



## NeutronOptics 125x100mm CMOS Laue Camera

We have developed various Laue crystal alignment cameras for x-rays, and similar cameras can be used with a neutron beam. They allow rapid crystal alignment, and can also be used for hands-on teaching of crystallography. A finely collimated white beam produces a number of "Bragg spots" from a single crystal, and by measuring the positions of these spots the crystal orientation is determined.

Greater precision is obtained with backscattering, but the intensities are weaker, especially for x-rays because of the scattering "form-factor". A classic bench-top x-ray generator with a spot size of  $\sim 1\text{mm}$  and power of **30-50 kV and 30-50 mA is required**. The photo shows our new 125x100mm CMOS camera, the same size, but x6 more efficient than our old 1-CCD Laue camera for the same price.



Our old 1" Sony ICX694 12.5x10mm chip, with an f/1.4 lens, is replaced by our 24x16mm APS-C IMX571 detector with a faster f/0.95 lens. The area of the APS-C chip is x3 larger, and the lens aperture is x2 greater, so **the total gain in efficiency is x6 !**

The photo shows our compact APS-C Laue camera, which is the same size and price as our old 1-CCD Laue camera.

- **Camera dimensions:** 222x146x90mm
- **Field-Of-View:** 125x100 mm
- **Optical Aperture:** f/0.95
- **Sensor:** Sony CMOS IMX571
- **Chip size:** 23.5x15.7mm (APS-C)
- **Resolution:** 6248x4176
- **Pixel Size:** 3.75 x 3.75  $\mu\text{M}$
- **Binning:** from 2x2 to 8x8
- **High sensitivity:** (QE $\sim$ 90%)
- **Low dark current:** 0.003@-10 °C
- **Full well capacity:** 50,000 electrons
- **ADC:** 16 bit grey scale image
- **Readout Noise:** 3 e- typical
- **Readout Time:** <1s
- **Interface:** USB 3.0 with 10-20m cables
- **Power:** 12v DC to local standards
- **Cooling:** Thermoelectric:  $\Delta T = -35^\circ\text{C}$
- **Typical Laue Exposure Time:** 30-60s

## Installing the NeutronOptics Laue Camera on the x-ray beam

A classic **W x-ray generator** with a spot size of  $\sim 1\text{mm}$  and power of **30-50 kV** and **30-50 mA** is better than a modern fine focus tube. **Mount the camera as close to the source as reasonable** using the 4mm bolt holes at the back; minor adjustments to position and orientation are necessary.

**You will need to make an adapter for your source** to fit the 2mm collimator. The 1mm collimator slides into the 2mm tube, with the nose extending toward **the crystal  $\sim 40\text{mm}$  from the window**.



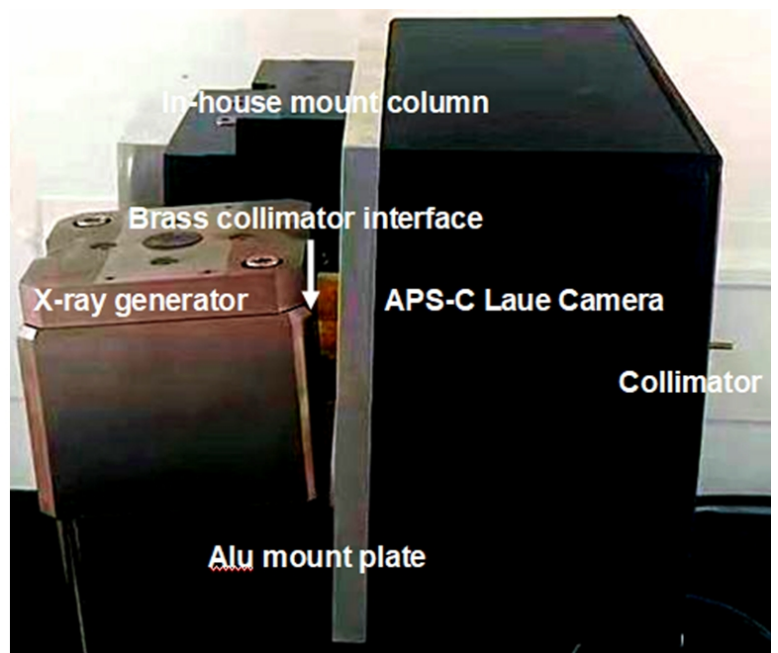
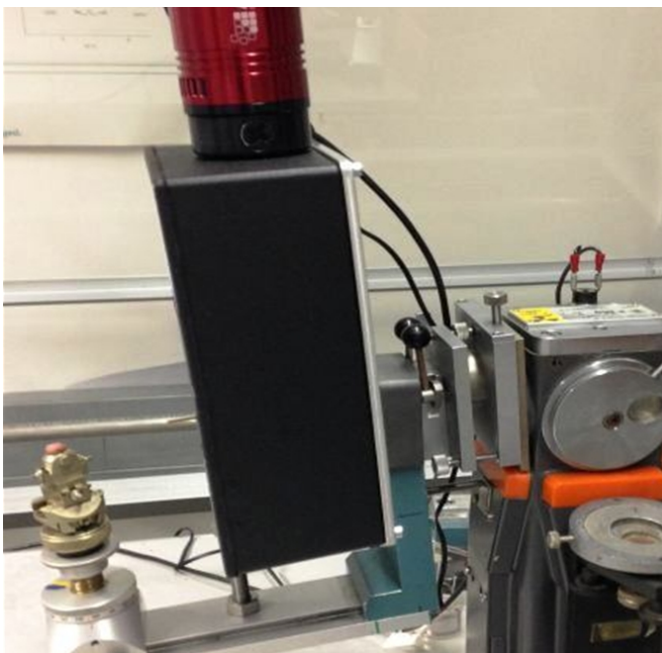
1mm Collimator nose

The collimator must be precisely aligned, and the source voltage and current set for **maximum intensity through the collimator**. The carbon fibre window & scintillator are not fragile. To remove collimator tubes, **pull them out from the back of the camera**, and insert them from the back. **The O-ring can be sealed** with a very small amount of black mastic or eventually black paint.

**You need maximum x-ray transmission through the collimator, & minimum x-ray background.**

The camera mount must allow **small adjustments to x-y position and orientation** to maximise x-ray transmission. That can be checked with a small detector, or even a scintillator “wand” in the beam.

The **left photo below** shows how **Prof. W. Donner and Dr L. Diop at the T.U. Darmstadt** converted a Huber Image Plate (IP) Laue camera mount to use the older NeutronOptics 1-CCD Laue camera. The CCD camera was simply bolted on in place of the IP cassette, with the beam tube and orientation mechanics retained. A simple bolt was added to support the extra weight of the camera. **The CMOS camera can be installed in the same way, since the detector box is the same size.**



The **right photo above** shows how another user mounted the similar 1-CMOS camera using a custom column to support the camera, with a brass collimator interface to the x-ray generator. Optional Pb shielding is used between the generator and the camera. **This close mount is better.**

**Apart from poor alignment, a common problem is background due to x-ray leakage through the back of the camera, especially around the collimator. Extra Pb shielding may be necessary. Because backscattered Laue intensity is low, it is vital to maximise signal/noise.**



## NeutronOptics APS-C CMOS Camera Operation

Install the ASI Camera Driver & Software for Windows, Linux or Macintosh

- Install the Windows camera driver `toupcam.dll` (x64) from the DVD, or download it from [https://www.touptek-astro.com/downloads?atfWidgetNav=box\\_win](https://www.touptek-astro.com/downloads?atfWidgetNav=box_win)
- You can use [ToupView](#) to control the camera, but we recommend [SharpCap4](#)
- [ToupTekDshowAstro](#) provides alternative Dshow support
- If you want to develop your own software, download the [SDK zip](#) Software Development Kit. Read the HTML documentation under `/doc/en.html` or `/doc/hans.html` for the Chinese version
- You may want to install the [ASCOM Platform Driver](#) if you want to use [ImageJ-for-ASCOM](#)
- **Do not update the camera firmware** if you don't have problems with that already installed
- General [ToupTek software](#) for other computer systems can be downloaded from their web site

