the bottom right shows "1 Warning".

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148	☒	☒
84	83.00 - 84.00	222	0	0	105	☒	☒
Total		516	0	0	253		

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Even if not mosaic, try different thresholds, in range 5-100.

The screenshot shows the iMosfilm software interface. The main window has a menu bar (Session, View, Help) and a toolbar with various icons. The left sidebar contains icons for Images, Indexing, Strategy, Cell Refinement, Integration, and History. The main area is titled "Autoindexing" and displays a table of indexed images. A dialog box with a yellow warning icon is overlaid on the main window, indicating a failure in the indexing process.

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1

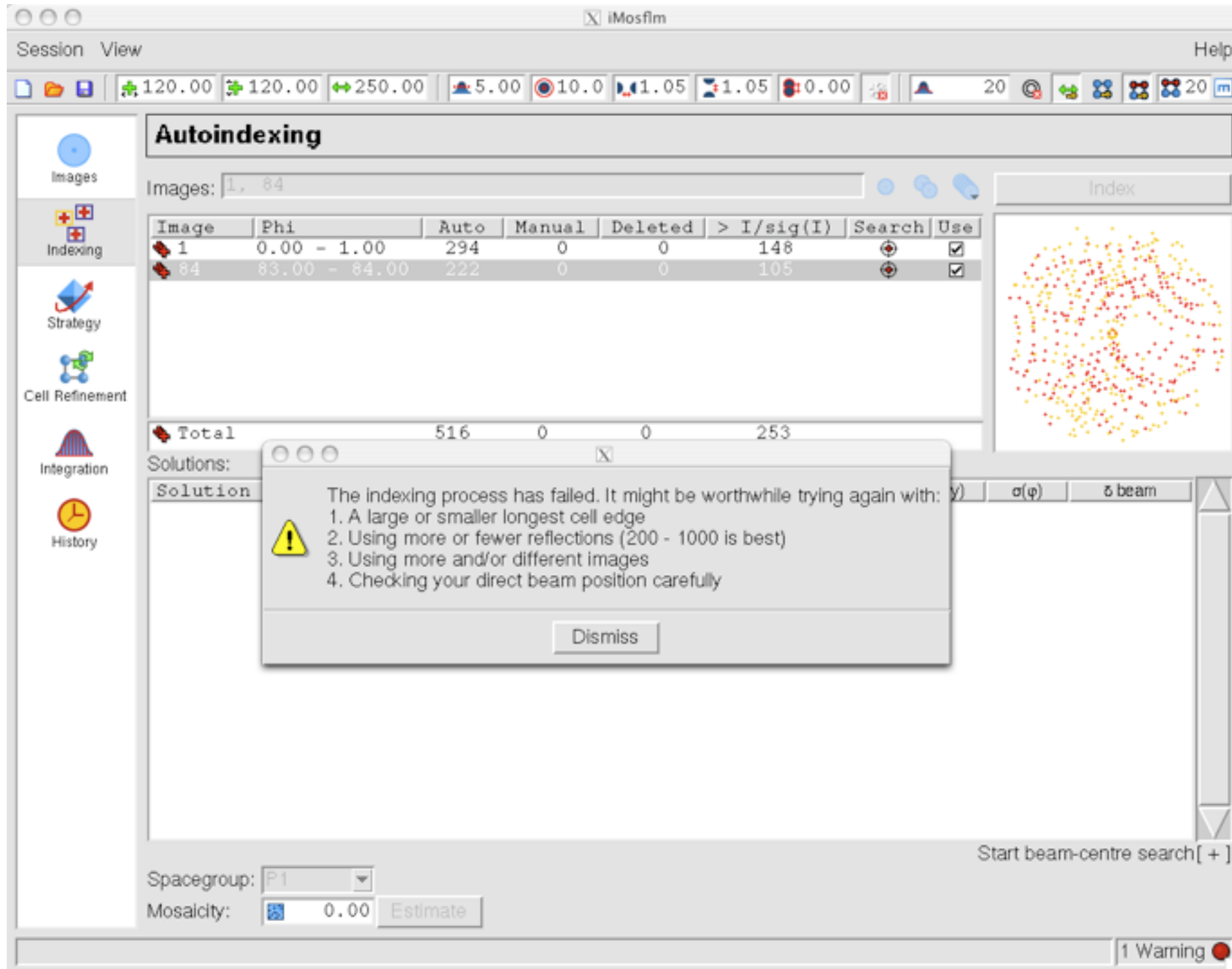
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Decrease the maximum cell length (worked out based on the spot size, so for small spots may be very large, eg 700Å).



The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a menu bar with "Session", "View", and "Help". Below the menu bar is a toolbar with various icons. The left sidebar contains icons for "Images", "Indexing", "Strategy", "Cell Refinement", "Integration", and "History". The main area is titled "Autoindexing" and contains a table of indexed images. The table has columns: Image, Phi, Auto, Manual, Deleted, > I/sig(I), Search, and Use. The table shows two images: 1 and 84. Image 1 has a Phi range of 0.00 - 1.00, 294 Auto reflections, 0 Manual reflections, 0 Deleted reflections, and a signal-to-noise ratio of 148. Image 84 has a Phi range of 83.00 - 84.00, 222 Auto reflections, 0 Manual reflections, 0 Deleted reflections, and a signal-to-noise ratio of 105. The "Total" row shows 516 Auto reflections, 0 Manual reflections, 0 Deleted reflections, and a signal-to-noise ratio of 253. A dialog box is open in the center of the screen, titled "The indexing process has failed. It might be worthwhile trying again with:". The dialog box contains a list of four suggestions: 1. A large or smaller longest cell edge, 2. Using more or fewer reflections (200 - 1000 is best), 3. Using more and/or different images, and 4. Checking your direct beam position carefully. The dialog box has a "Dismiss" button. The bottom of the iMosfilm window shows the "Spacegroup" set to "P1" and the "Mosaicity" set to "0.00". There is an "Estimate" button next to the Mosaicity field. The status bar at the bottom right shows "1 Warning" with a red warning icon.

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148	☒	☒
84	83.00 - 84.00	222	0	0	105	☒	☒
Total		516	0	0	253		

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Try using more images (if only a few spots on each image). Indexing usually works best with a few hundred reflections.

The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a "Session View" menu. The "Autoindexing" tab is active, showing a table of indexed reflections. The table has columns: Image, Phi, Auto, Manual, Deleted, > I/sig(I), Search, and Use. The data rows are for images 1 and 84. A dialog box with a yellow warning icon is overlaid on the main window, stating: "The indexing process has failed. It might be worthwhile trying again with:" followed by a list of four suggestions. The suggestions are: 1. A large or smaller longest cell edge, 2. Using more or fewer reflections (200 - 1000 is best), 3. Using more and/or different images, and 4. Checking your direct beam position carefully. The dialog box has a "Dismiss" button. The main window also shows a "Total" row with values 516, 0, 0, and 253. The "Index" button is visible on the right. The bottom of the window shows "Spacegroup: P1" and "Mosaicity: 0.00" with an "Estimate" button. A status bar at the bottom right indicates "1 Warning".

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

Autoindexing

Images: 1, 84

Solutions:

Solution

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1

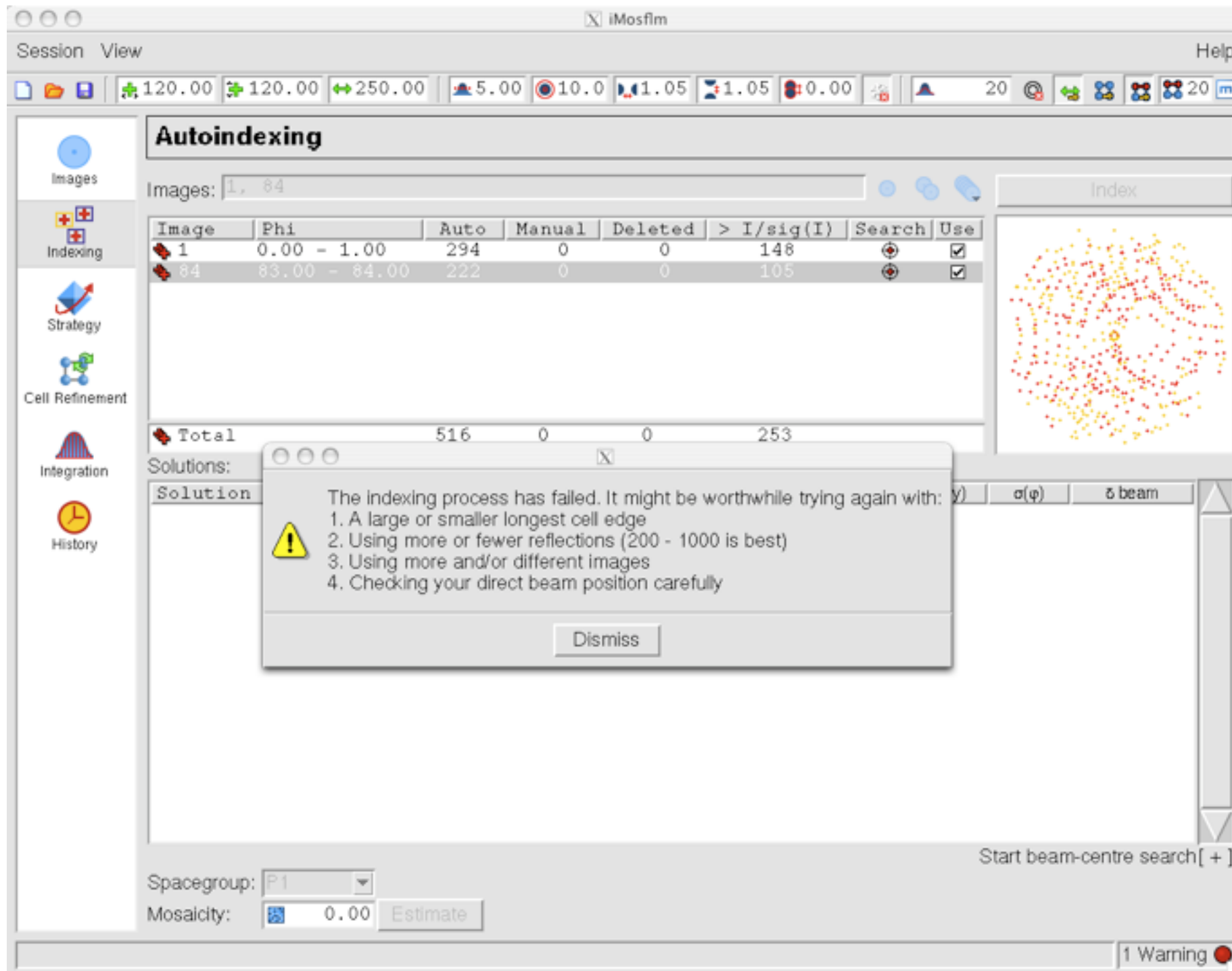
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Many of the parameters that influence the spotfinding and indexing can be changed in the top line of the gui.



What can be done if indexing fails ?

What can be done if indexing fails ?

The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a "Session View" menu. The top toolbar contains various icons for file operations and data manipulation. The left sidebar has icons for "Images", "Indexing", "Strategy", "Cell Refinement", "Integration", and "History". The main area is titled "Autoindexing" and displays a table of indexed images. The "Images" field shows "1, 84". The table has columns: Image, Phi, Auto, Manual, Deleted, > I/sig(I), Search, and Use. The "Total" row shows 516 total reflections, 0 manual, 0 deleted, and 253 reflections with > I/sig(I) > 3. A dialog box with a yellow warning icon is overlaid on the main window, stating: "The indexing process has failed. It might be worthwhile trying again with:" followed by a list of four suggestions. The "Dismiss" button is at the bottom of the dialog. The bottom of the main window shows "Spacegroup: P1" and "Mosaicity: 0.00" with an "Estimate" button. A status bar at the bottom right indicates "1 Warning".

Session View

Help

120.00 120.00 250.00 5.00 10.0 1.05 1.05 0.00 20

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution

! The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1

Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Check the direct beam (shown as a green cross on the image), if uncertain try a direct beam search (works best with 2 images)

Session View

119.55 120.09 250.00 5.00 10.0 1.05 1.05 0.00 20 25

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.0 - 1.0	294	0	0	148		☒
84	83.0 - 84.0	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution	Lat.	Pen.	a	b	c	α	β	γ	$\sigma(x,y)$	$\sigma(\varphi)$	δ beam
4 (ref)	mC	1	101.4	58.5	62.1	90.0	122.9	90.0	0.20	0.39	0.45 (0.2)
5 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45 (0.2)
6 (ref)	hR	2	58.6	58.6	156.4	90.0	90.0	120.0	0.21	0.54	0.46 (0.3)
7 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45 (0.2)

Start Beam-centre search [-

Beam x	Beam y	Beam x ref	Beam y ref	a	b	c	α	β	γ	$\sigma(x,y)$	$\sigma(\varphi)$	δ beam
118.5	119.1	119.57	120.09	58.5	58.5	62.1	90.1	118.0	119.9	0.22	0.34	1.40
118.5	119.6	119.57	120.09	58.5	58.6	62.1	90.1	118.0	120.0	0.19	0.54	1.10
118.5	120.1	119.57	120.09	58.5	58.6	62.1	90.1	118.0	120.0	0.19	0.54	1.00
118.5	120.6	119.57	120.09	58.5	58.6	62.1	90.1	118.0	120.0	0.19	0.54	1.10
118.5	121.1	119.56	120.09	58.6	58.5	62.1	118.0	90.1	120.0	0.21	0.54	1.40
119.0	119.1	119.57	120.08	58.5	58.5	62.1	118.0	90.1	119.9	0.21	0.35	1.10
119.0	119.6	119.57	120.09	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.72
119.0	120.1	119.57	120.09	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.52
119.0	120.6	119.57	120.08	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.72
119.0	121.1	119.57	120.08	58.5	58.5	62.1	118.0	90.1	119.9	0.21	0.35	1.10
119.5	119.1	119.57	120.08	58.5	58.5	62.1	90.1	118.0	119.9	0.21	0.35	0.99
119.5	119.6	119.57	120.09	58.5	58.5	62.1	90.1	118.0	120.0	0.20	0.35	0.50

Spacegroup: h3

Mosaicity: 0.00 Estimate

No Warnings

Beam
search

What can be done if indexing fails ?

iMosfilm

Session View Help

120.00 120.00 250.00 5.00 10.0 1.05 1.05 0.00 20

Autoindexing

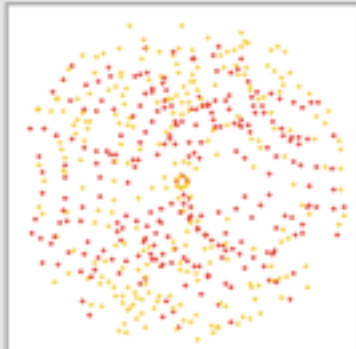
Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution

Index



Start beam-centre search [+]

Spacegroup: P1

Mosaicity: 0.00 Estimate

1 Warning

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

What can be done if indexing fails ?

Try only using one image, especially if disorder/multiple lattices are only present in one of the images or if the crystal has “died” by the last image.

The screenshot shows the iMosfilm software interface. The main window has a menu bar (Session, View, Help) and a toolbar with various icons. The left sidebar contains icons for Images, Indexing, Strategy, Cell Refinement, Integration, and History. The main area is titled "Autoindexing" and displays a table of indexed images. A dialog box with a yellow warning icon is overlaid on the main window, indicating a failure in the indexing process.

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒

Total 516 0 0 253

Solutions:

Solution

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1

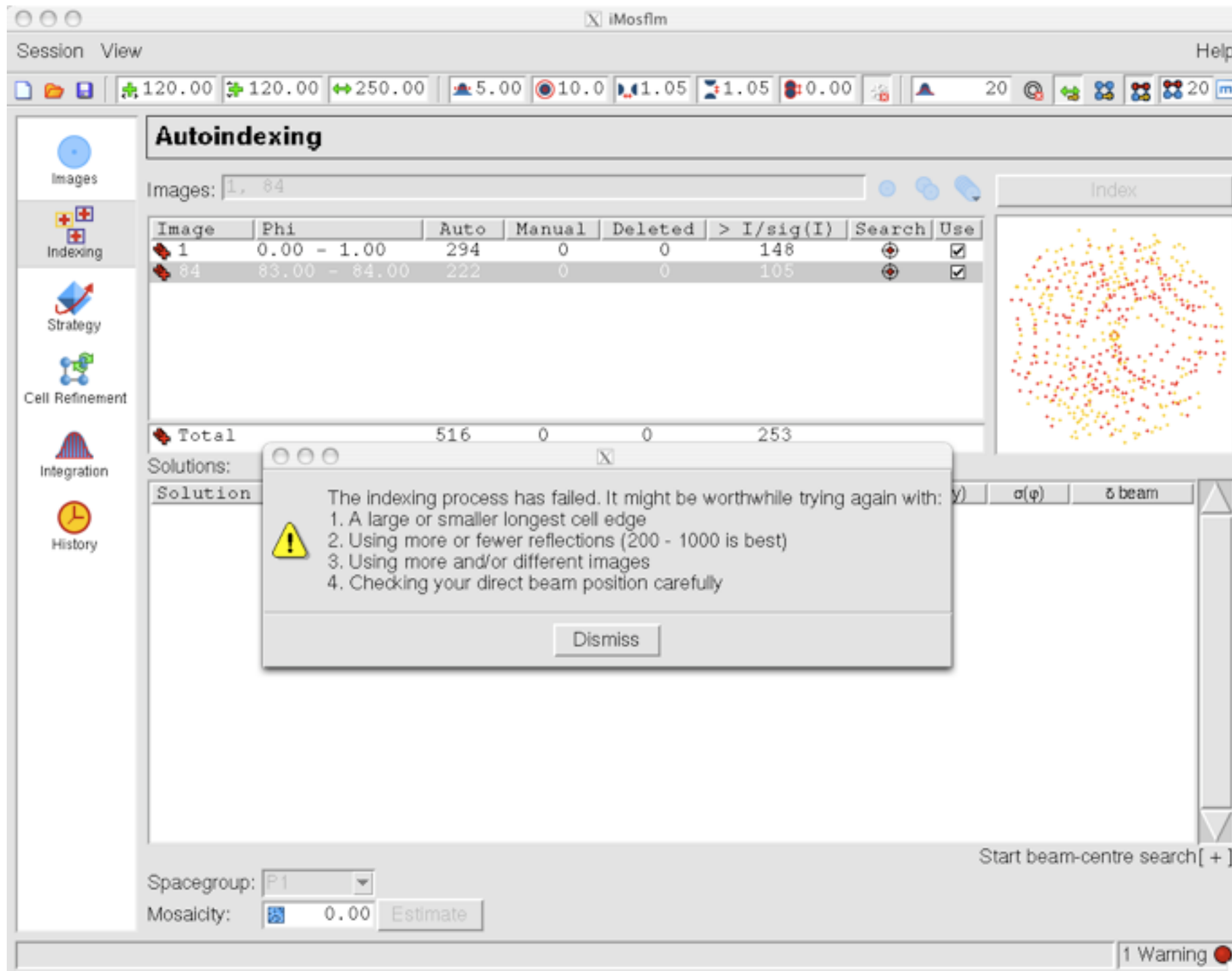
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

If very mosaic, or there are multiple lattices, increase the threshold for spots to be used up to ~100 (this is set automatically to 5, 10 or 20 by mosfilm depending on strength of the image).



The screenshot shows the iMosfilm software interface. The main window has a menu bar (Session, View, Help) and a toolbar with various icons. The left sidebar contains icons for Images, Indexing, Strategy, Cell Refinement, Integration, and History. The main area is titled "Autoindexing" and displays a table of indexed images. A dialog box with a yellow warning icon is overlaid on the main window, indicating a failure in the indexing process.

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒

Total: 516 0 0 253

Solutions:

Solution

The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

Spacegroup: P1

Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Even if not mosaic, try different thresholds, in range 5-100.

The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a menu bar with "Session", "View", and "Help". Below the menu bar is a toolbar with various icons. The left sidebar contains icons for "Images", "Indexing", "Strategy", "Cell Refinement", "Integration", and "History". The main area is titled "Autoindexing" and contains a table of indexed images. The table has columns: Image, Phi, Auto, Manual, Deleted, > I/sig(I), Search, and Use. The data rows are:

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

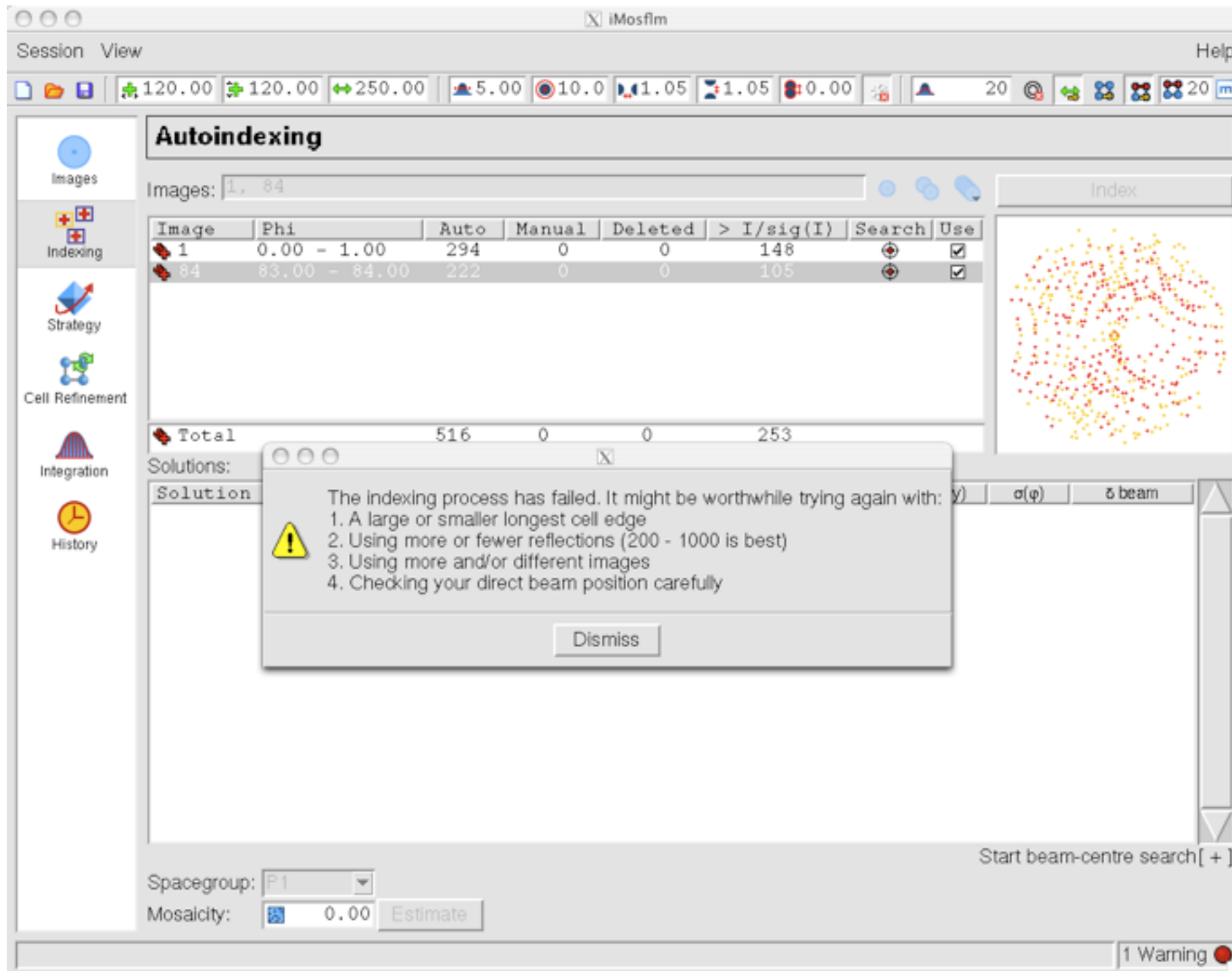
Below the table is a "Solutions:" section with a "Solution" button. A dialog box is open in the center of the screen, titled "The indexing process has failed. It might be worthwhile trying again with:". The dialog box contains a list of suggestions:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

The dialog box has a "Dismiss" button. In the bottom right corner of the iMosfilm window, there is a status bar that says "1 Warning" with a red warning icon.

What can be done if indexing fails ?

Decrease the maximum cell length (worked out based on the spot size, so for small spots may be very large, eg 700Å).



The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a "Session View" menu. The "Autoindexing" tab is active, showing a table of indexed images and a list of solutions. A dialog box with a yellow warning icon is displayed in the center, indicating that the indexing process has failed. The dialog box provides four suggestions for troubleshooting: 1. A large or smaller longest cell edge, 2. Using more or fewer reflections (200 - 1000 is best), 3. Using more and/or different images, and 4. Checking your direct beam position carefully. The dialog box has a "Dismiss" button. The background window shows a table of indexed images with columns for Image, Phi, Auto, Manual, Deleted, > I/sig(I), Search, and Use. The table lists two images, 1 and 84, with their respective parameters. The "Total" row shows 516 images, 0 manual, 0 deleted, and 253 indexed. The "Solutions" section shows a single solution. The "Index" button is visible on the right. The bottom of the window shows the "Spacegroup" set to "P1" and "Mosaicity" set to "0.00". A status bar at the bottom right indicates "1 Warning".

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒
Total		516	0	0	253		

Solutions:

Solution

Spacegroup: P1
Mosaicity: 0.00 Estimate

Start beam-centre search [+]

1 Warning

What can be done if indexing fails ?

Try using more images (if only a few spots on each image). Indexing usually works best with a few hundred reflections.

The screenshot shows the iMosfilm software interface. The main window is titled "iMosfilm" and has a "Session View" menu. The "Autoindexing" tab is active, showing a table of indexed images and a list of solutions. A dialog box with a yellow warning icon is displayed in the center, indicating that the indexing process has failed. The dialog box provides four suggestions for troubleshooting: 1. A large or smaller longest cell edge, 2. Using more or fewer reflections (200 - 1000 is best), 3. Using more and/or different images, and 4. Checking your direct beam position carefully. The dialog box has a "Dismiss" button. The background interface includes a toolbar with various icons, a sidebar with icons for Images, Indexing, Strategy, Cell Refinement, Integration, and History, and a status bar at the bottom showing "Spacegroup: P1", "Mosaicity: 0.00", and "1 Warning".

Session View

Help

120.00 120.00 250.00 5.00 10.0 1.05 1.05 0.00 20

Autoindexing

Images: 1, 84

Image	Phi	Auto	Manual	Deleted	> I/sig(I)	Search	Use
1	0.00 - 1.00	294	0	0	148		☒
84	83.00 - 84.00	222	0	0	105		☒

Total 516 0 0 253

Solutions:

Solution

Index

Start beam-centre search [+]

Spacegroup: P1

Mosaicity: 0.00 Estimate

1 Warning

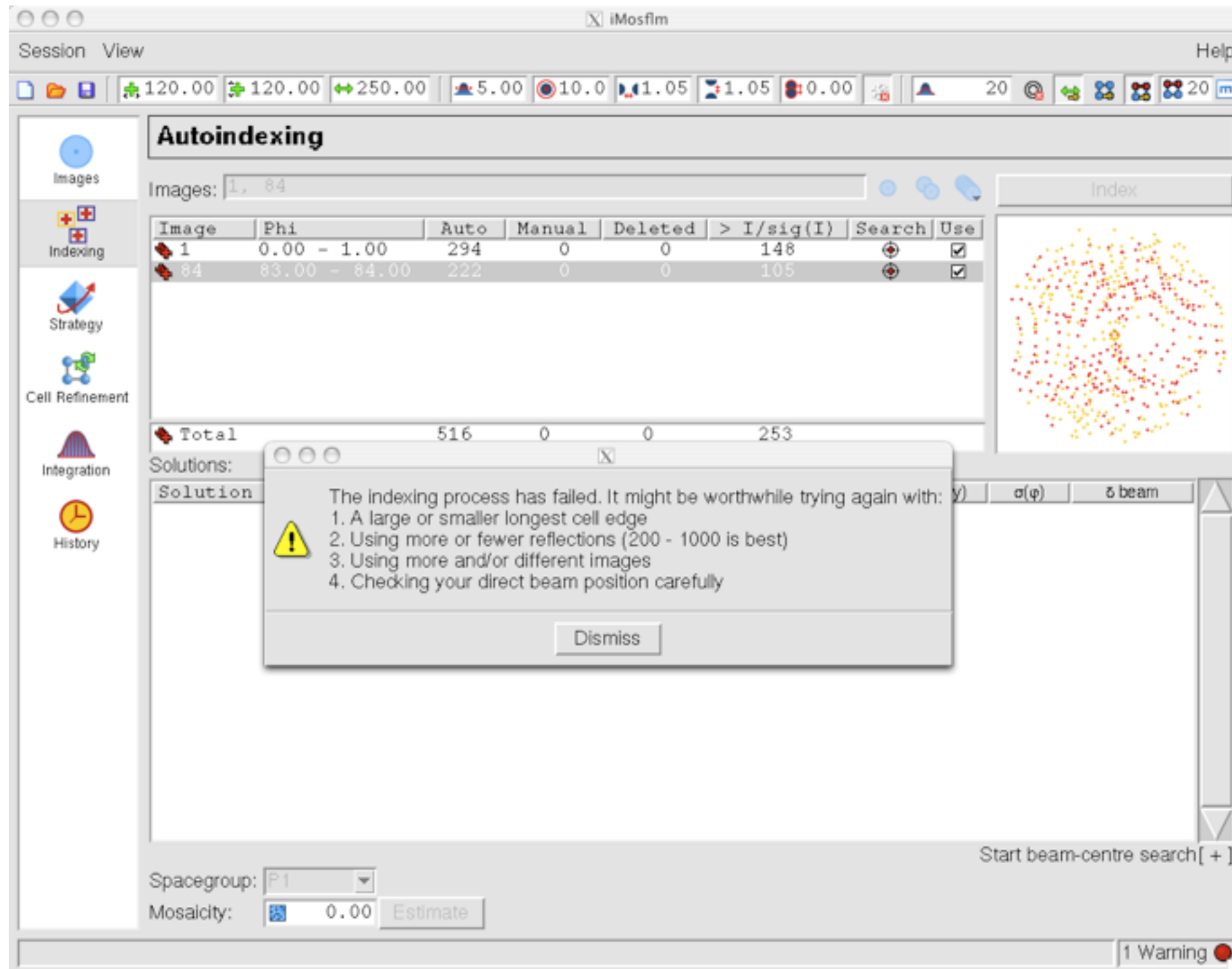
The indexing process has failed. It might be worthwhile trying again with:

1. A large or smaller longest cell edge
2. Using more or fewer reflections (200 - 1000 is best)
3. Using more and/or different images
4. Checking your direct beam position carefully

Dismiss

What can be done if indexing fails ?

Many of the parameters that influence the spotfinding and indexing can be changed in the top line of the gui.



Indexing – choosing the “best” solution

Solution	Lat.	Pen.	a	b	c	α	β	γ	$\sigma(x,y)$	$\sigma(\phi)$	δ beam
1 (ref)	aP	0	81.3	81.9	82.3	90.0	90.1	90.0	0.17	0.43	0.01 (0.0)
2 (ref)	mP	0	81.3	81.9	82.3	90.0	90.1	90.0	0.16	0.43	0.00 (0.0)
3 (ref)	aP	0	81.3	81.9	82.3	90.0	89.9	90.0	0.17	0.43	0.01 (0.0)
4 (ref)	mP	1	81.3	82.3	81.8	90.0	90.0	90.0	0.18	0.44	0.00 (0.0)
5 (ref)	mP	1	81.8	81.3	82.3	90.0	90.0	90.0	0.18	0.44	0.00 (0.0)
6 (ref)	oP	1	81.3	81.8	82.3	90.0	90.0	90.0	0.18	0.44	0.00 (0.0)
7 (ref)	mC	3	116.2	115.8	81.4	90.0	90.2	90.0	0.18	0.48	0.00 (0.0)
8 (ref)	tP	3	82.1	82.1	81.3	90.0	90.0	90.0	0.22	0.45	0.00 (0.0)
9 (ref)	oC	3	116.0	116.1	81.3	90.0	90.0	90.0	0.21	0.46	0.00 (0.0)
10 (ref)	mC	3	116.2	115.8	81.4	90.0	90.2	90.0	0.18	0.48	0.00 (0.0)
11 (ref)	mC	4	115.5	115.3	82.2	90.0	90.1	90.0	0.24	0.43	0.01 (0.0)
12 (ref)	oC	4	115.5	115.3	82.3	90.0	90.0	90.0	0.24	0.42	0.01 (0.0)
13 (ref)	tP	4	81.6	81.6	82.3	90.0	90.0	90.0	0.24	0.42	0.01 (0.0)
14 (ref)	mC	4	115.5	115.3	82.2	90.0	90.1	90.0	0.24	0.43	0.01 (0.0)
15 (ref)	hR	6	115.5	115.5	142.4	90.0	90.0	120.0	0.28	0.49	0.01 (0.0)
16 (ref)	hR	6	115.7	115.7	141.7	90.0	90.0	120.0	0.35	0.44	0.01 (0.0)
17 (ref)	cP	7	81.8	81.8	81.8	90.0	90.0	90.0	0.34	0.44	0.01 (0.0)
18 (reg)	mC	248	81.3	183.3	81.9	90.0	90.0	90.0	-	-	-
19 (reg)	oC	248	81.3	183.3	81.9	90.0	90.0	90.0	-	-	-

Spacegroup: P23

Mosaicity: 0.92 Estimate

Normally the solution with the highest symmetry from the group of solutions with low penalties is correct. However, beware of pseudosymmetry !

Note here that the chosen solution (cubic) has a $\sigma(xy)$ value of 0.34mm while for the (correct) orthorhombic solution this value is 0.18mm

The true symmetry can only be determined by integrating some of the images

If known, the true space group can be selected from the drop down menu

Indexing – Other tips

- If even the triclinic solution (solution 1) has a high positional error ($\sigma(xy)$), sometimes selecting this triclinic solution and then repeating the indexing will help find the correct solution. This is because the direct beam coordinates are refined as part of the indexing.

Incorrect direct beam coordinates are the most common cause of indexing failure.

- **Beware !** Indexing from a single image can give incorrect results for low symmetry space groups. The prediction will fit for the image used in the indexing, but not for images at very different phi values.
- Beware of pseudo centering or lattice repeats which result in a class of reflections being systematically weaker than the rest (eg a pseudo lattice translation of $a/2$ will mean that all h odd reflections are weak). If only the strongest reflections are used in indexing, the resulting cell will be too small.

Indexing – Mosaicity estimation

History

2 (ref)	aP	0	58.5	58.6	62.1	61.9	62.0	60.0	0.20	0.35	0.44	(0.1)
3 (ref)	mC	1	101.3	58.6	62.2	90.0	123.0	90.0	0.21	0.42	0.44	(0.1)
4 (ref)	mC	1	101.4	58.5	62.1	90.0	122.9	90.0	0.20	0.39	0.45	(0.2)
5 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45	(0.2)
6 (ref)	hR	2	58.6	58.6	156.4	90.0	90.0	120.0	0.21	0.54	0.46	(0.3)
7 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45	(0.2)
8 (reg)	hR	60	60.4	60.4	144.8	90.0	90.0	120.0	-	-	-	-
9 (reg)	mC	60	103.5	62.2	58.5	90.0	124.4	90.0	-	-	-	-
10 (reg)	mC	60	85.3	85.4	58.5	90.0	133.2	90.0	-	-	-	-
11 (reg)	oI	60	58.6	62.2	85.3	90.0	90.0	90.0	-	-	-	-
12 (reg)	mC	61	101.4	58.6	62.1	90.0	122.9	90.0	-	-	-	-
13 (reg)	tI	61	60.4	60.4	85.3	90.0	90.0	90.0	-	-	-	-
14 (reg)	oI	61	58.5	62.2	85.4	90.0	90.0	90.0	-	-	-	-
15 (reg)	mC	61	101.5	58.5	62.2	90.0	122.9	90.0	-	-	-	-

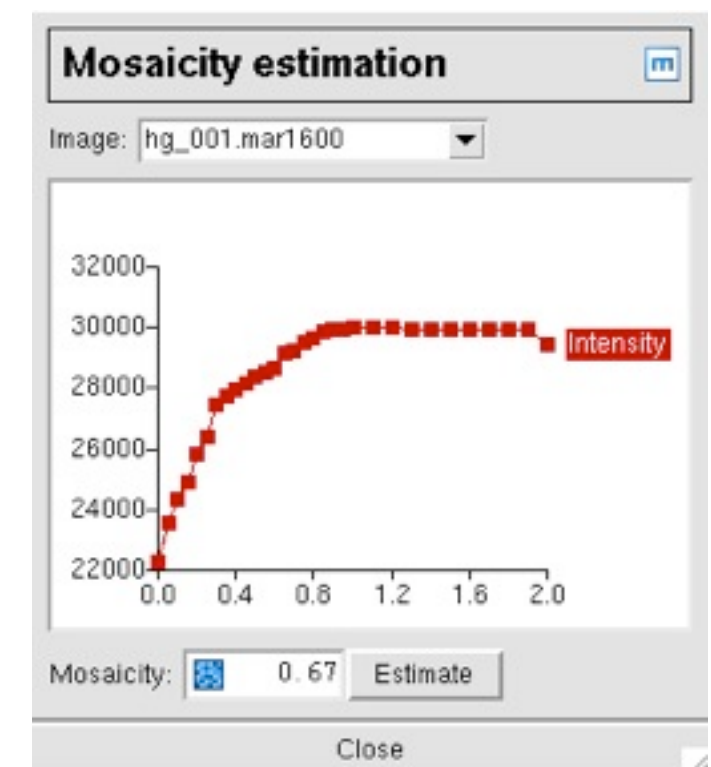
Spacegroup: h3

Mosaicity: 0.00 Estimate

Start beam-centre search [+]

No Warnings

The image is integrated many times with increasing values of the mosaic spread, and the total intensity of all predicted spots is plotted against mosaicity. A point corresponding to the shoulder of this curve is taken as the best estimate.