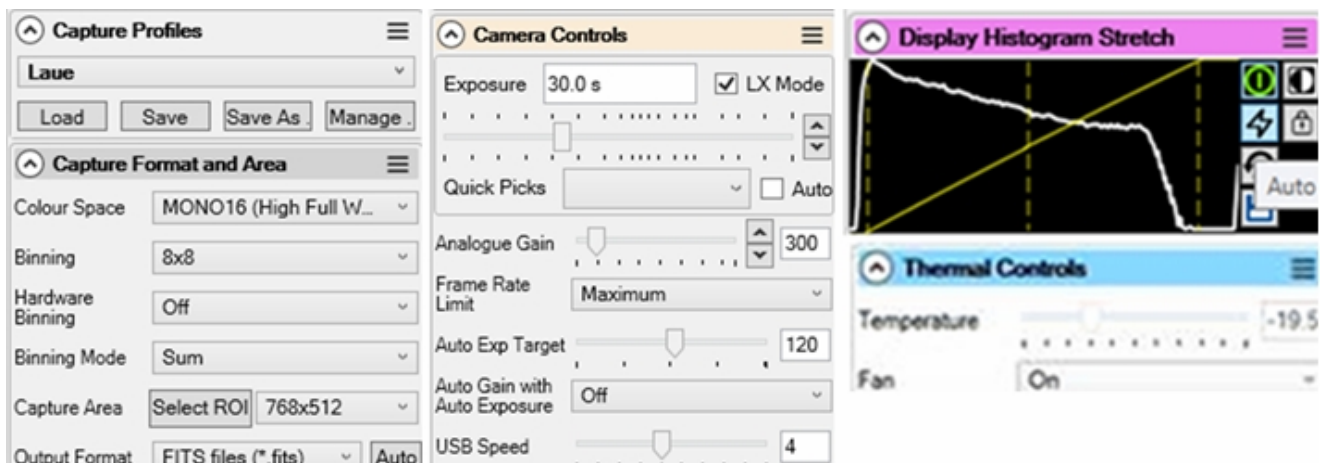
**ToupView** may be sufficient for simple beam monitoring, and is available for both Windows, MacOS and Linux computers, but Windows **SharpCap4** offers more features suitable for Laue diffraction.

### Installing the Recommended SharpCap4 Viewer

Use [SharpCap4](#) from the DVD or download it from <https://www.sharpcap.co.uk/sharpcap/downloads>. SharpCap was designed for low-light imaging for astronomers, with more complete controls, including many you will not need for imaging. Prefer the 64-bit version for memory management.

**The camera will be automatically recognised if it is plugged in, and you just need to choose it from the "Cameras" menu.** A window will open with the image and camera controls on the right.

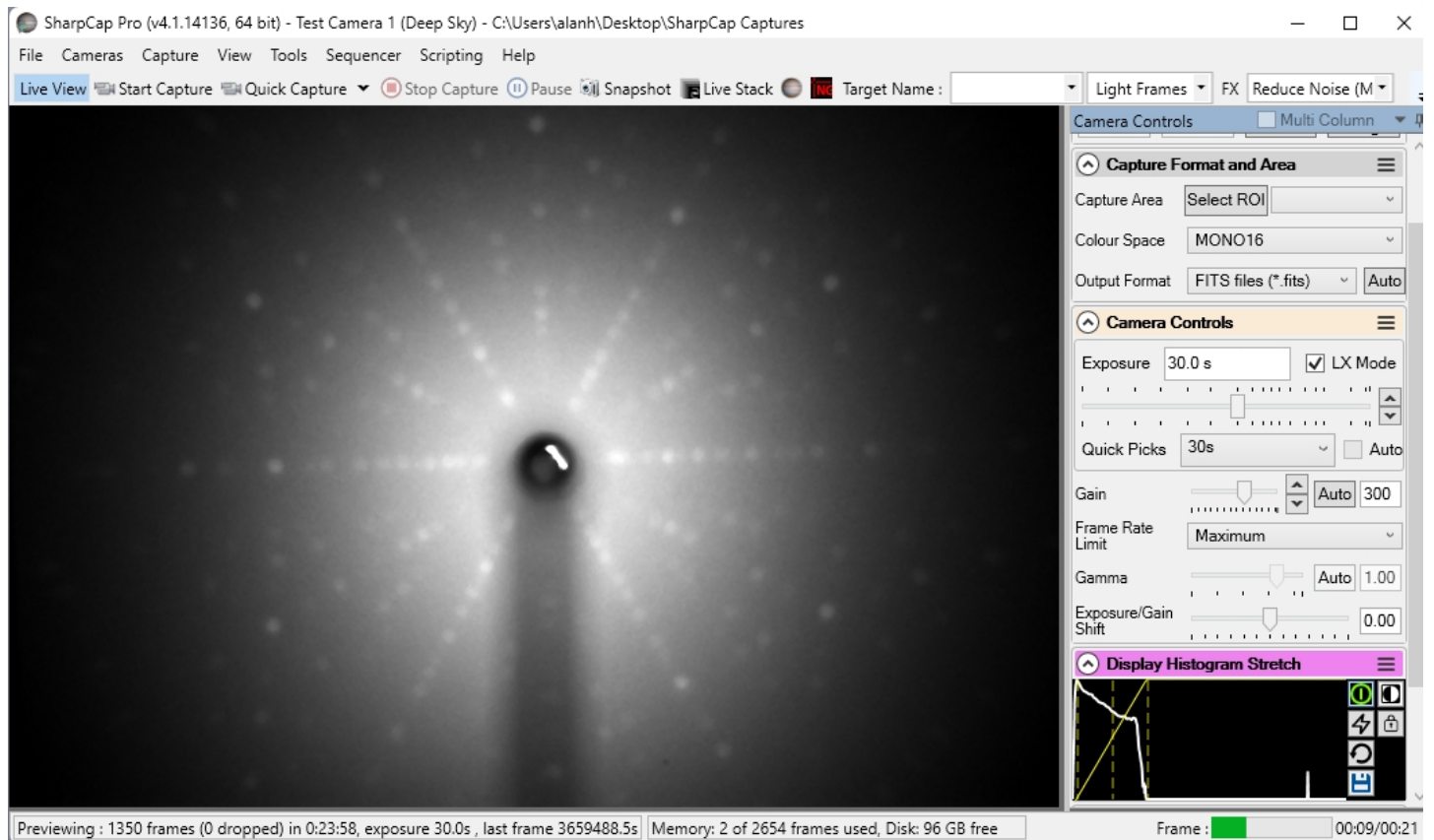
**Select MONO16, 8x8 binning in SUM mode for FITS** or TIFF output with **30s** exposure at **-10C**. The Histogram "lightning" icon sets an automatic display range, and you can pull the dotted lines. You can **mouse-drag the Camera Controls** to another part of the screen, or even hide them.



Tip: Copy [https://neutronoptics.com/soft/Laue\(ATR2600M\(USB2.0\)\).ini](https://neutronoptics.com/soft/Laue(ATR2600M(USB2.0)).ini) to **C:\Users\. Select and load it from the **Capture Profiles** menu at the top of the Sharpcap Controls to load parameters appropriate for our ATR2600M Laue camera.**

You can test the camera by shining a bright light on its face to see a light leak around the collimator.

A **Manual** <https://docs.sharpcap.co.uk/4.1/> is available, but these instructions may be sufficient.



Click **"Snapshot"** to save a single image frame. [FITS files can be opened with imageJ](#) and the [Windows Store QuickLook with the FitsViewer plugin](#). Open FITS files with a text editor such as [NotePad++](#) to read image parameters. In menu **"File/Settings"** check auto connect and restore.