Indexing – Mosaicity estimation

History

2 (ref)	aP	0	58.5	58.6	62.1	61.9	62.0	60.0	0.20	0.35	0.44	(0.1)
3 (ref)	mC	1	101.3	58.6	62.2	90.0	123.0	90.0	0.21	0.42	0.44	(0.1)
4 (ref)	mC	1	101.4	58.5	62.1	90.0	122.9	90.0	0.20	0.39	0.45	(0.2)
5 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45	(0.2)
6 (ref)	hR	2	58.6	58.6	156.4	90.0	90.0	120.0	0.21	0.54	0.46	(0.3)
7 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45	(0.2)
8 (reg)	hR	60	60.4	60.4	144.8	90.0	90.0	120.0	-	-	-	-
9 (reg)	mC	60	103.5	62.2	58.5	90.0	124.4	90.0	-	-	-	-
10 (reg)	mC	60	85.3	85.4	58.5	90.0	133.2	90.0	-	-	-	-
11 (reg)	oI	60	58.6	62.2	85.3	90.0	90.0	90.0	-	-	-	-
12 (reg)	mC	61	101.4	58.6	62.1	90.0	122.9	90.0	-	-	-	-
13 (reg)	tI	61	60.4	60.4	85.3	90.0	90.0	90.0	-	-	-	-
14 (reg)	oI	61	58.5	62.2	85.4	90.0	90.0	90.0	-	-	-	-
15 (reg)	mC	61	101.5	58.5	62.2	90.0	122.9	90.0	-	-	-	-

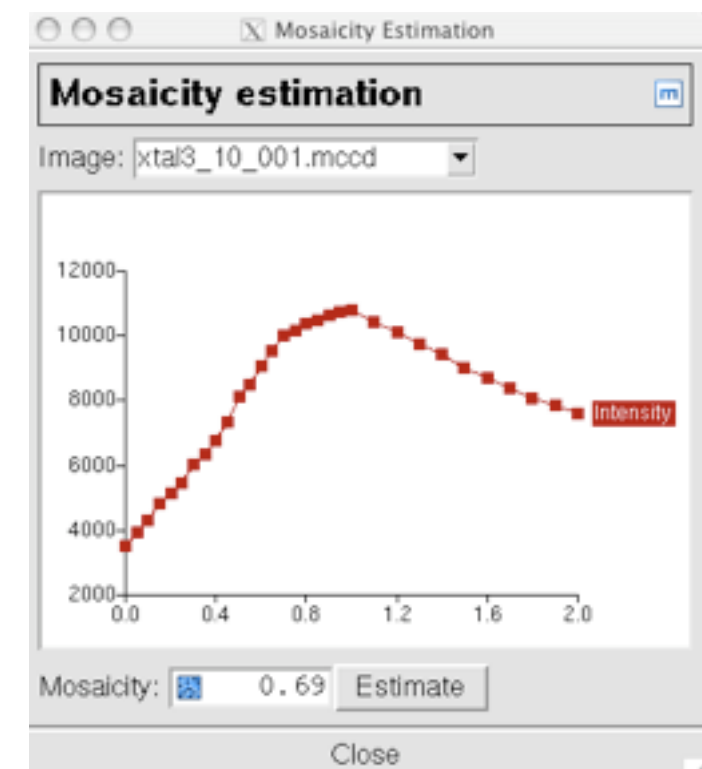
Spacegroup: h3

Mosaicity: 0.00 Estimate

Start beam-centre search [+]

No Warnings

If the unit cell is large, the total intensity will drop at high values of mosaic spread, because overlapping reflections are not included.



Indexing – Mosaicity estimation

History

2 (ref)	aP	0	58.5	58.6	62.1	61.9	62.0	60.0	0.20	0.35	0.44	(0.1)
3 (ref)	mC	1	101.3	58.6	62.2	90.0	123.0	90.0	0.21	0.42	0.44	(0.1)
4 (ref)	mC	1	101.4	58.5	62.1	90.0	122.9	90.0	0.20	0.39	0.45	(0.2)
5 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45	(0.2)
6 (ref)	hR	2	58.6	58.6	156.4	90.0	90.0	120.0	0.21	0.54	0.46	(0.3)
7 (ref)	mC	2	101.5	58.5	62.1	90.0	122.9	90.0	0.20	0.36	0.45	(0.2)
8 (reg)	hR	60	60.4	60.4	144.8	90.0	90.0	120.0	-	-	-	-
9 (reg)	mC	60	103.5	62.2	58.5	90.0	124.4	90.0	-	-	-	-
10 (reg)	mC	60	85.3	85.4	58.5	90.0	133.2	90.0	-	-	-	-
11 (reg)	oI	60	58.6	62.2	85.3	90.0	90.0	90.0	-	-	-	-
12 (reg)	mC	61	101.4	58.6	62.1	90.0	122.9	90.0	-	-	-	-
13 (reg)	tI	61	60.4	60.4	85.3	90.0	90.0	90.0	-	-	-	-
14 (reg)	oI	61	58.5	62.2	85.4	90.0	90.0	90.0	-	-	-	-
15 (reg)	mC	61	101.5	58.5	62.2	90.0	122.9	90.0	-	-	-	-

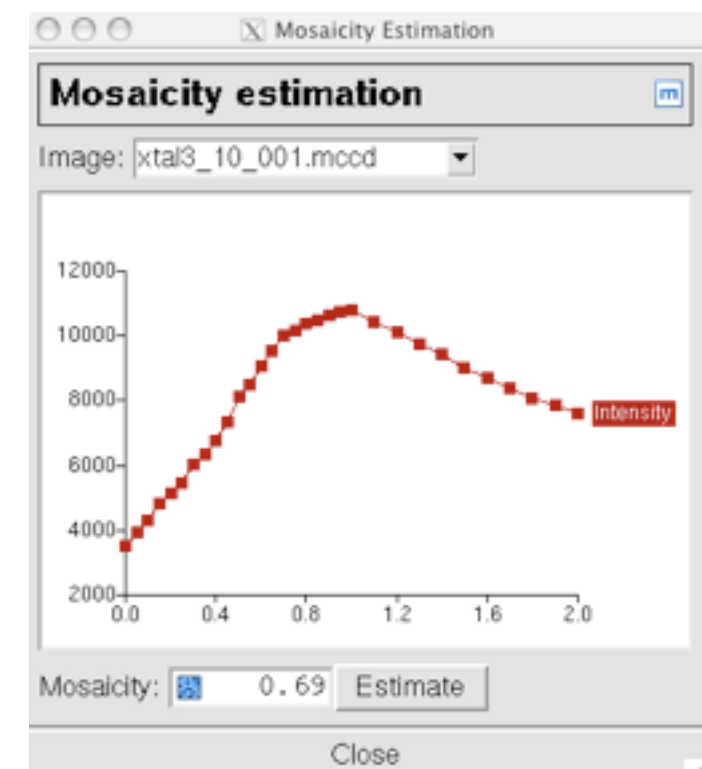
Spacegroup: h3

Mosaicity: 0.00 Estimate

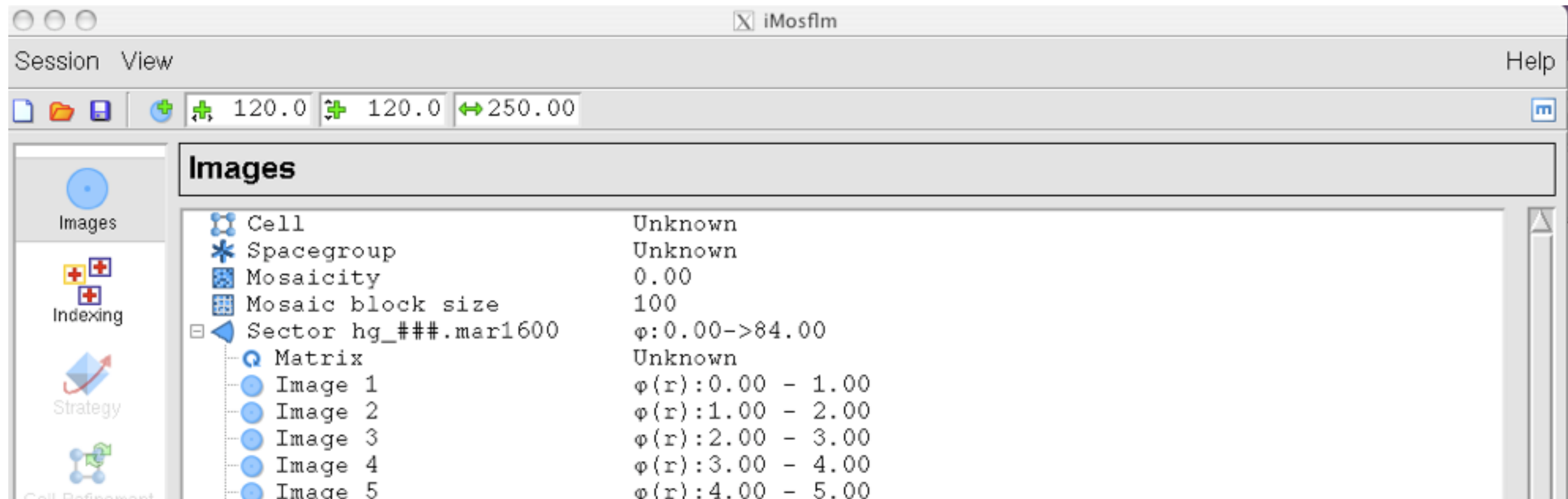
Start beam-centre search [+]

No Warnings

If the initial orientation is incorrect, the mosaicity will be over-estimated. This will be corrected during integration.



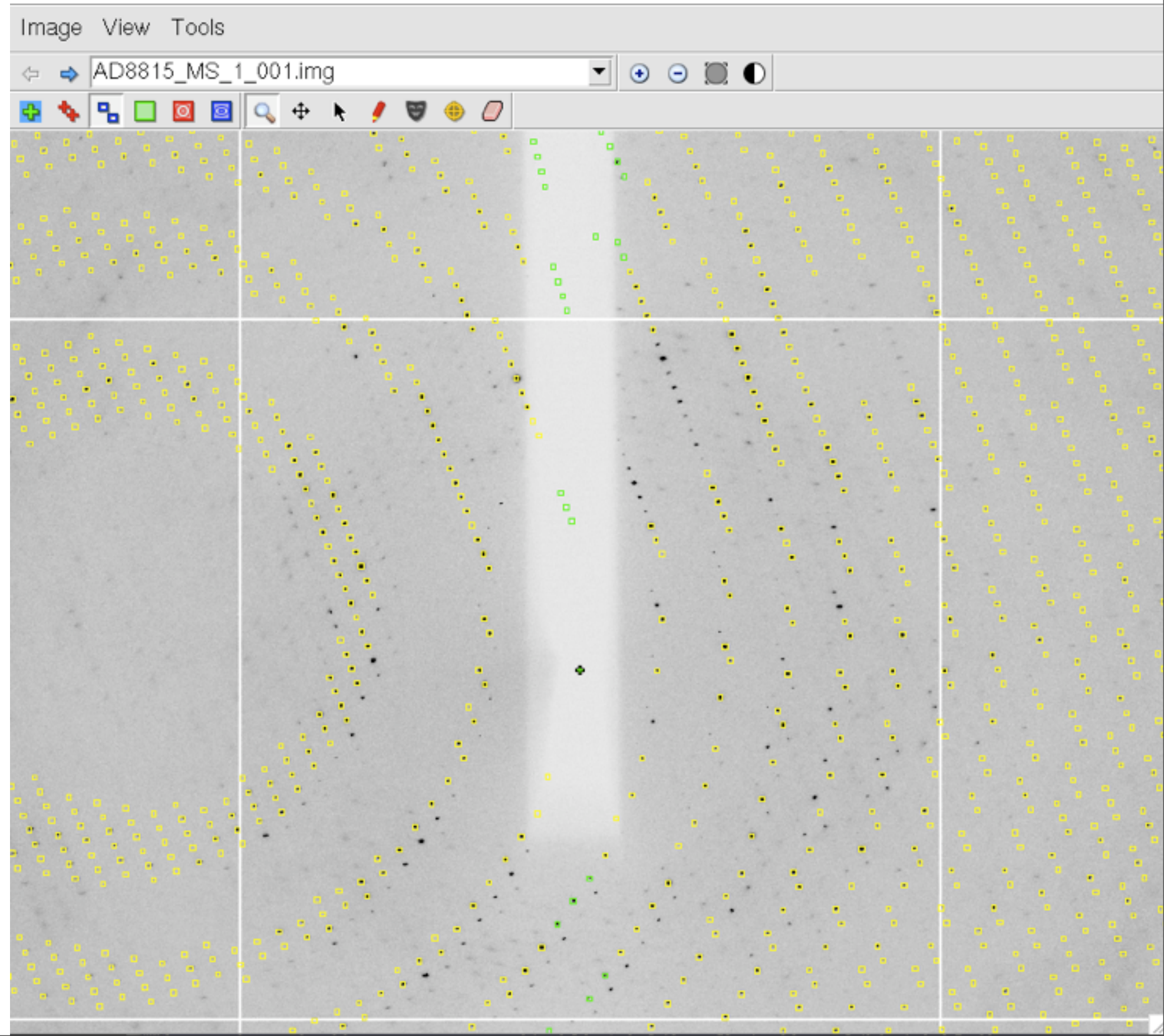
Mosaicity – the effect of the mosaic block size



Decreasing the mosaic block size has the effect of increasing the apparent mosaic spread at low resolution (Nave, C. (1998) Acta Cryst D54, 848-853)

Mosaicity – the effect of the mosaic block size

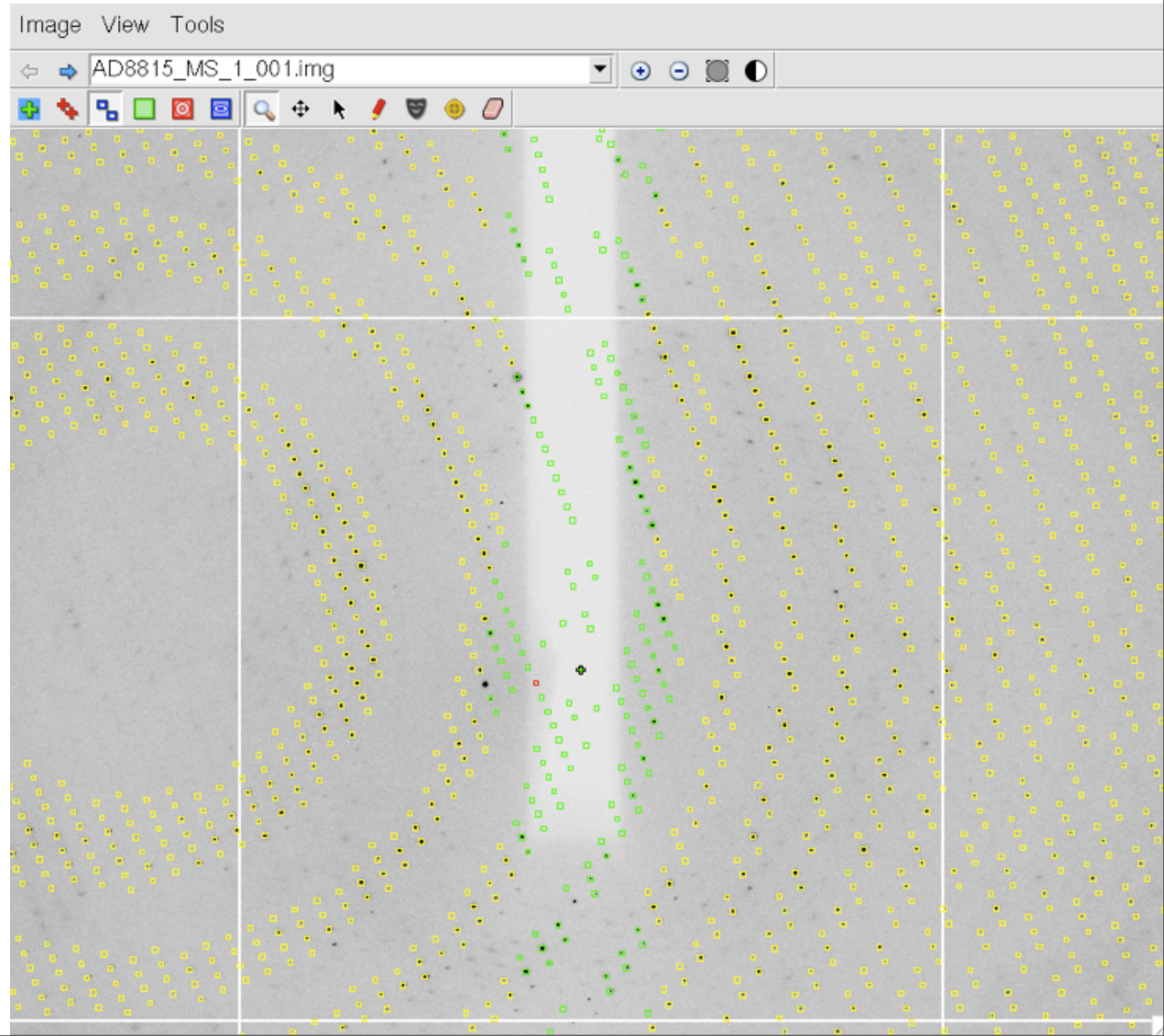
Blocksize 100 μ



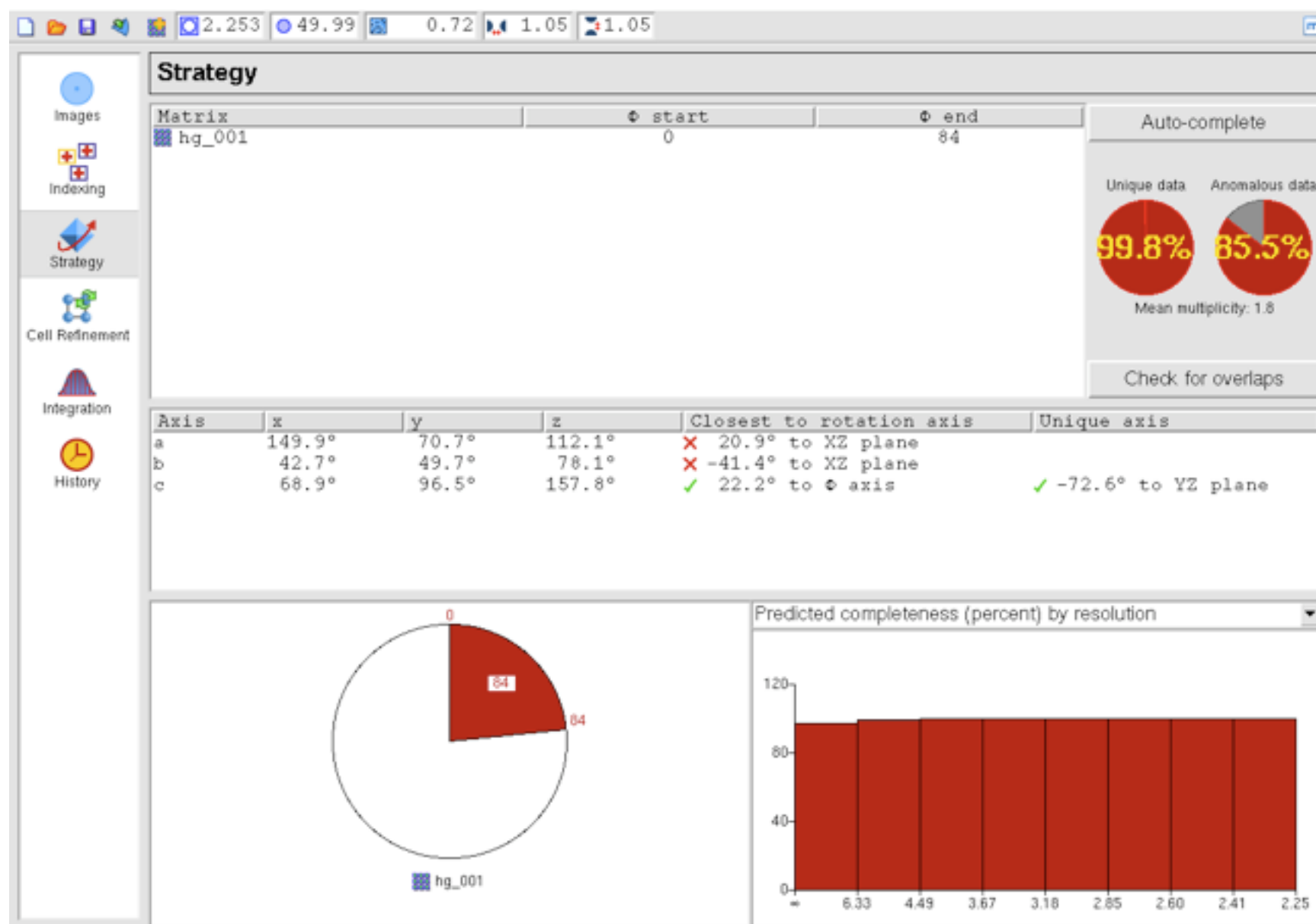
Mosaicity – the effect of the mosaic block size

Blocksize 0.2μ

It may be necessary to increase the maximum reflection width to avoid losing reflections (green boxes)



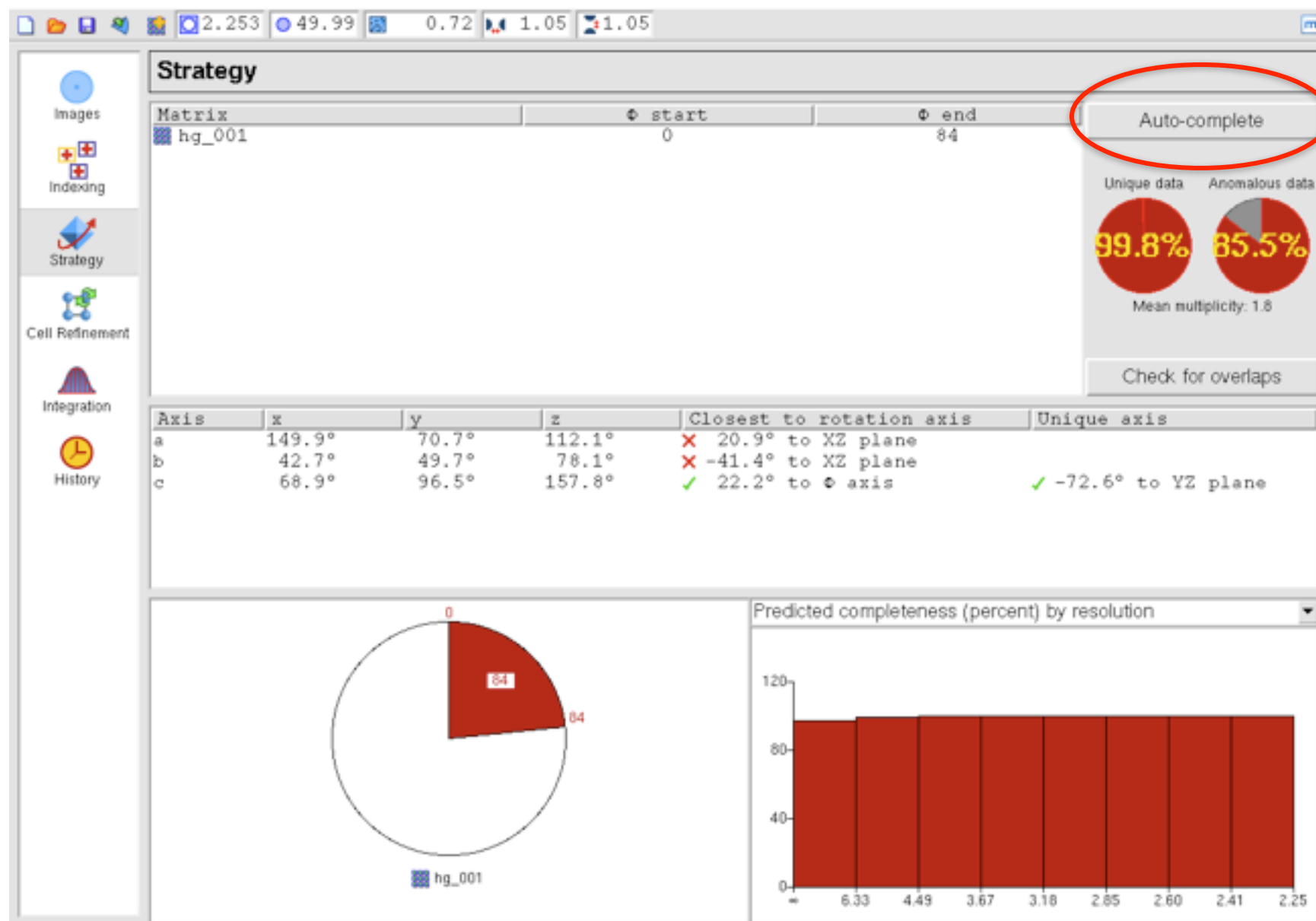
Strategy



Initial strategy results assume that all data between phi start and phi end have been collected !

To calculate a strategy, select the “Auto-complete” button.

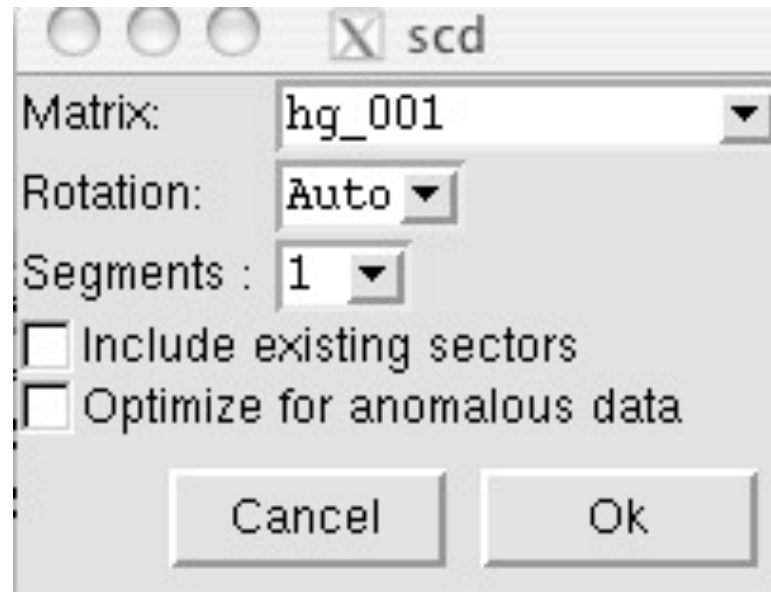
Strategy



Initial strategy results assume that all data between phi start and phi end have been collected !

To calculate a strategy, select the “Auto-complete” button.

Strategy

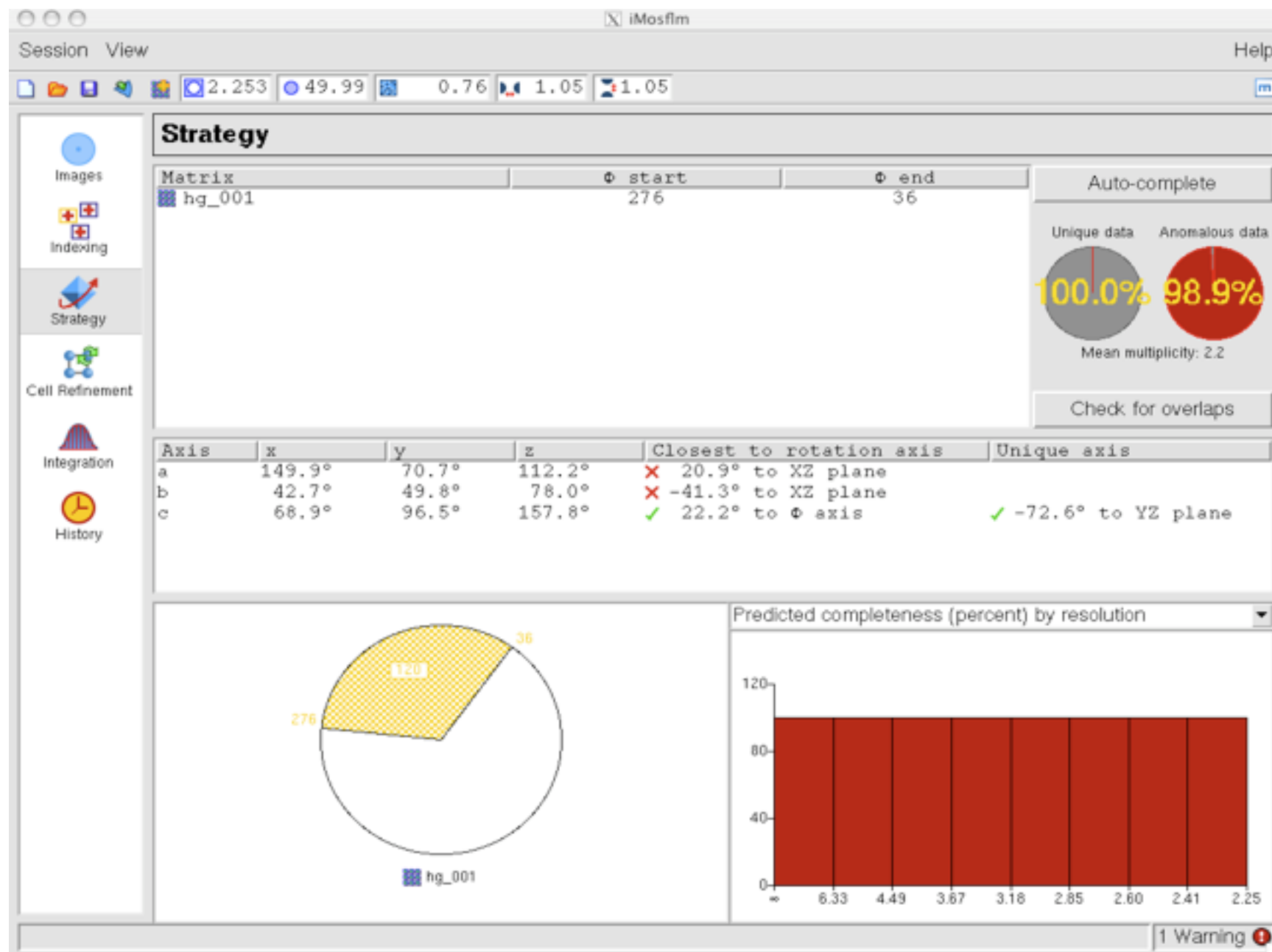


Use defaults for a normal strategy calculation

High completeness (>94%) can be achieved with a smaller total rotation by collecting the data in segments. Eg 2 segments of 30° each for orthorhombic. Select the desired total rotation and the number of segments from pull down menus.

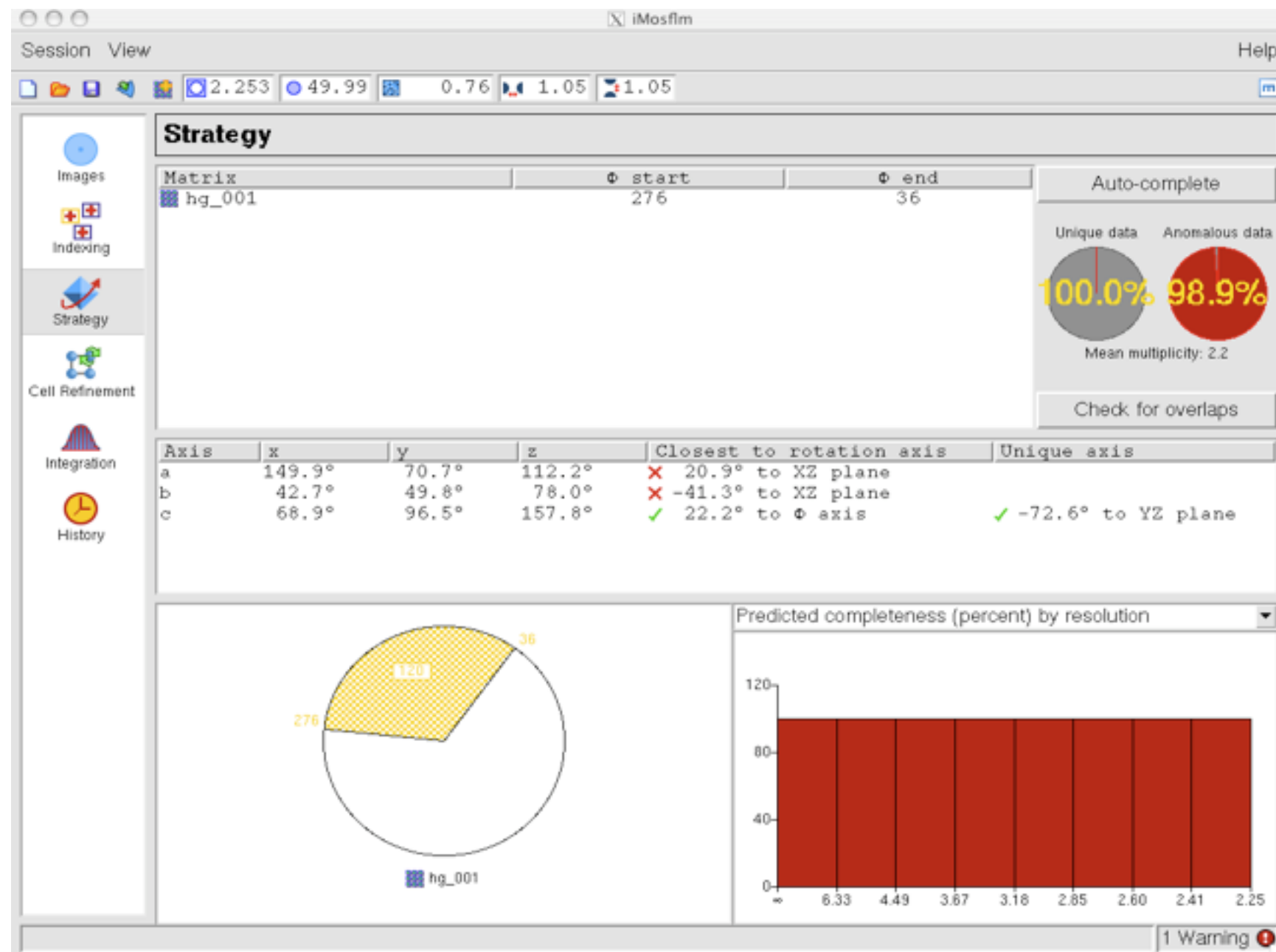
If collecting anomalous data, remember to tick the box !

Strategy



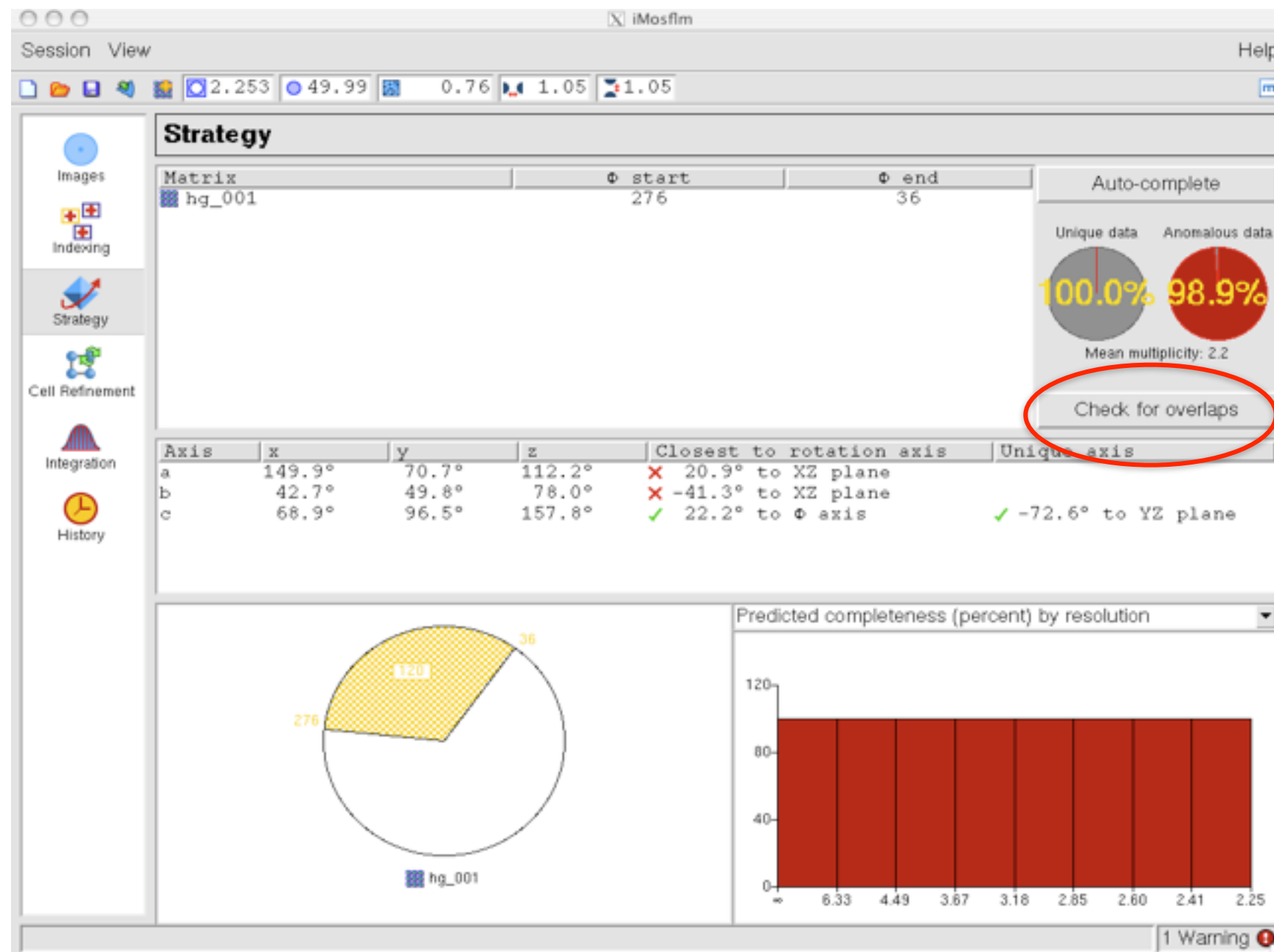
The start end end point of the suggested strategy can be dragged with the mouse to test other rotation ranges.