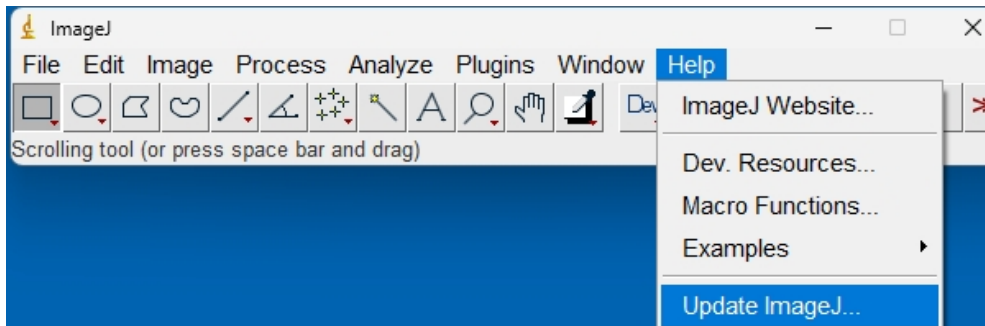
**If you do use SharpCap, consider paying £14 for a license** <https://store.astrosharp.co.uk/Store>  
You need a license to use advanced features like scripting, useful for automating imaging.

## Hints on getting Optimal Performance

- **Experiment thoroughly without radiation until you fully understand the camera controls**
- High Gain will multiply the intensity, but also increase noise and reduce the dynamic range
- Binning will multiply the intensity and speedup readout, but reduce optical resolution
- You can also limit readout to a "sub-frame" ROI region of the full image
- The "Display" panel controls what you see, but has no effect on what you collect
- Drag the vertical dashed line in the display panel to adjust the displayed intensity
- Click the lightning icon on the display panel to automatically adjust displayed intensity
- "Zoom" (and the wheel mouse button) zooms the size of the image display
- Image display is for guidance. **Open the image with ImageJ for measurement**
- The CMOS chip is cooled to reduce noisy pixels. You can also use [ImageJ Despeckle](#) filter
- The Window heater prevents fogging below 0°C (the CMOS chamber contains a desiccant)
- The centre of the image doesn't correspond precisely to the centre of the window

## Image Treatment with ImageJ

[ImageJ](#) will open the 16-bit raw [FITS](#) files, filter noise, modify intensity/contrast, and save them in various formats. An ImageJ installation is included on the NeutronOptics software CD under "Extras". **Copy the ImageJ folder to your C: disk, launch ImageJ and do Help/Update imageJ.**



We recommend you systematically use **"Subtract Diffuse Bkgd.txt"** to subtract diffuse background.

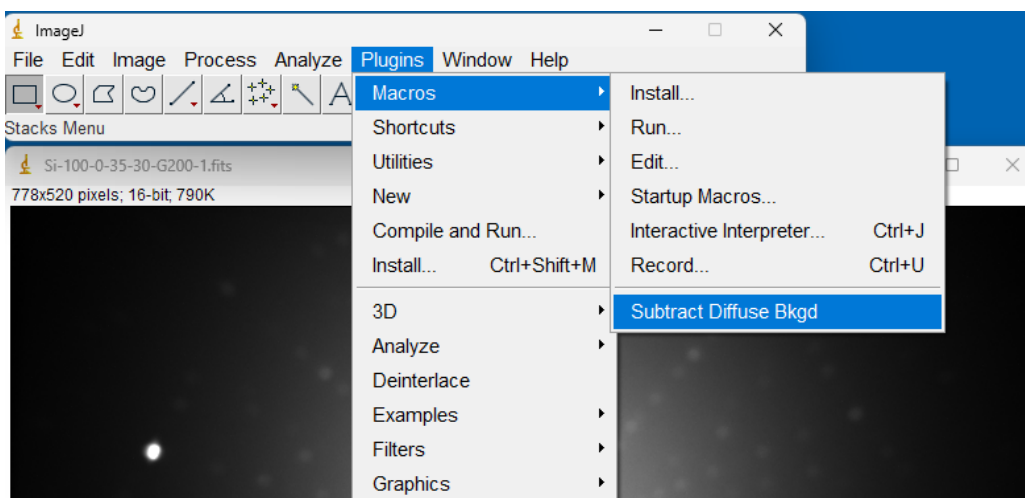
## Removing Diffuse Background with ImageJ – An Essential Step

Download <https://www.neutronoptics.com/downloads/Subtract%20Diffuse%20Bkgd.txt> and put it into the **C:\ImageJ\macros\toolsets** folder if it's not already there. (Read it with a text editor if you wish).

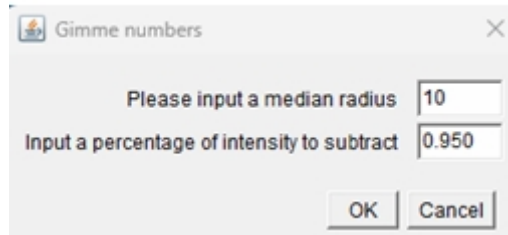
Launch imageJ, click the **red >>** arrow on the right of the menu, and select **"Subtract Diffuse Bkgd"**



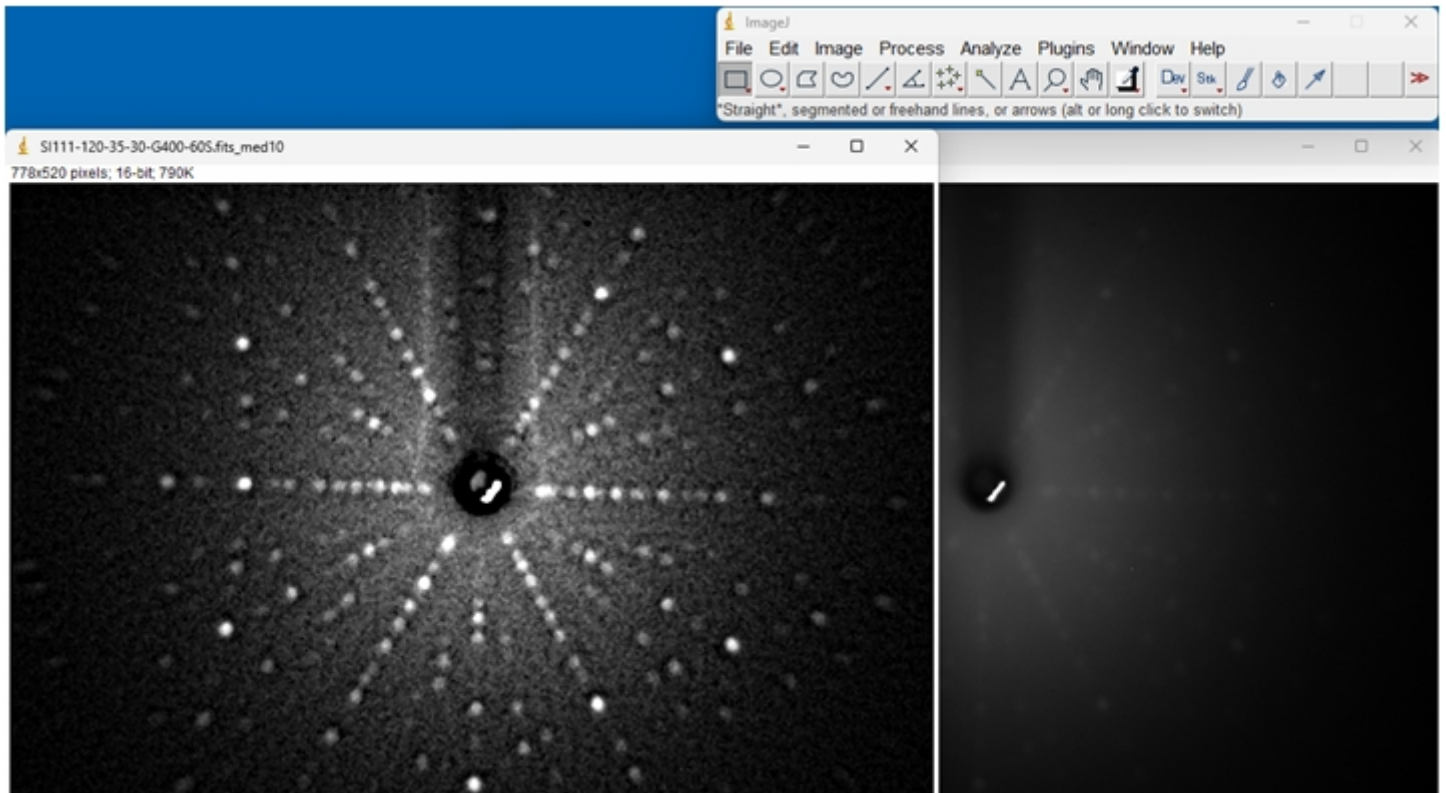
Now open your FITS image and run **imageJ/Plugins/Macros/Subtract Diffuse Bkgd** as below