Strategy



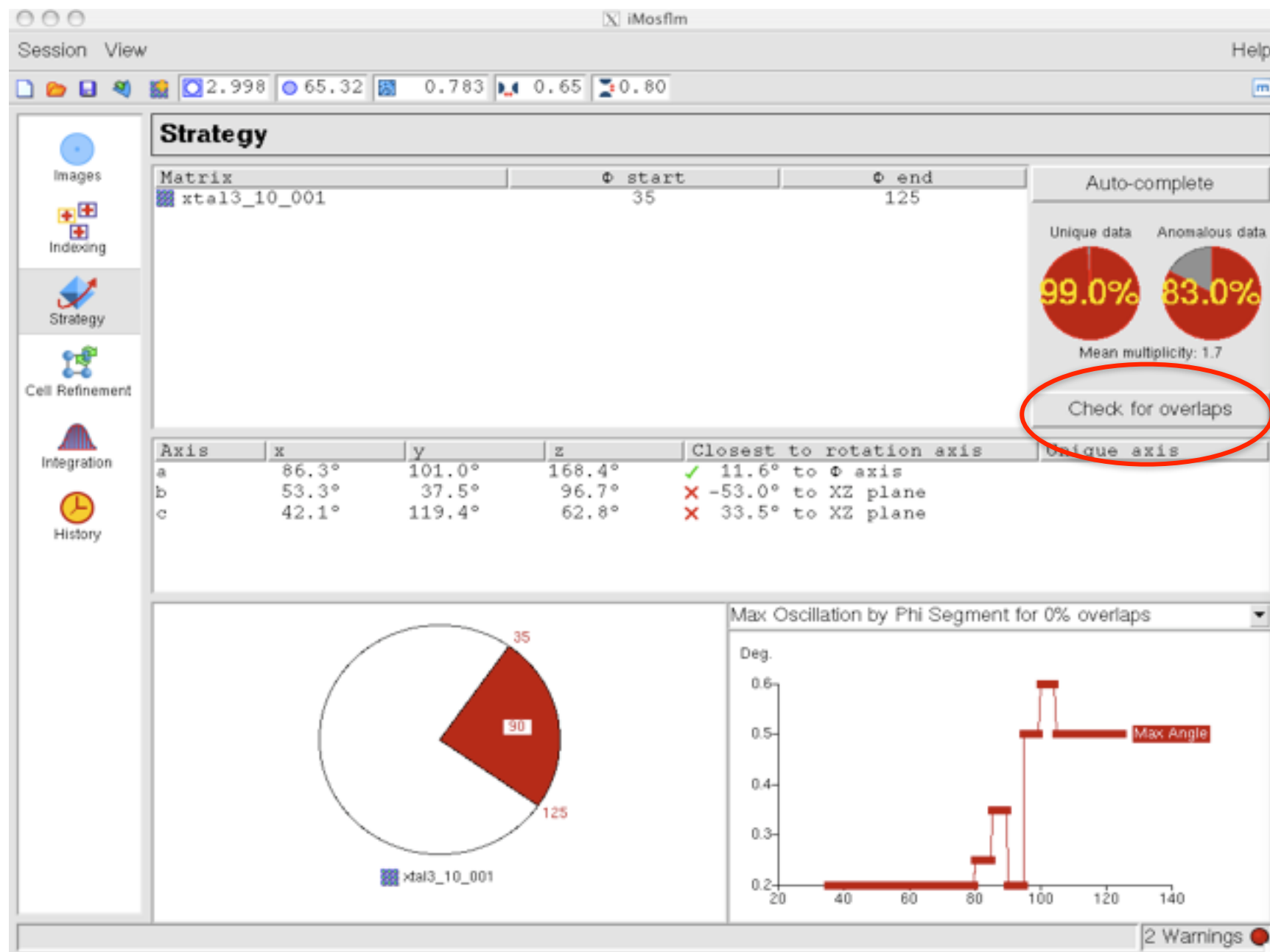
Select “Check for overlaps” to determine maximum oscillation angle without overlaps

Strategy



Select "Check for overlaps" to determine maximum oscillation angle without overlaps

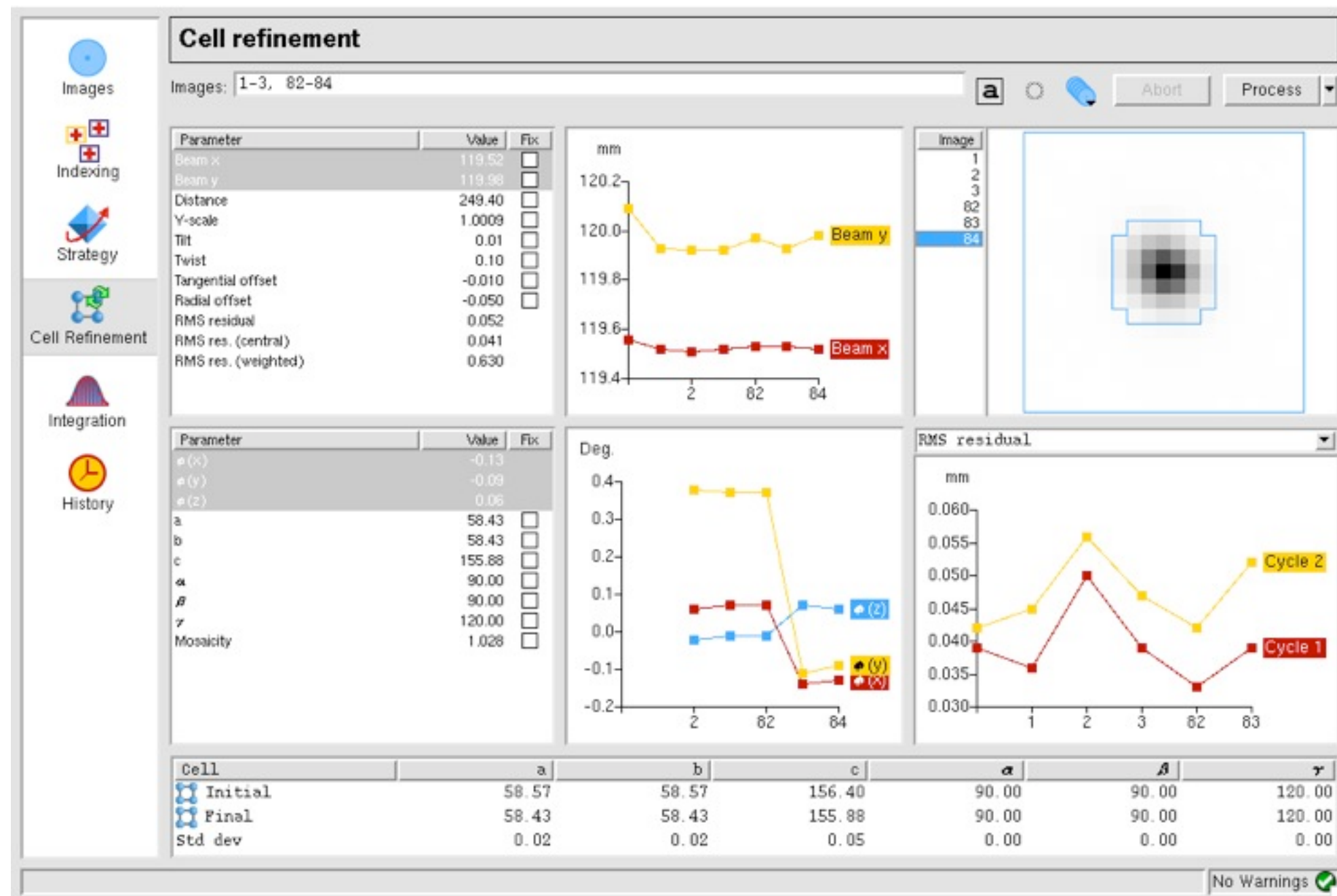
Strategy



Select “Check for overlaps” to determine maximum oscillation angle without overlaps

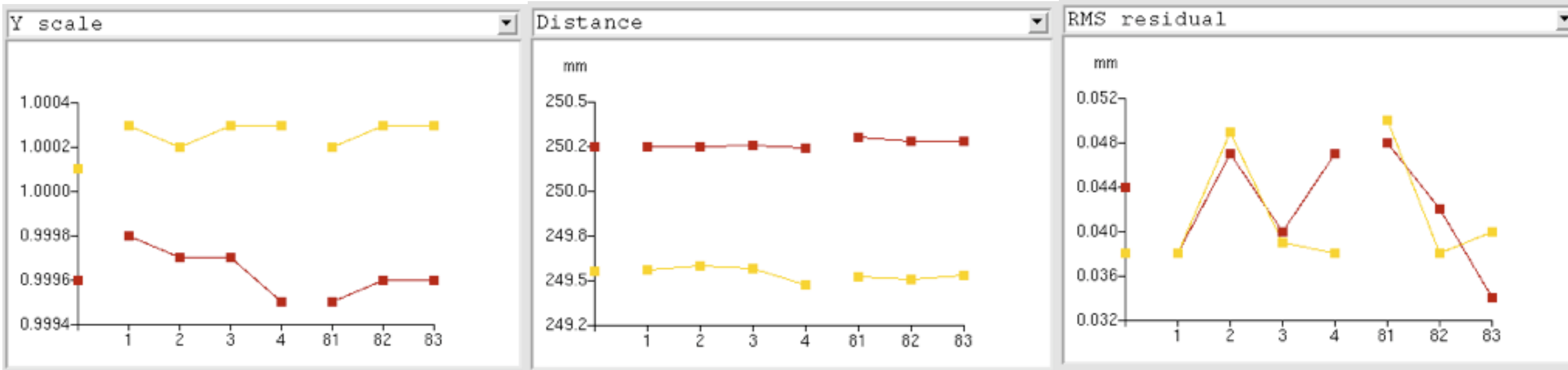
Cell refinement

For cell refinement, two small wedges of data separated by about 90° in phi are integrated. The way in which the total spot intensity of partially recorded reflections is distributed across adjacent images is used to refine crystal cell parameters, orientation and mosaicity. Final cell sds should ideally be less than 0.1 Å.



Cell refinement

Has it worked ?



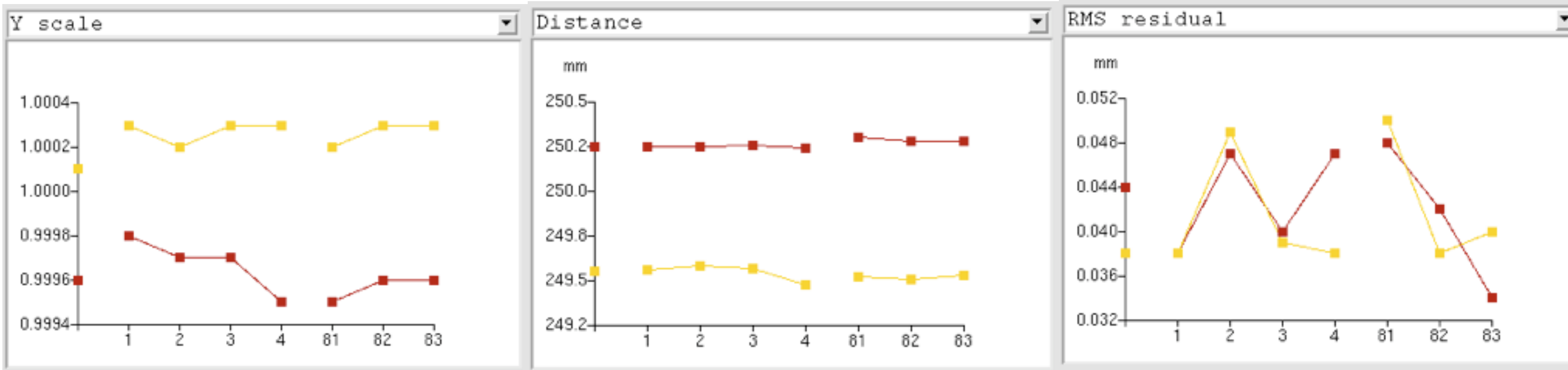
At resolutions less than $\sim 3.3\text{\AA}$, the cell refinement may not work well.

Indicators that it has worked are:

- Yscale is close to 1.0 for all images
- The detector distance is the same for all images
- The rms residual is smaller at the end of refinement.

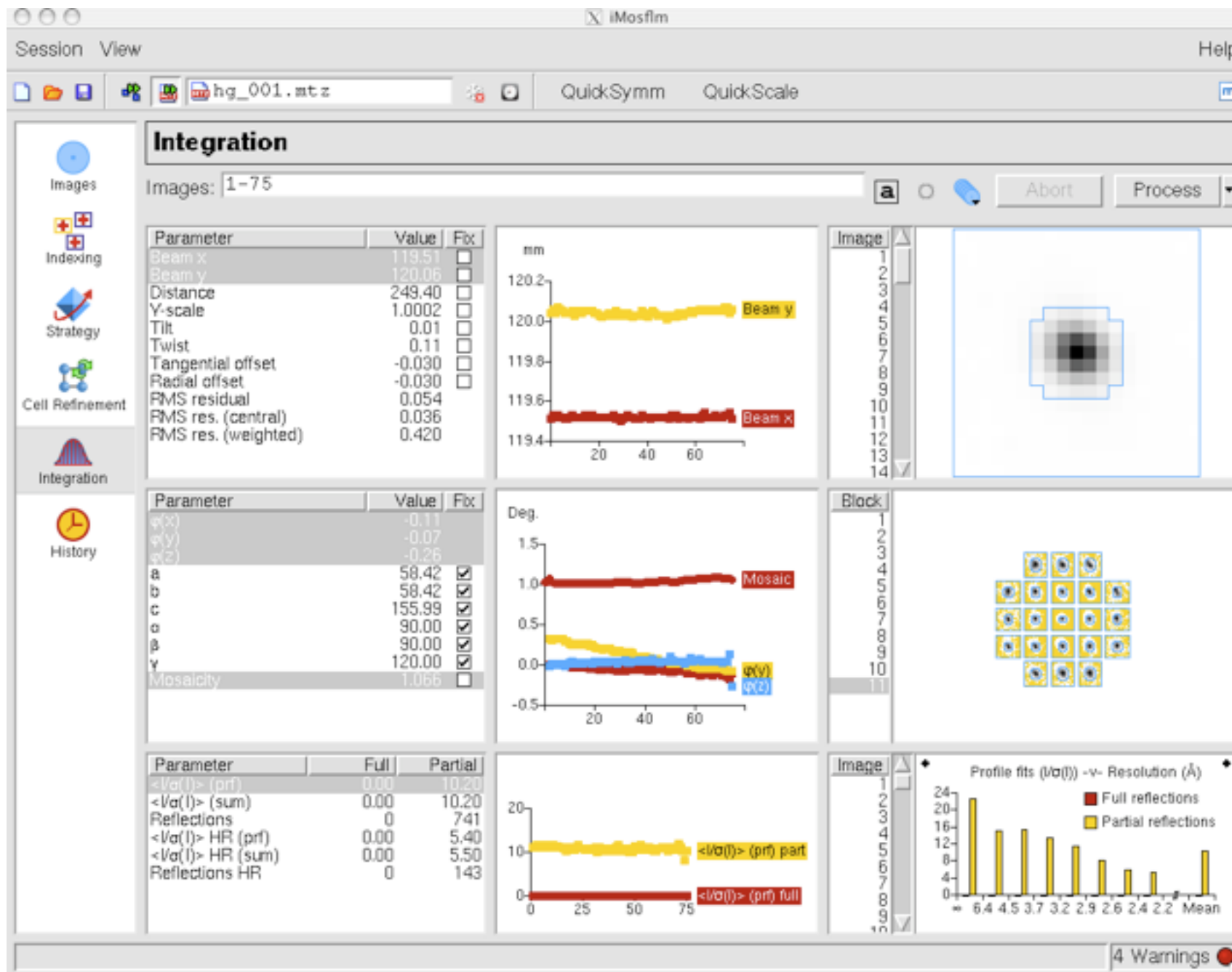
Cell refinement

Has it worked ?



If cell refinement does not work well, simply use the cell derived from autoindexing on two images (or more for low symmetries).

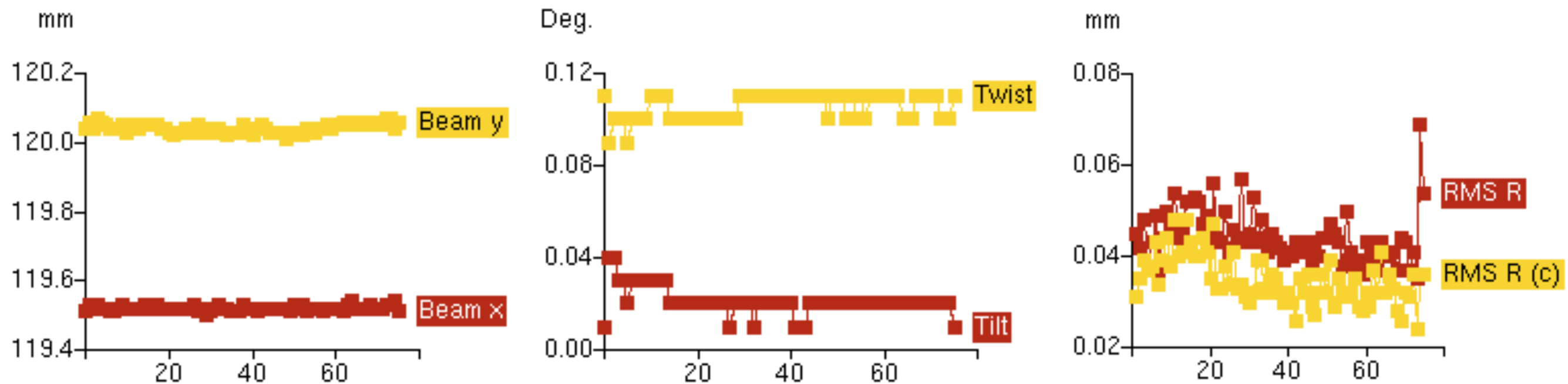
Integration



During integration, the refined detector and crystal parameters are plotted as a function of image number.

Also displayed are the average spot profile in the centre of the detector and the standard profiles and an indication of data quality ($I/\sigma(I)$) as a function of resolution)

Integration - Stability of refined detector parameters

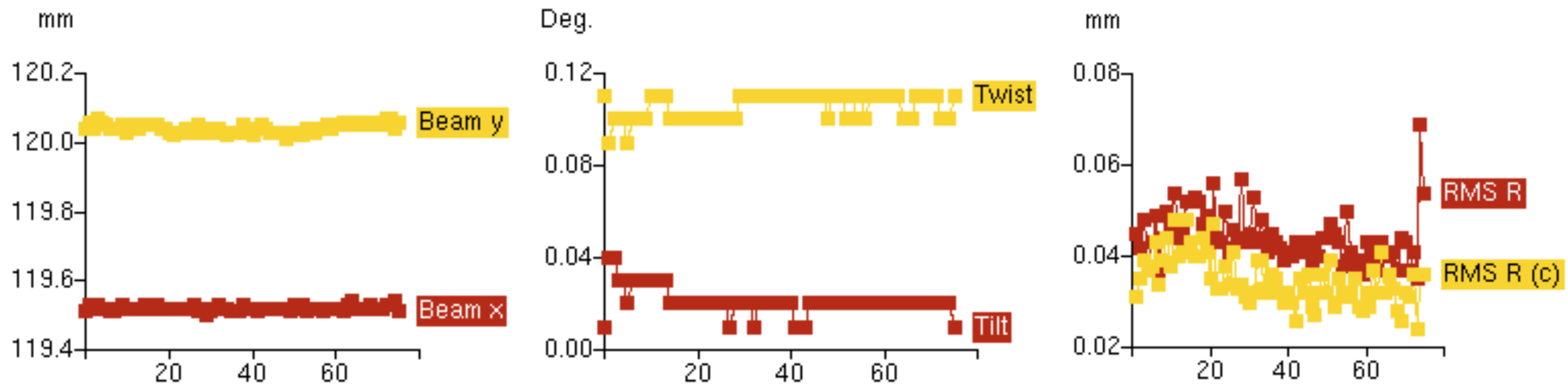


Detector parameters should remain stable during integration

- Direct beam coordinates should not vary by more than 0.1-0.2mm
- Detector tilt and twist should not vary more than 0.2-0.3 degrees
- Rms error in spot positions should be more or less constant (unless spot size/quality or strength of diffraction is changing significantly).

Parameters can be fixed if necessary, but only as a last resort !

Integration - Stability of refined detector parameters



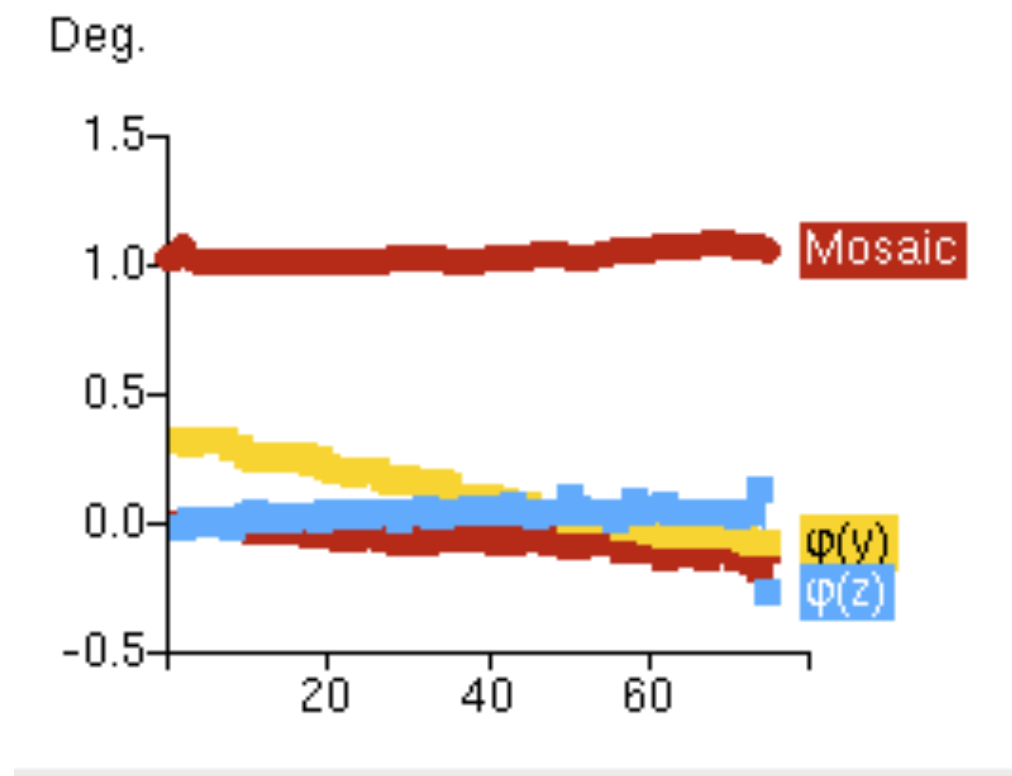
Detector parameters should remain stable during integration

- Direct beam coordinates should not vary by more than 0.1-0.2mm
- Detector tilt and twist should not vary more than 0.2-0.3 degrees
- Rms error in spot positions should be more or less constant (unless spot size/quality or strength of diffraction is changing significantly).

Parameters can be fixed if necessary, but only as a last resort !

Beware: Beam Y coordinate will appear to change if Yscale parameter changes (compensates for error in cell parameters).

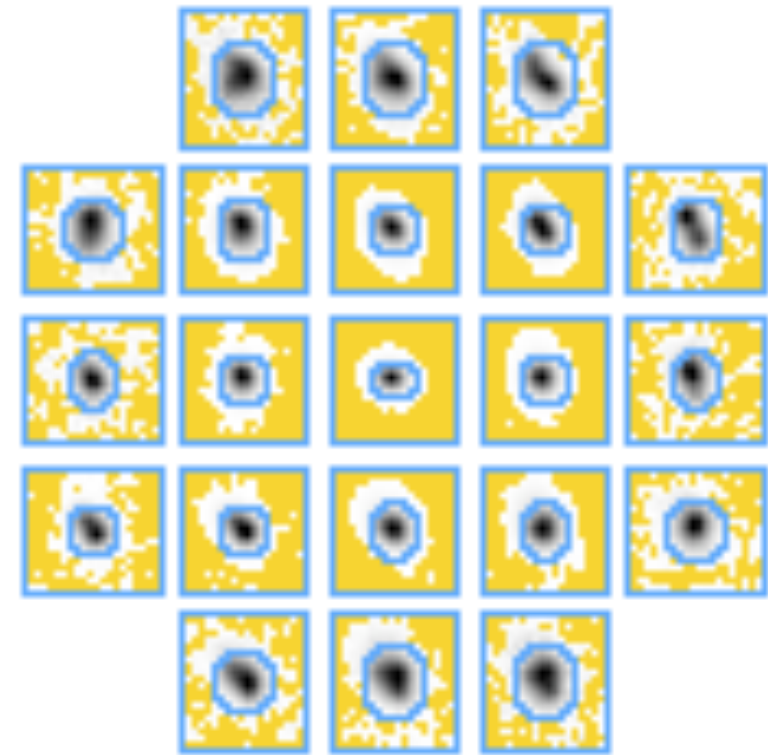
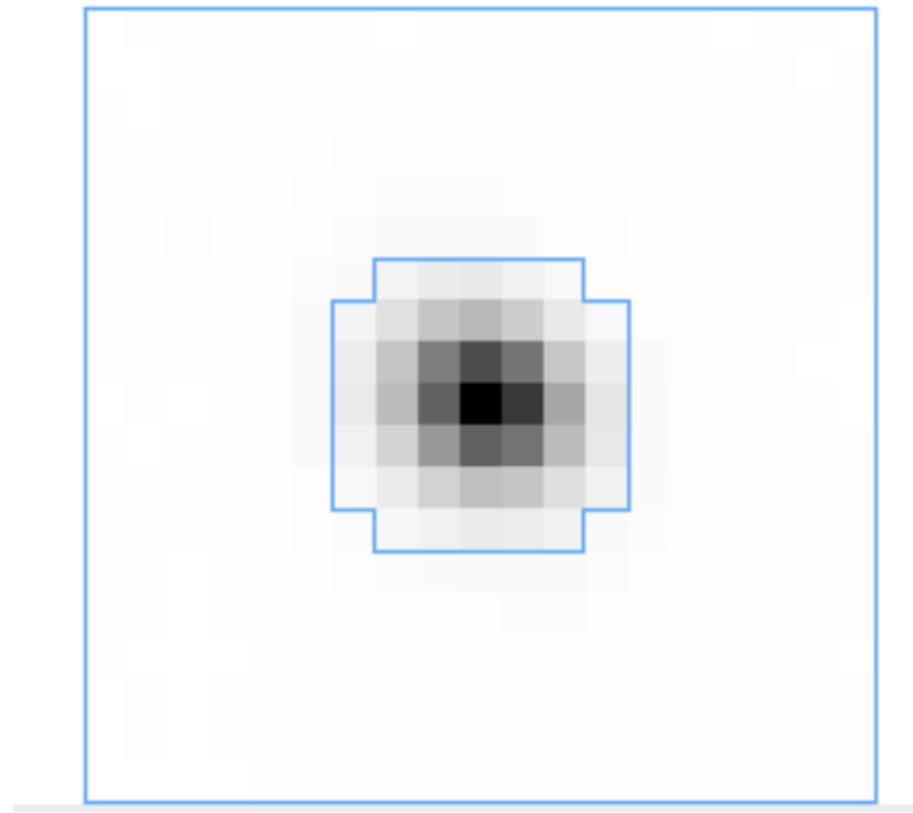
Integration – Stability of refined crystal parameters



Refined “missets” $\varphi(x)$, $\varphi(y)$, $\varphi(z)$ should vary less than $0.1 \times$ mosaic spread from one image to the next. A smooth variation is probably compensating for a non-orthogonal beam and rotation axis.

Refined mosaic spread should vary smoothly.

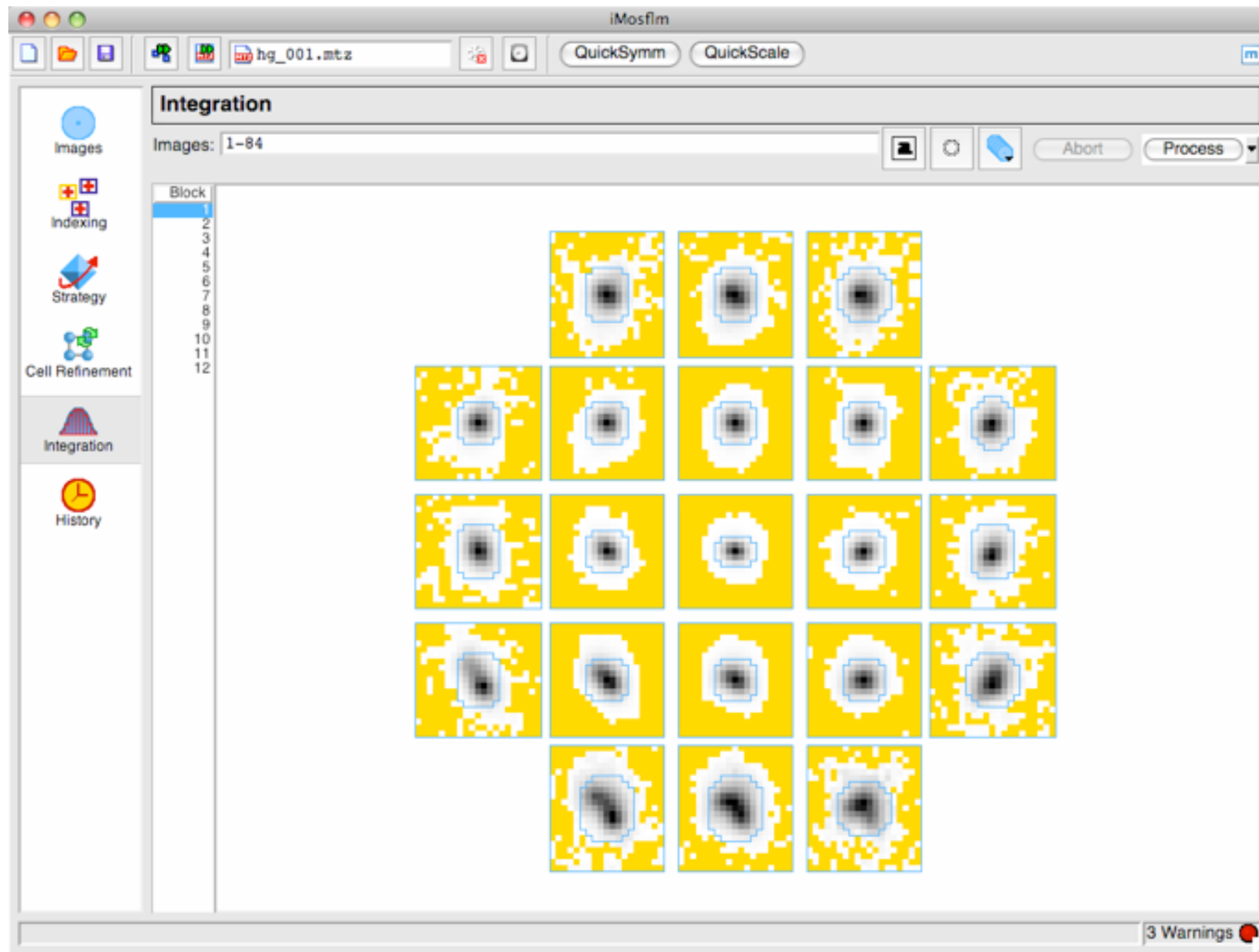
Integration – Spot profiles



The average spot profile in the central region of the detector is displayed for every image, and the standard profiles are displayed for every block of images.

The spot should be positioned centrally within the peak region of the box (inner blue boundary). The Profile Tolerance parameters can be used to make the peak region smaller or larger for special cases.

Integration – Spot profiles

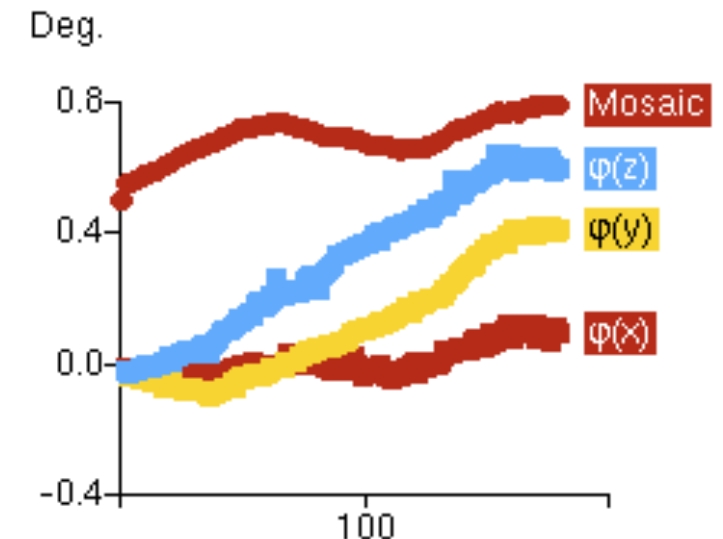
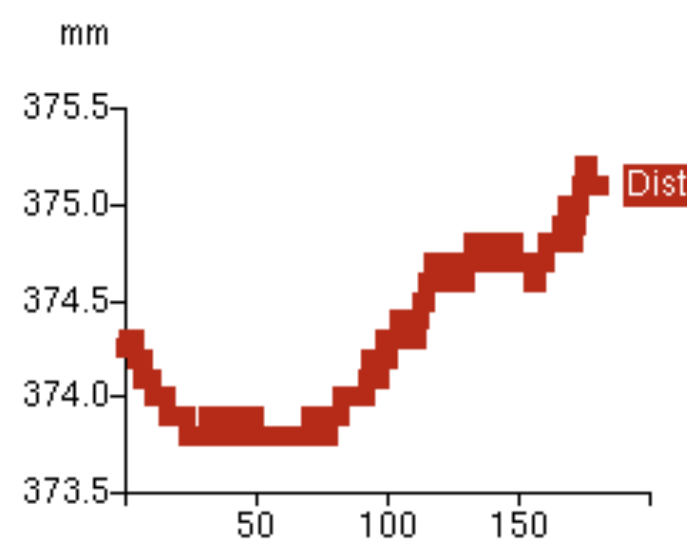
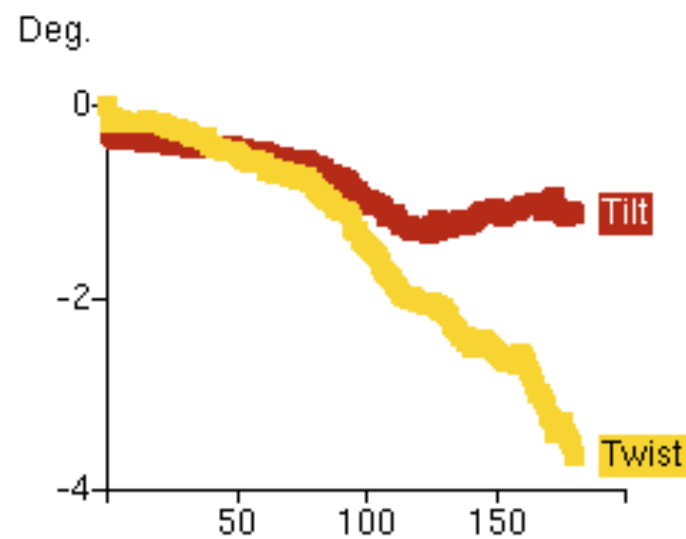
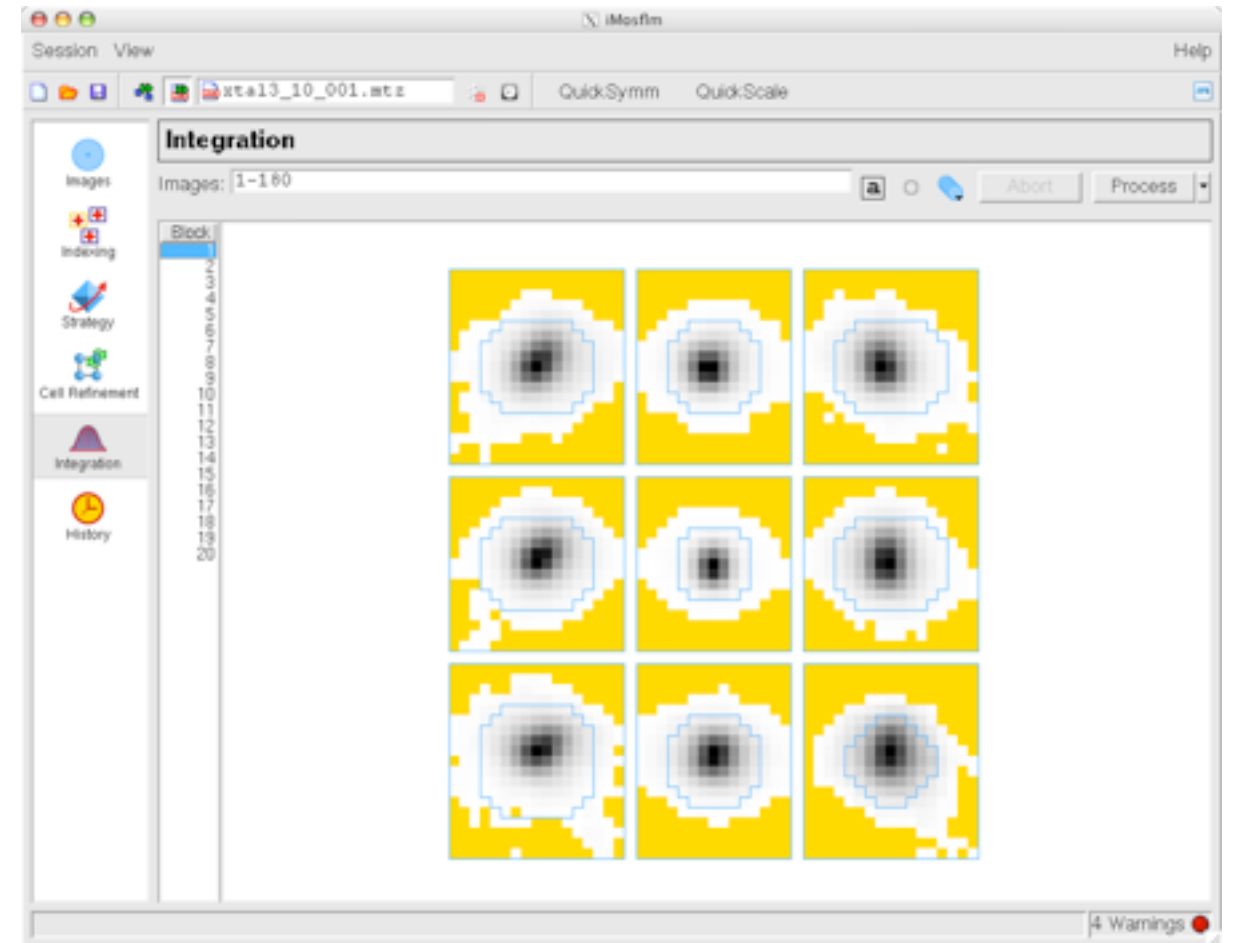