You will get a parameters box as below. Choose e.g. radius 10 and subtract percentage 0.950

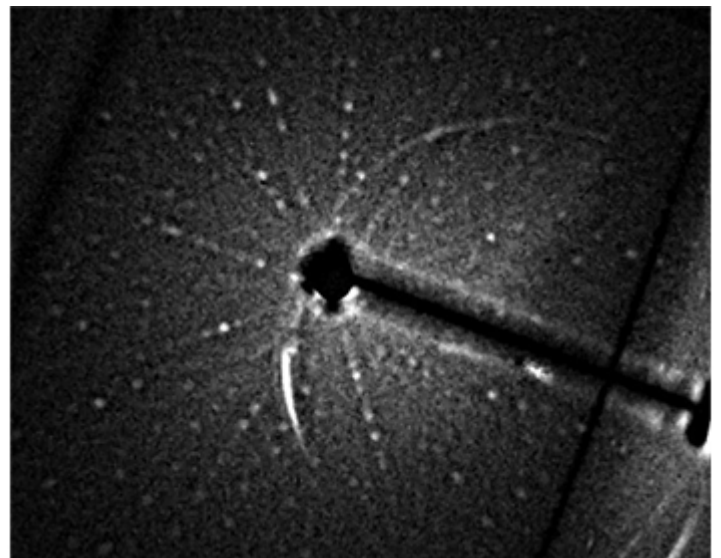
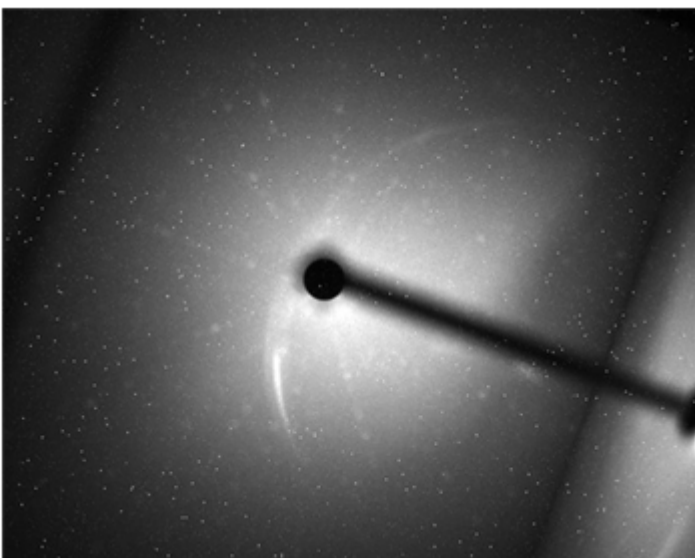


On clicking OK, you will immediately get the image with the diffuse background subtracted as below (left image) compared to the original weak image (below right, partly hidden by left image).



Note the light leak (oblique bar) in the centre of both images, and **the huge signal improvement**.

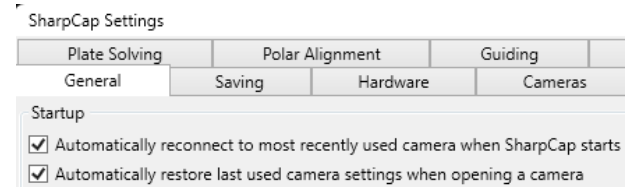
The left image below shows a very poor image with isolated bright pixels with no obvious Laue pattern. The right image shows the astonishing effect of this macro written by [M. Cammer](#).



## ImageJ for SharpCap – Automating Laue Imaging and Background Filtering

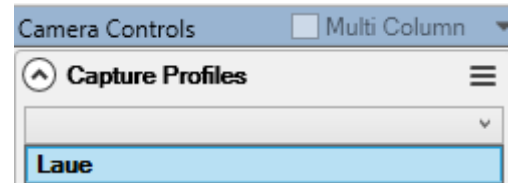
If you purchase the SharpCap Pro licence for £14 from <https://store.astrosharp.co.uk/Store>, you can use its scripting capability to control image acquisition, filtering and display, directly from imageJ. This also simplifies the GUI interface.

1) **Open File/SharpCap Settings** and choose to automatically reconnect to the last used camera, and use its settings. (These options will also be set by the [SharpCap imageJ macro tool](#)).



2) **Download the Laue imaging Profile** (it is also installed by the [SharpCap imageJ macro tool](#)) to **C:\Users\**

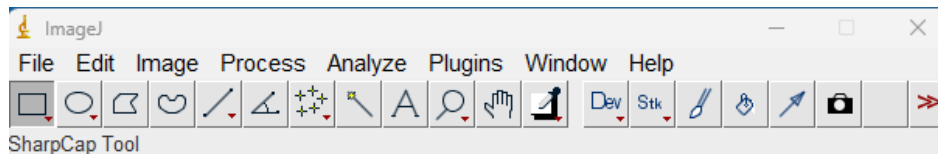
Run SharpCap and select this Laue profile from the Capture Profiles menu on the top right. This loads recommended settings for Laue imaging with the NeutronOptics CMOS camera.



You can now click on the SharpCap's **"Snapshot"** icon to acquire a raw image. But below we will see how to do that from imageJ.

3) **Install ImageJ** and download the [SharpCap imageJ macro tool](#) to place it in Windows folder "C:\ImageJ\macros\toolsets\" or wherever you have installed imageJ.

4) **Open imageJ**, click the **red arrow >>** at the top right, and select the **"SharpCap" macro tool**. A new camera icon appears on the right of the menu. **Right-click this new imageJ camera icon**.



You will obtain a simplified SharpCap capture menu. **Click "OK"** after eventually changing the exposure time or other settings. The **"Help"** button on the bottom left displays these instructions.

**Left-click the camera icon to collect an image** which will be displayed directly in imageJ, after eventually subtracting the Calculated Diffuse Background (recommended). You can even hide the SharpCap interface if you wish.

The **Calculated Diffuse Background** is simply the intensity averaged over a radius of 10 pixels, and 95% of this calculated diffuse background is subtracted from the original image to emphasise the sharp Laue spots.

Alternatively you can enter any BG file to be subtracted.

A new image under the same conditions will be collected every time you left-click the camera icon.

**Right-click the camera icon to change parameters.**

This imageJ tool has been designed for Laue imaging with the [Touptek ATR2600M camera](#), but will also work with other cameras. If particular settings are not available, the nearest available settings will be used.

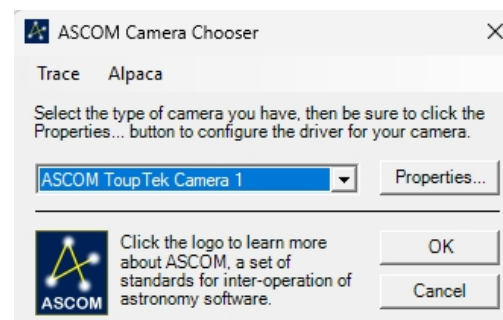
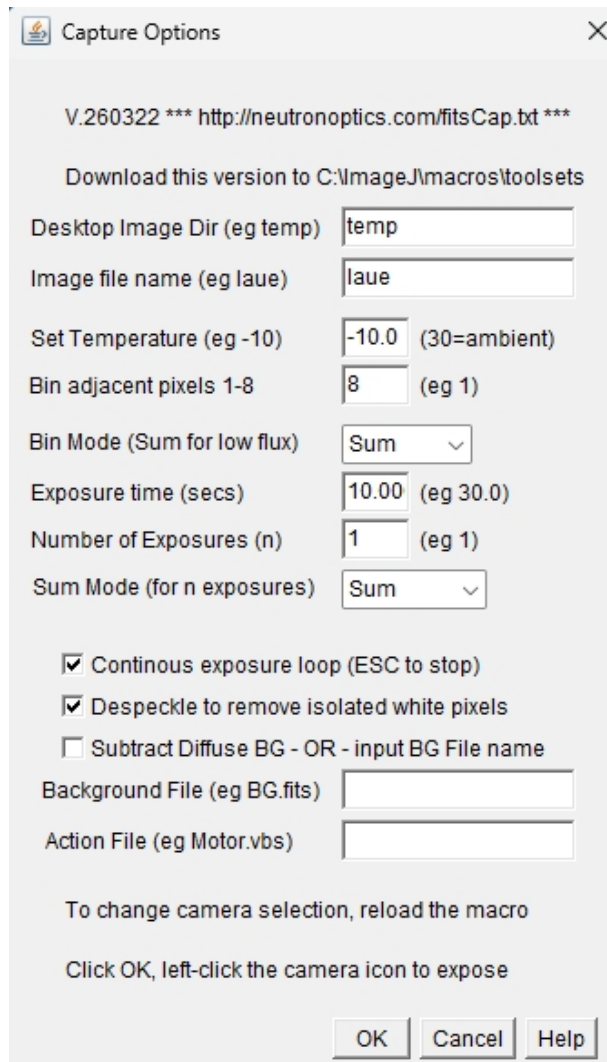
## fitsCap – Automating Laue or Tomographic Imaging & Background Filtering

**fitsCap.txt** is an imageJ Macro plugin using the [FITS.DLL](#) for cameras with an [ASCOM](#) driver, including NeutronOptics imaging and Laue diffraction cameras using Touptek & ZWO detectors.

- The GUI is very simple, and the images are opened directly in **imageJ** for treatment
- Exposure time, binning etc can be set and the temperature plotted for each image
- A number of images can be acquired individually, averaged or summed
- Note that **Bin Mode** can be “summed” or “averaged”. **Sum Mode** can also be “Individual”
- Background can be subtracted using either a calculated diffuse BG (Laue) or a BG file
- A command file can be run after each image to e.g. change sample orientation
- This help file can be displayed from the Help button on the user interface (below)

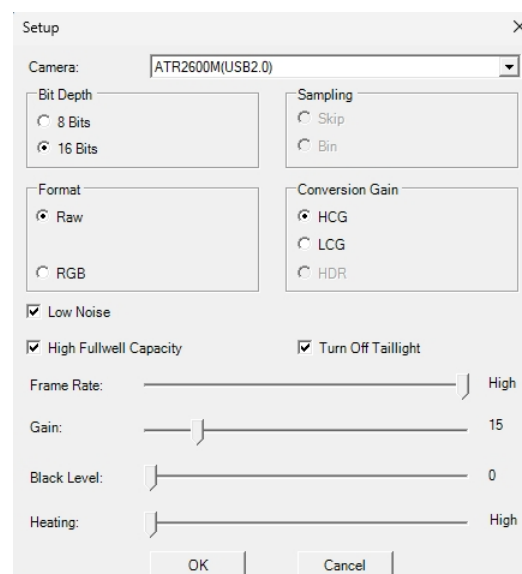
### To install this fitsCap.txt imageJ macro plugin:

- Copy <https://neutronoptics.com/fitsCap.txt> to the `\ImageJ\macros\toolsets` directory
- Install the ASCOM Platform environment from <https://www.ascom-standards.org/>
- Install the [Touptek ASCOM](#) (blue detector) or [ZWO ASCOM](#) (red detector) drivers
- Download **FITS.zip** from <https://www.easysky.de/ASCOM/Image/FITS.htm> and unzip it
- Copy **FITS.dll** to `C:\Program Files (x86)\Common Files\ASCOM\Image\`
- Register FITS.DLL by typing `regsvr32 FITS.dll` into a Windows Administrator cmd shell
- Download <https://neutronoptics.com/ASCap.vbs> to a **VBScript** directory under **ImageJ**
- Click the **red >> icon** at the top right of the ImageJ toolbar and select the fitsCap tool
- **Right-click** the camera tool icon that appears, select the camera & options
- **Left-click** the camera icon to capture a FITS image and display it with ImageJ



The **ASCOM Camera Chooser** (above) appears when you right-click the imageJ Camera icon. Usually select the default ASCOM Touptek Camera 1 for NeutronOptics cameras.

### Temperature control works less well for ZWO cameras



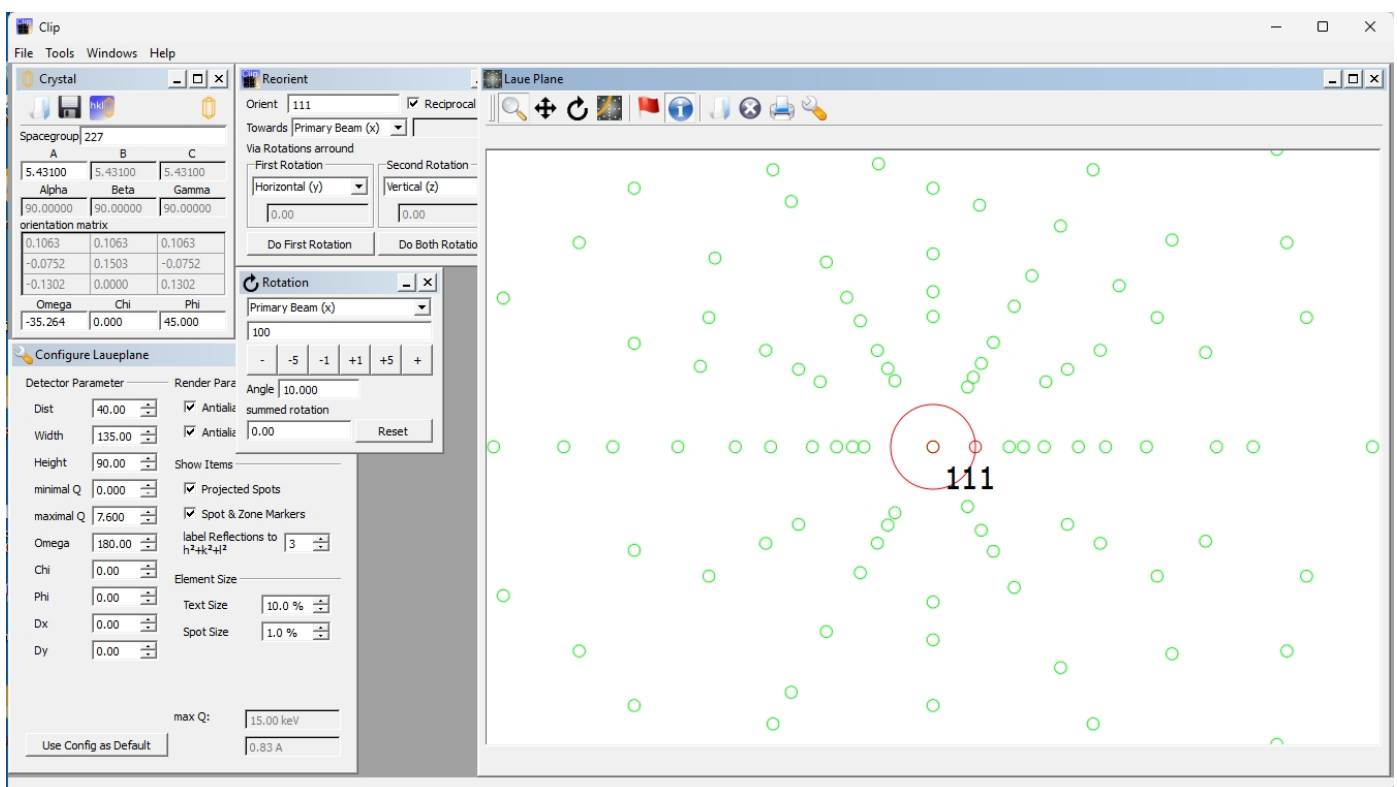
## The CLIP program for Simulating a standard Si [111] Laue Pattern

**CLIP** (<https://clip4.sourceforge.net/>) is a Windows application by Olaf Schumann that may be used for Laue indexing and crystal orientation. (Note that the **CLIP manual** does not describe all features <https://neutronoptics.com/soft/CLIP.pdf>. Open **CLIP**, drag the window to enlarge it, and then drag the **Laue Plane** window to uncover the **Crystal** window. (If closed, these windows can be opened with the **File/New Crystal** and **File/New Laue Orientation** menus). Enter the **Space Group** (number or symbol) and **lattice constants** (A,B,C) with **angles** (Alpha, Beta, Gamma), which will be constrained by the **Space Group**. The Euler angles **Omega, Chi and Phi** represent rotations around the z-, x- and y-axis respectively in a Cartesian laboratory system, with the z-axis along the beam.