The standard profiles should be well defined for all blocks of data in the dataset

Integration – what should NOT happen

3Å weakly diffracting data,
monoclinic cell

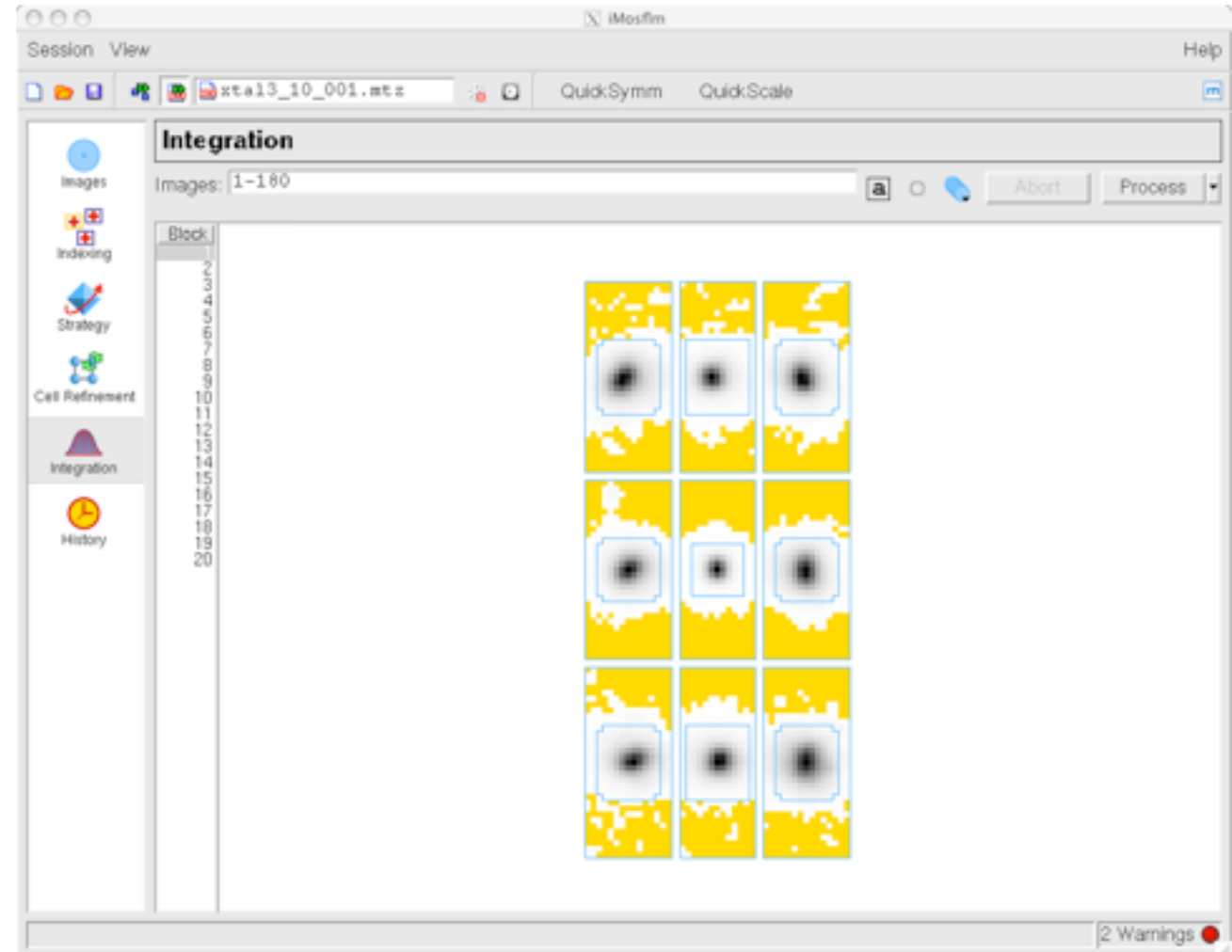
indexed from the first image only



Excessive variation in detector Tilt/Twist and distance also indicate a problem

Integration – what should NOT happen

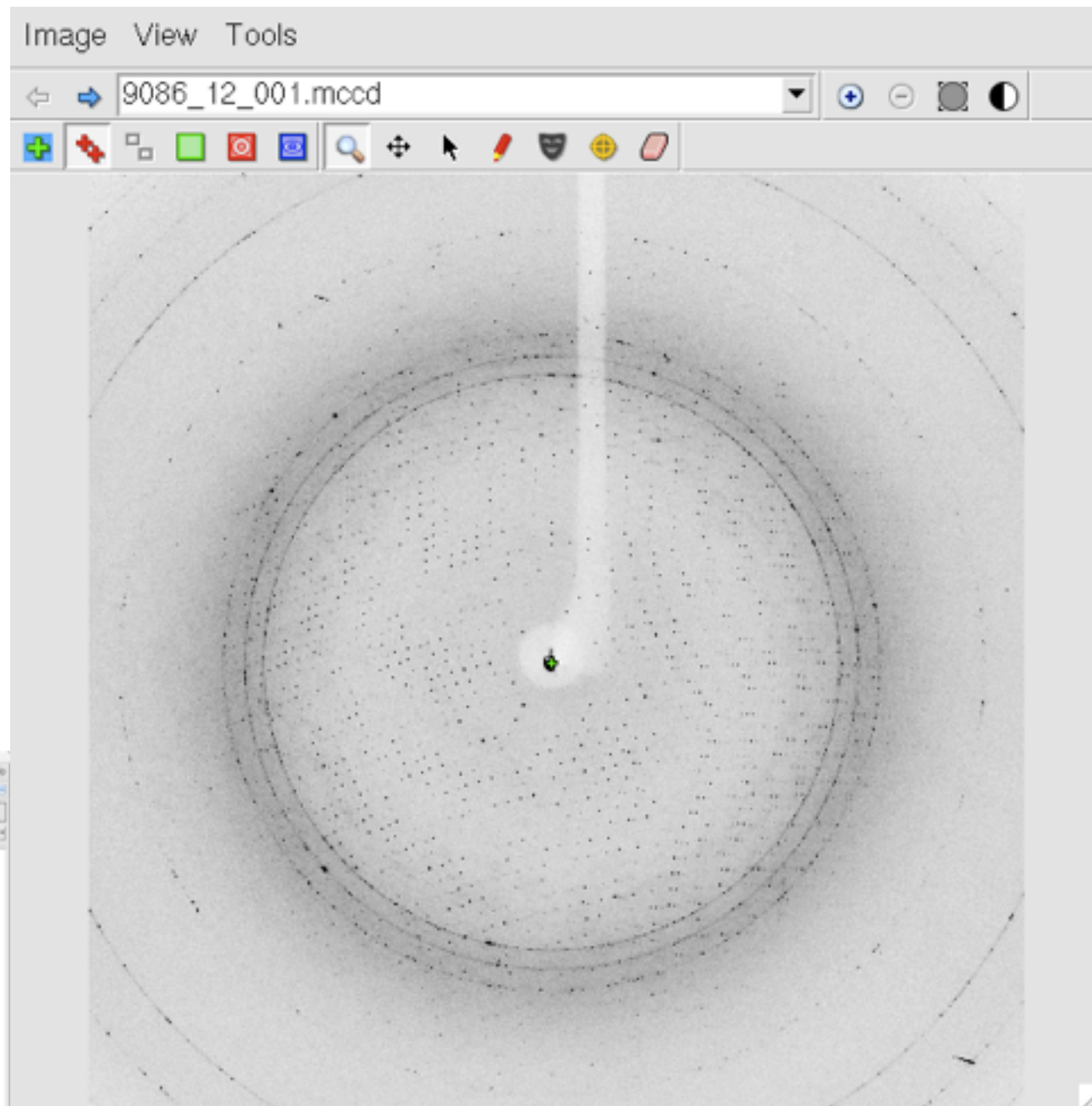
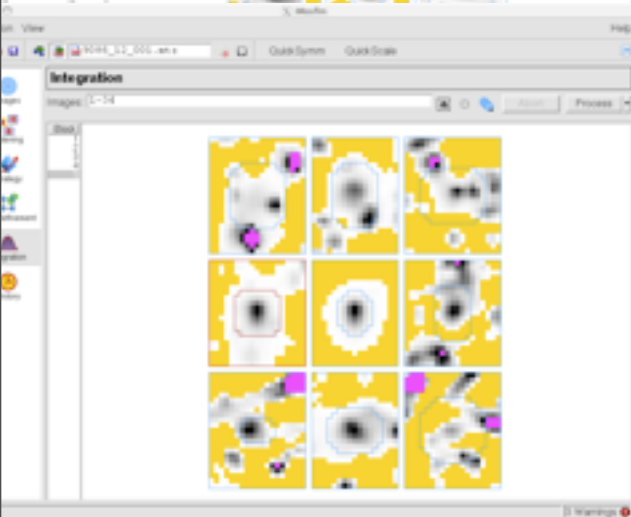
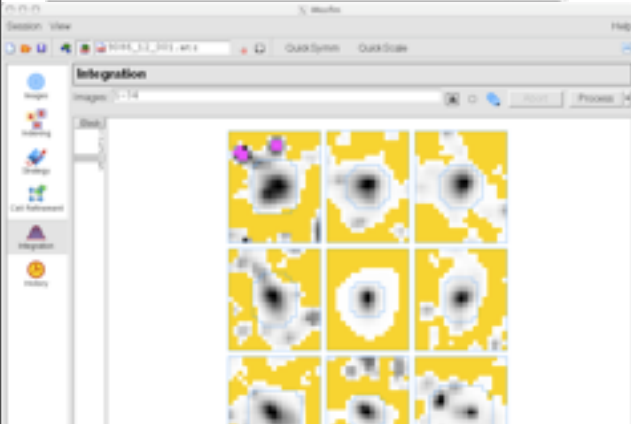
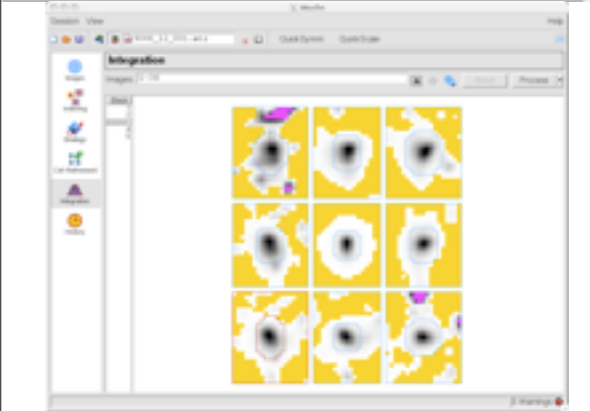
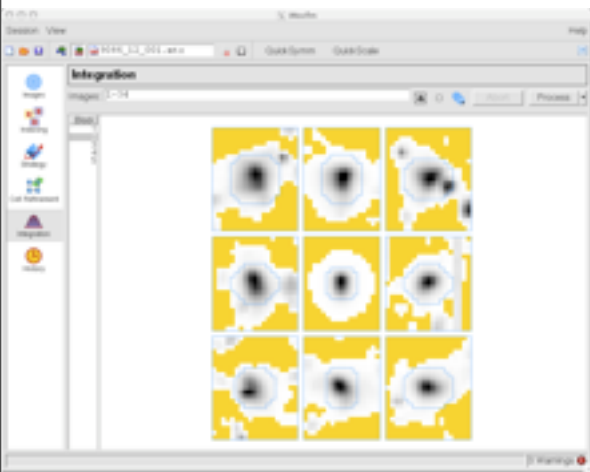
The situation improves significantly if the cell is refined (using 2 segments of data)



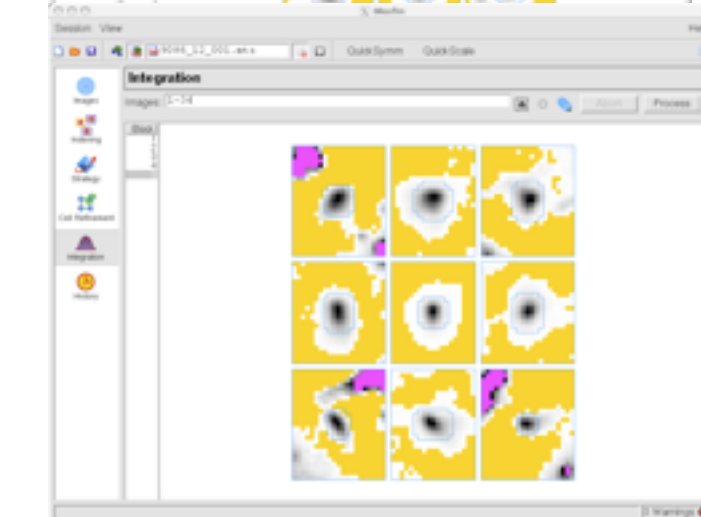
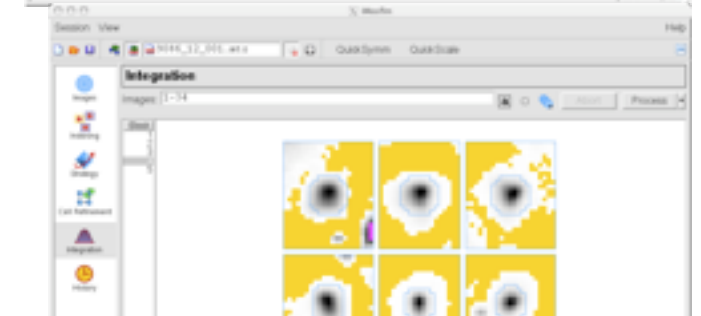
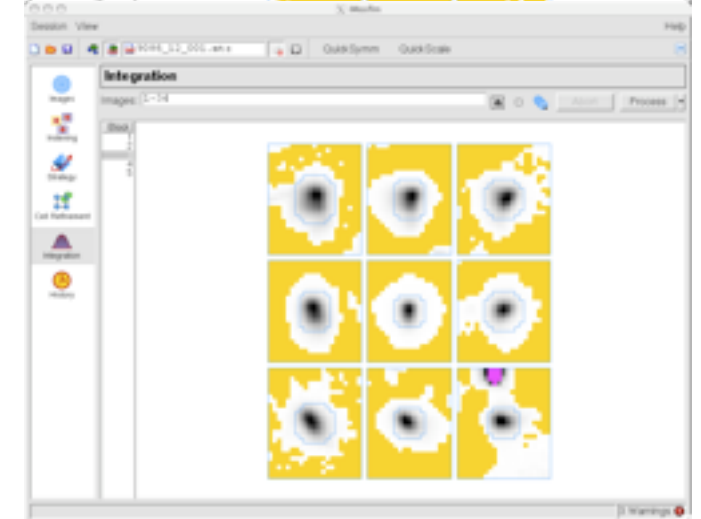
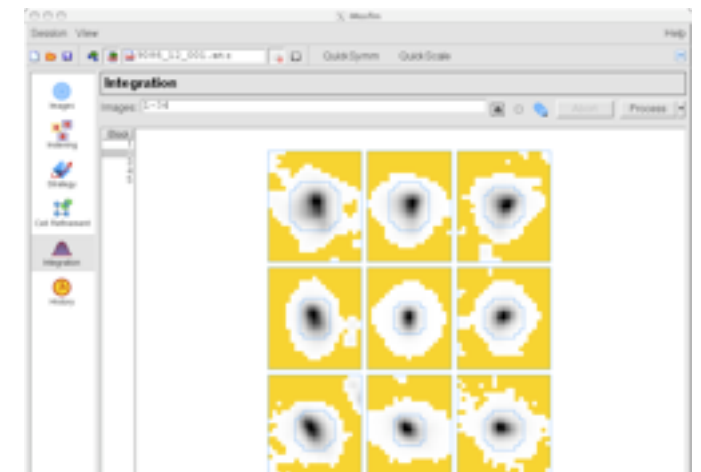
Cell parameters:

Initial	$a=148.4$	$b=130.8$	$c=209.6$	$\beta=107.3$
Refined	$a=147.8$	$b=130.8$	$c=210.4$	$\beta=108.0$

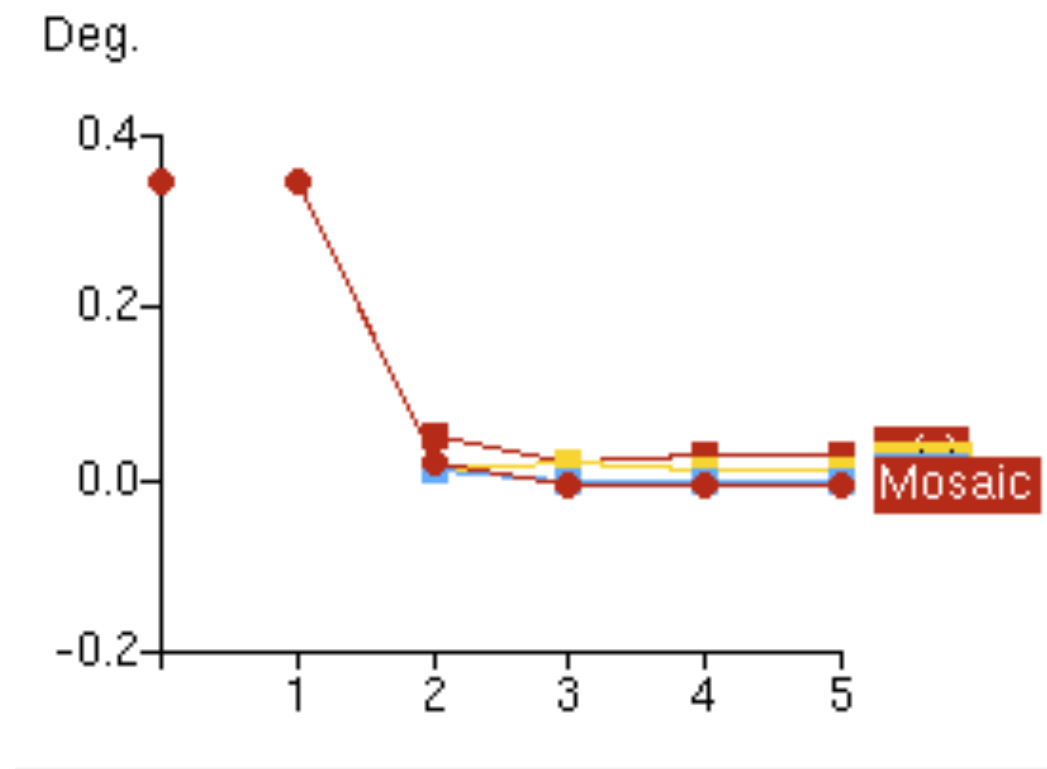
Icy Issues



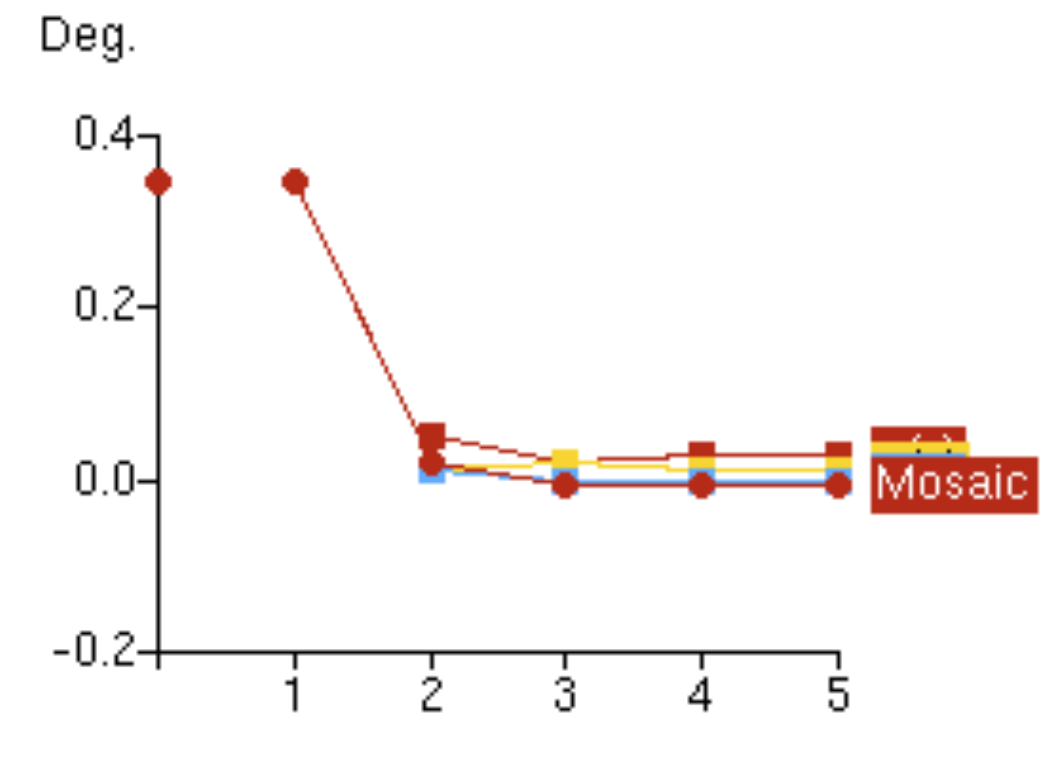
Excluding spots in the resolution shells corresponding to the rings helps improve the profiles, but leads to lower completeness (eg 98->89% at 2.6 Å)



More on what should not happen ...