For Si the group is 227 and the cubic cell 5.431 Å. The **space group constrains** the lattice constants, and the systematic extinctions of Laue spots. Use the Rhombohedral setting eg R3m for trigonal crystals, with  $a=b=c$  and  $\alpha=\beta=\gamma$ . Click the Crystal **floppy disk icon** to save the cell information to a file \*.cell, or load an existing \*.cell file with the first book icon. You can drag the **Crystal** icon on the right to the Laue Plane window to **connect them**.

Click the **Laue/Spanner** icon to configure the Laue Plane by entering the **Distance** of the crystal from the camera window (typically 40 mm), plus the **Width** and **Height** of the window. The 3:2 NeutronOptics 1-CMOS detector sees a window of ~135x90 mm. The **minimal and maximal Q** (0, 7.6) define an x-ray energy band up to 15 keV. These numbers determine the number of visible Laue spots. Most importantly the angle **Omega** between the incident and reflected beam is **180 for Back Reflection** (or 0 for Transmission Laue). (**Chi, Phi**) define the orientation around the beam, and (**Dx, Dy**) the displacement of the beam centre. Click **Use Config by Default** to save this as the default.

The default orientation [100] can be changed by opening the **Tools/Reorientation** menu, and entering an **Orient** vector, here [111] towards the Primary Beam. Clicking **Do Both Rotations** will perform both an **Omega** and a **Phi** rotation to align the chosen vector along the beam. **Tools/Rotation** will perform minor rotations if required. **Try simulating any Laue pattern** this way. **Clicking a reflection** identifies it, and drag-clicking can pan or rotate the pattern (**special icons**).



## Defining Zones and Orienting a standard Si [111] Laue Pattern

Click the 4th last **book icon** in the Laue Plane window to open a Laue Image file, in this case Si111. Most 8-bit image formats are accepted. We have temporarily switched off the [100] spot display and reset the calculated Laue pattern back to the default [100] orientation, but this is not essential. Click the small red circle and move it to the **centre of the pattern** (the intersection of rows of spots, not the central bright spot). Click the small circle on the large red circle to adjust the **excluded central zone**.

Now click the **Zone Mark mode**, the 4th icon in the Laue Plane window. Click on a Laue spot and, holding down the mouse button, **drag and click** on a second Laue spot on the same arc. In this high symmetry pattern, many are straight lines through the centre, plus less obvious hyperbolas for back-scattering (or ellipses for transmission). You can also remove **Zone arcs** by right clicking them.

Click the 3rd **HKL icon** in the CLIP Crystal menu to open the **Indexing/Refinement window**. In that window, click **Start** and then click **Stop**. Indexing is very fast and multiple solutions will be listed with increasing **Deviation**, with **Mean** and **RMS** deviations listed. Click on the best fit (**lowest Idx**) to display the calculated Laue spots and the corresponding axis. In this case, the best fit is [111].

The screenshot shows the CLIP software interface. The main window displays a Laue pattern image with overlaid zone lines. A text box over the image reads: "Zone mark mode. Left click and drag insert a zone marker with control points at drag start and drag end position." The Indexing/Refinement window is open, showing a table of deviation and indexing results.

Deviation	Idx mean	Idx rms
11.79	1.04	1.22
53.79	2.59	3.03
18.55	2.07	3.16
56.22	2.70	3.51
38.49	2.70	3.74
37.83	2.70	3.74
38.48	3.30	3.99
61.16	3.07	4.00
36.81	3.19	4.14
44.84	3.19	4.15
28.40	3.07	4.18
36.98	3.00	4.19
36.26	2.81	4.23
26.34	3.11	4.32
37.40	3.00	4.32
36.31	3.00	4.32

T	h	k	l	h	k	l	angula	Spatia	HK /
Zone	0	-1	-1	-0.00	-1.00	-1.00	0.05	0.06	0.13
Zone	-2	-1	1	-2.00	-1.00	1.00	0.05	0.17	0.23
Zone	-1	-1	-2	-1.00	-1.00	-2.00	0.11	0.39	0.46
Zone	-1	-1	0	-1.00	-1.00	-0.00	0.25	0.60	0.61
Zone	-1	0	-1	-1.00	-0.01	-1.00	0.35	0.42	0.87
Zone	-1	-1	-1	-1.00	-0.99	-1.01	0.51	3.18	1.55
Zone	-1	1	1	-1.01	1.01	0.97	1.04	6.93	3.16
Zone	1	0	-3	0.98	0.03	-3.01	0.76	5.25	4.17
Sum							3.27	17.57	11.79

Note that we assumed a distance of 40 mm for the distance of the crystal from the camera window. This distance, along with the dimensions of the camera window, will determine the scale of the pattern and the location of the individual spots. Yet even without these precise geometric parameters **we were able to determine the crystal alignment simply from the zone lines**.

The precise dimensions of the window could be determined by placing fine lead markers on it. Eventually, small optical distortions could be corrected using a larger absorbing grid with a barrel distortion routine in imageJ ( <https://neutronoptics.com/downloads/Barrel%20Distortion.txt> )

## Refining the Orientation of a standard Si [111] Laue Pattern

To obtain a better correspondence between calculated and observed Laue spots, first hide the zone lines in the **Configure Laueplane**. Use the **I-tool** to click on the individual spots to identify them or open the **CLIP/Tools/ReflexInfo** and move the mouse over the pattern to identify individual spots.

Choose **Refinement** instead of Indexing, and select all parameters except the centre **Det.x & Det.y**. Clicking on **Start** Refinement gives a better correspondence with the green calculated spots. Some spots will only be calculated if you increase the **maximal Q** (x-ray energy). You can also increase the minimal Q because low energy x-rays don't diffract. Click **Start** Refinement again a couple of times.

The screenshot shows the CLIP software interface. The main window displays a Laue pattern with green calculated spots and a red circle around the central spot labeled '111'. The 'Indexing / Refinement' dialog is open, showing the 'Refinement' tab with a table of parameters and their values and errors. The 'Configure Laueplane' dialog is also visible, showing detector parameters and rendering options.

Name	Value	Error
Crystal		
<input checked="" type="checkbox"/> ome...	0.0000	0.1317
<input checked="" type="checkbox"/> chi	0.0000	0.0873
<input checked="" type="checkbox"/> phi	0.0000	0.1269
Laue Plane		
<input checked="" type="checkbox"/> Dist...	42.657	0.488
<input checked="" type="checkbox"/> Om...	180.4695	0.4195
<input checked="" type="checkbox"/> Chi	1.0731	0.4763
<input type="checkbox"/> Det_x	0.8304	
<input type="checkbox"/> Det_y	1.2422	

T	h	k	l	h	k	l	Angula	Spatia	4K /
Zone	0	-1	-1	-0.00	-1.00	-1.00	0.05	0.21	0.13
Zone	-1	-2	-1	-1.00	-2.00	-1.00	0.03	0.06	0.14
Zone	1	0	-3	1.00	0.00	-3.00	0.03	0.22	0.19
Zone	-1	1	1	-1.00	1.00	1.00	0.08	0.53	0.24
Zone	-1	-1	-2	-1.00	-1.00	-2.00	0.07	0.28	0.31
Zone	-2	-1	1	-2.00	-1.00	1.00	0.10	0.38	0.43
Zone	-1	-1	0	-1.00	-1.00	-0.00	0.22	0.21	0.54
Zone	-1	-1	-1	-1.00	-1.00	-1.00	0.19	1.21	0.57
Zone	1	0	-1	1.00	-0.01	-1.00	0.30	0.30	0.74
Sum							1.08	3.38	3.29

The refinement is stable and all spots have been calculated in good correspondence with the observed spots. Note that no information about the atomic coordinates has been provided, so the intensities of the spots cannot be calculated. Some calculated spots are therefore not observed.