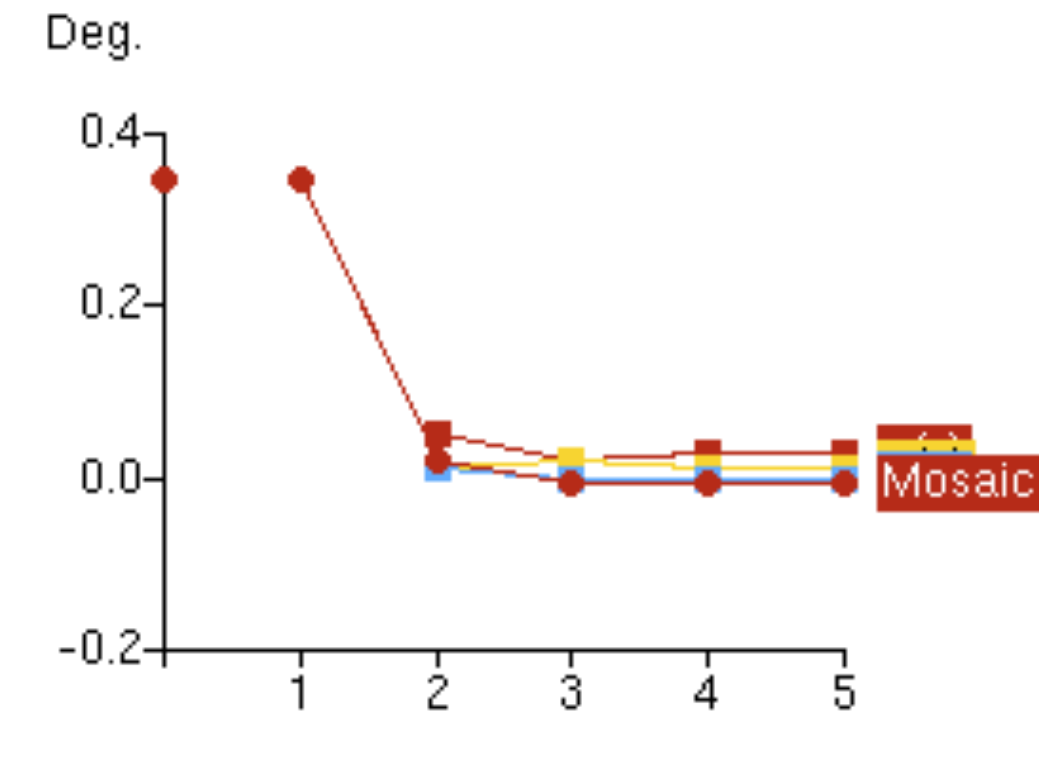


More on what should not happen ...



If the mosaicity refines to a value close to zero, all subsequent processing will be junk !

More on what should not happen ...



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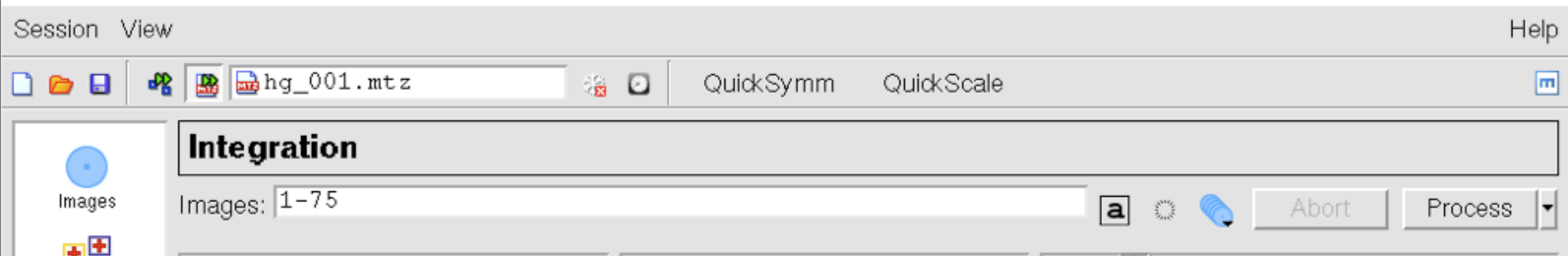
Possible causes:

- Inaccurate cell parameters
- Inaccurate crystal orientation

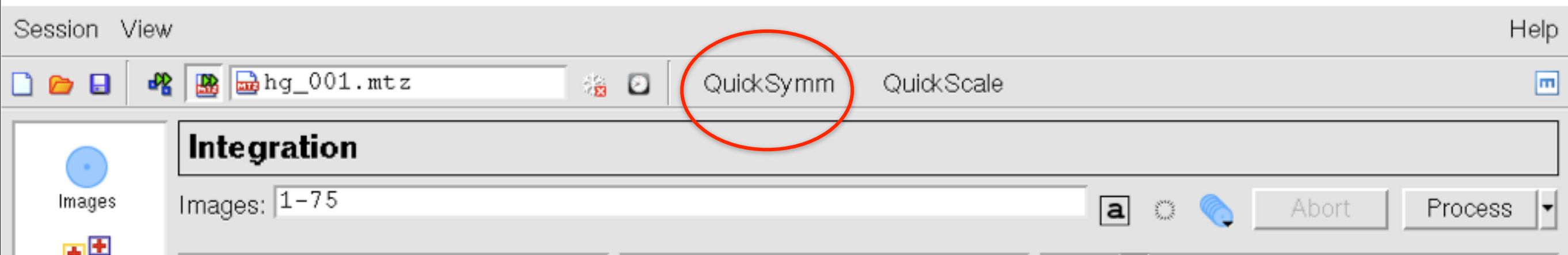
Possible solutions:

- Try to get an accurate cell (Cell refinement)
- Reset the mosaicity to a sensible value and repeat integration of a few images (5-10), so that orientation is updated.
- **Fix** the mosaic spread at a suitable value (look at the predicted spots).

After integration ... Pointless and Aimless/Scala

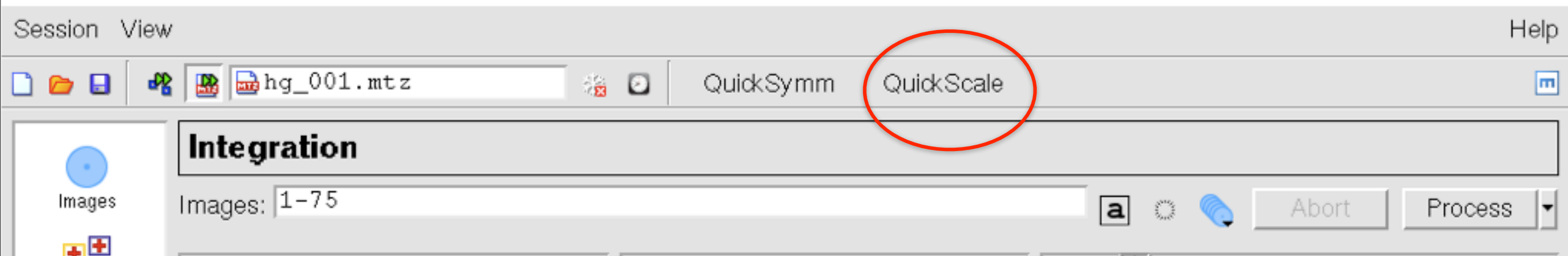


After integration ... Pointless and Aimless/Scala



Selecting “Quicksymm” will run POINTLESS to determine the true symmetry. The results will be displayed in a browser window.

After integration ... Pointless and Aimless/Scala



Selecting “Quicksymm” will run POINTLESS to determine the true symmetry. The results will be displayed in a browser window.

Selecting “Quickscale” will run POINTLESS, followed by running AIMLESS or SCALA with the space group symmetry assigned by POINTLESS. Results are displayed in a browser window.

At present, both programs can only be run with the default options.

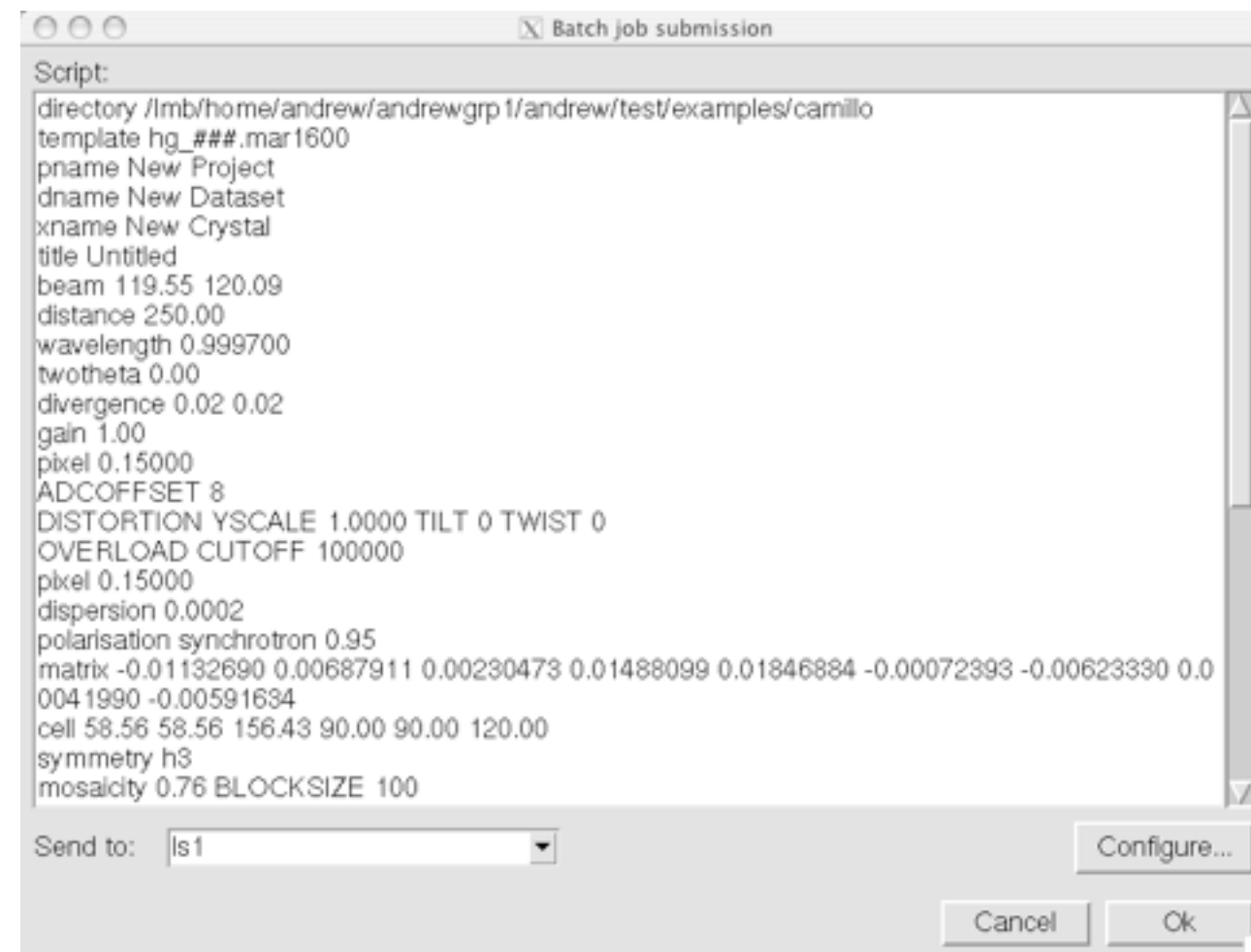
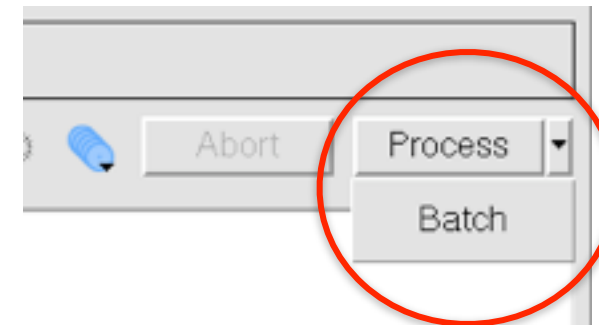
Go faster ... background job submission from the GUI

Selecting “Batch” from the Process pull down menu allows submission of an integration run in background.



Go faster ... background job submission from the GUI

Selecting “Batch” from the Process pull down menu allows submission of an integration run in background.

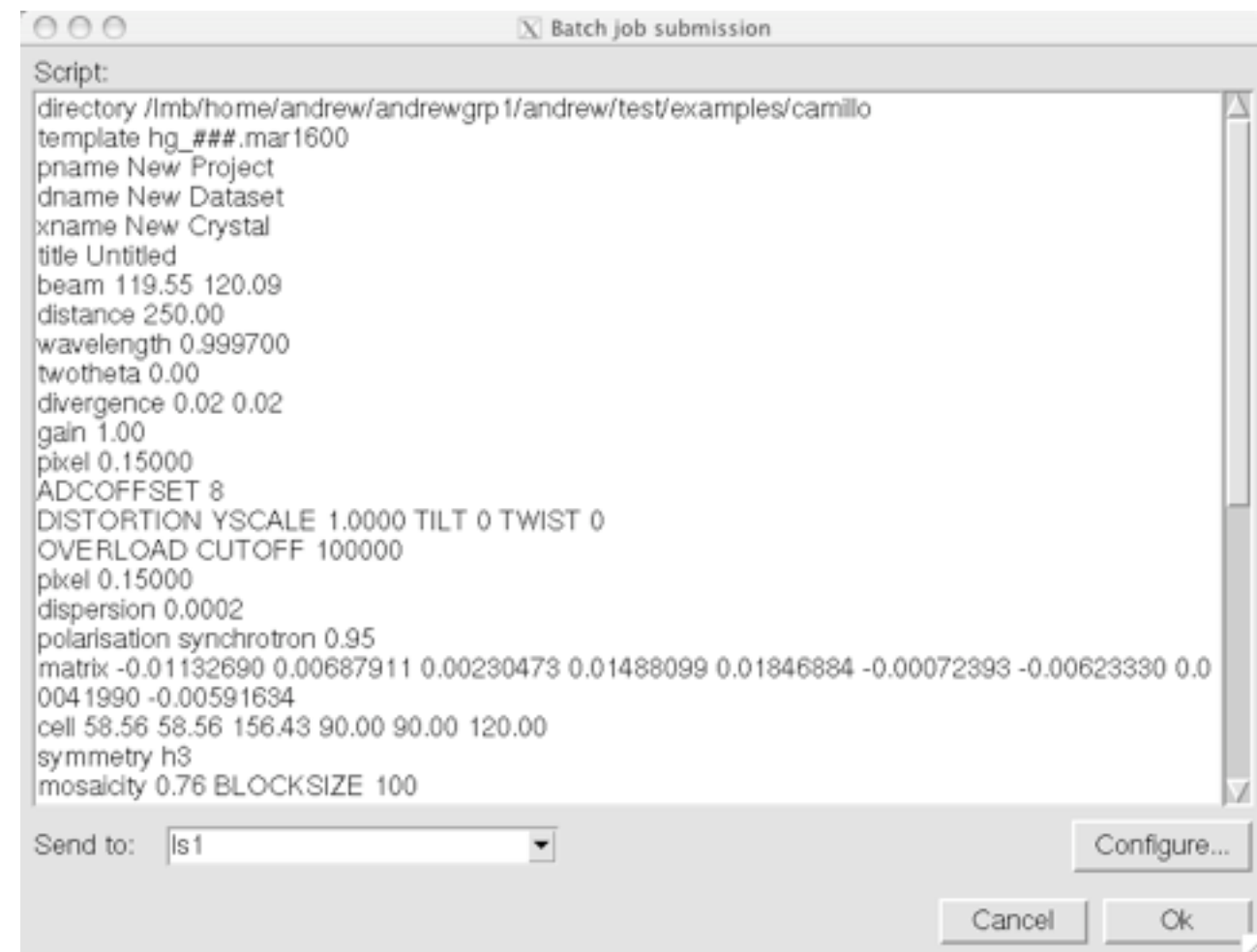
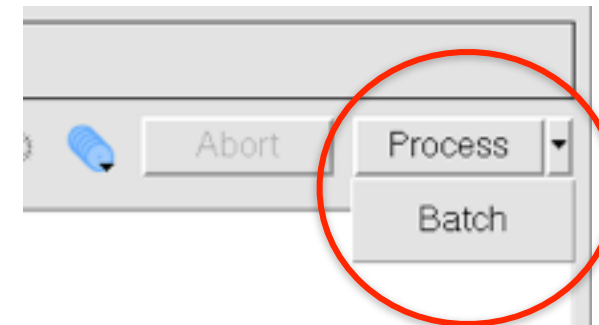


Go faster ... background job submission from the GUI

Selecting “Batch” from the Process pull down menu allows submission of an integration run in background.

This will be quicker, but the imosflm graphical output is lost (although very similar graphs are produced by running loggraph on the mosflm summary file).

This also provides a way of adding keywords for features not yet available in imosflm, or the commands can be cut and pasted into a “standard” command script.



Acknowledgements



The Mosflm team

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Luke Kontogiannis*

** past team members*

Thanks to Andrew for slides

Data collection is your last experimental step: don't mess it up