Note that the refined distance to the crystal has increased from 40 to 42.66 mm; it is difficult to measure it precisely. The orientation of the Laue plane has hardly changed and neither has the orientation of the crystal. The calculated **Errors** in these angles, **with the estimated errors in the crystal orientation only ~0.1 degrees**.

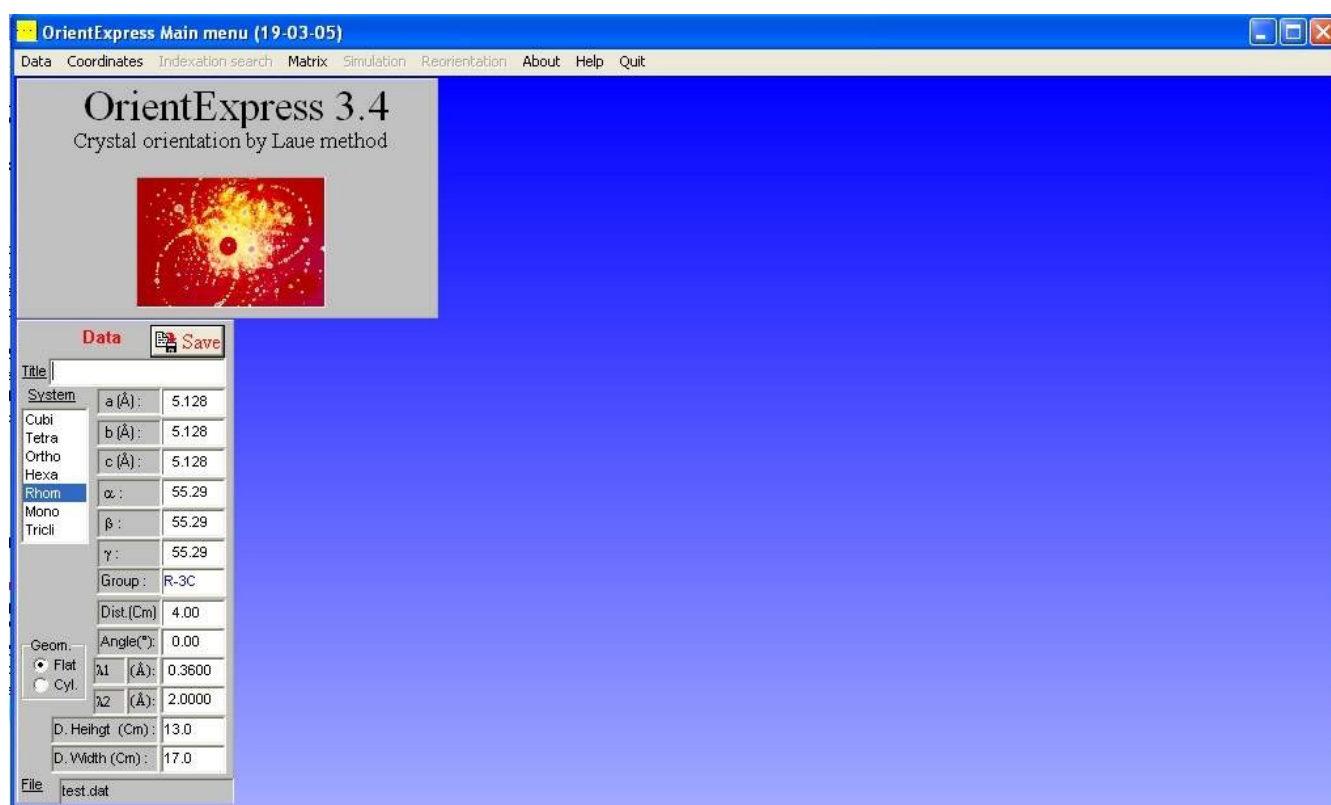
With such a simple crystal as Silicon, it has been possible to obtain a precise alignment with a 10s exposure, provided the camera was well aligned close to a strong x-ray generator, and provided the background was low, with diffuse background removed with the imageJ routine.

Please check the latest version of this Neutronoptics Laue Camera manual by downloading: <https://neutronoptics.com/soft/Manual-NeutronOptics-1CMOS-Laue-Camera.pdf>

## The OrientExpress program for Laue indexing

**OrientExpress** is an alternative Windows application for automatic Laue indexing, developed by Jean Laughier, with help from Bernard Bochu at LMGP, and Alain Filhol at ILL Grenoble. Old features such as "**Help**" don't work in Win-11 but have been transcribed to a PDF [OrientExpress Manual](#). Download OrientExpress with example files from <http://www.hewat.net/science/orientex.zip>  
**Install OrientExpress in a write-enabled directory, not "Program Files".**

Enter the crystal data from the **Data/Keyboard** menu, or use **Data/File** to open "**EXAMP1.DAT**", which contains lattice dimensions for a ruby test crystal (Al<sub>2</sub>O<sub>3</sub>) together with the characteristics of the camera (distance to crystal, angle between the beam and the camera normal, wavelength range, and camera screen dimensions). This is transmission Laue data, so the angle is 0°; it would be 180° for back reflection Laue. Al<sub>2</sub>O<sub>3</sub> is given on hexagonal axes, but allow the programme to convert to rhombohedral axes, for which indexing is easier. You can look up lattice dimensions in the [ICSD](#).

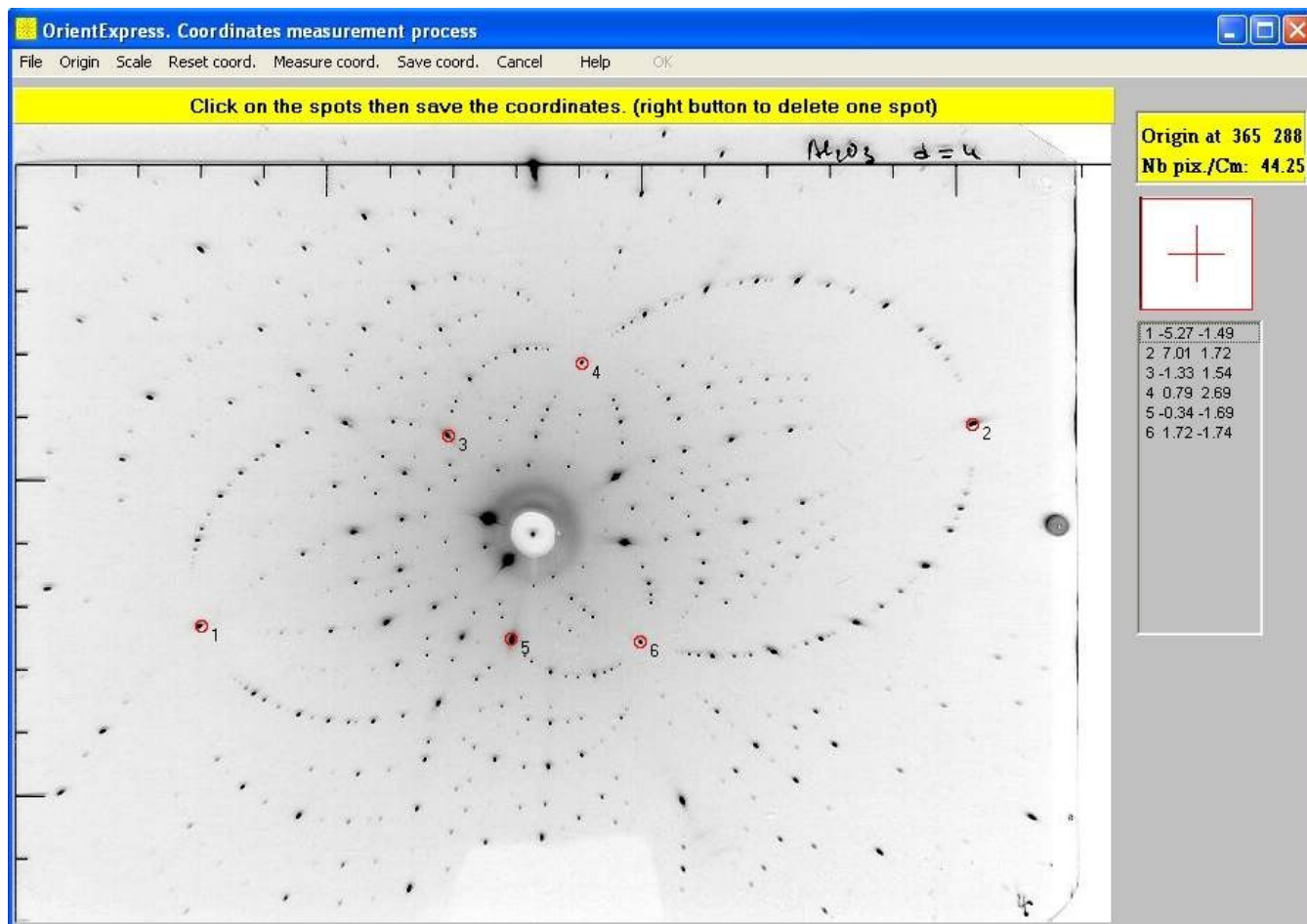


## Measuring the Laue peak coordinates

Under the **Coordinates/Image** menu select "**examp1b.jpg**" or a Laue pattern you saved from your camera. Select the **Origin/Circle** menu from the new Laue window that opens. Click and drag the **red circle** to define the beam axis of the Laue pattern (not always coincident with the centre of the beam hole) then click "**OK**". Select the **Scale/Enter** menu and enter the number of pixels/cm; 44.25 for the examples. Check these numbers at the top right of the screen. The Neutronoptics 125x100mm camera with 8x8 binning of 6248x4176 pixels will have approximately 4176/8=522 pixels for 9cm or ~58 pixels/cm. You should refine that number with a standard sample on your camera.

Now click "**Measure coord.**" and click on up to 10 spots (right click to remove a spot). It is best to select only 5-6 spots that are at the **intersections of arcs** of spots (zonal lines) which usually have small h,k,l indices. Finally, click "**Save coord.**" to a file or use the provided "**EXAMP1.COO**" file

Laue spots fall on **ellipses** for transmission Laue geometry; in backscattering geometry the spots fall on **hyperbolas**, the intersection of the scattering cones with the detector plane.



## Indexing the Laue pattern & crystal orientation

On the OrientExpress **main menu**, click "**Indexation search**" and simply click "**OK**" in the dialogue that opens. If indexing succeeds, a red Laue pattern will be super-imposed on your measured image corresponding to one of possibly several solutions (click on the different solutions if there are several). A correct solution will reproduce the observed spots (plus a lot more) and most importantly, **the intersecting arcs of spots**. If there is no good solution, check the centring, scale and cell parameters or select fewer Laue spots only on arc intersections. If all else fails, try **Simulation** below. Menu **Coordinates/Modification** modifies the coordinate list or centre/scale image constants.

## Refining the fit to the Laue pattern & orientation

On the OrientExpress main menu, select **Matrix/Refinement** and "**No additional coordinates**" then click "**OK**". Try refining again after adding more Laue spots. The resulting file "**Report.txt**" will list the (h,k,l) of all the Laue spots used for the refinement as well as their position on the pattern, their deviation from the calculated pattern, and the refined distance between the camera and crystal.

## Simulation and Rotating the Laue pattern


On the OrientExpress main menu, select **Simulation/Laue** and adjust the **spot size**. Then select the rotation axes under the **Options** of the simulation window and drag the mouse to rotate the Laue pattern around the selected axes. Choose the **Indexation** option and click on Laue spots to identify them. Even if you can't index the pattern, you can simulate it given the  $O_x, O_y, O_z$  crystal orientation axes by entering these under the **Matrix/Acquisition** menu then using the **Simulation/Laue/Options** menu as above to adjust the crystal orientation.

**OrientExpress Main menu (19-03-05)**

Data Coordinates Indexation search Matrix Simulation Reorientation About Help Quit

# OrientExpress 3.4

Crystal orientation by Laue method



**Crystal Orientation**

	Direct space (R31 matrix)			Recip. space (R13 transp. matrix)		
Crystal axis // to the beam (OX):	-0.251084	0.077323	0.068843	-4.41394	-0.69550	-0.79152
Crystal axis // to (OY):	-0.041606	0.067101	0.173058	2.50199	3.73285	4.93256
Crystal axis // to the camera axis (OZ):	-0.005606	0.233075	-0.173543	0.74402	3.44652	-1.15748

Display Hexagonal Indices and Matrix?  
 Yes  No

**Solutions**

Nb. resid.	h	k	l	h	k	l	h	k	l
1	0.0462	-1	-1	0	1	-1	0	1	0

**Data**

Title: \_\_\_\_\_

System

Cubi a (Å): 5.128

Tetra b (Å): 5.128

Ortho c (Å): 5.128

Hexa

Rhom α: 55.29

Mono β: 55.29

Tricli γ: 55.29

Group: R-3C

Dist.(Cm) 4.00

Angle(°): 0.00

Geom.

Flat

Cyl.

λ1 (Å): 0.3600

λ2 (Å): 2.0000

D. Height (Cm): 13.0

D. Width (Cm): 17.0

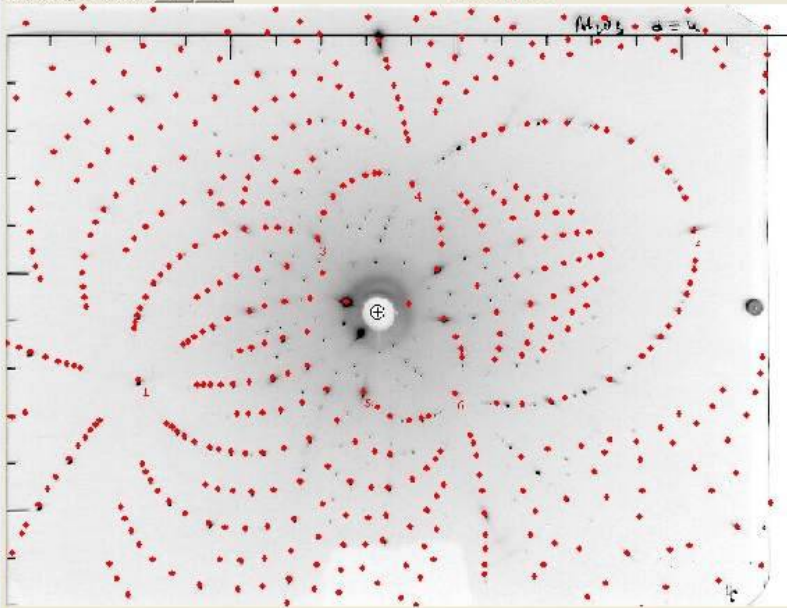
File test.dat File test.coo

**Coordinates**

Nb.	X(Cm)	Y(Cm)	h	k	l
1	-5.27	-1.49	-1	-1	-1
2	7.01	1.72	0	1	1
3	-1.33	1.54	-1	0	-2
4	0.79	2.69	0	1	0
5	-0.34	-1.69	-1	-2	0
6	1.72	-1.74	0	0	1
7					
8					
9					
10					

Adjust spot radius:

**Simulation**



The solution Nb. 1 is loaded

Note that we have chosen spots at the intersections of multiple arcs indicative of low order reflections in symmetry directions. Try removing the last 3 spots; you will still find a solution. Try adding spots at the intersections of fewer arcs; a solution is more problematic. Use only a few low order reflections to find a solution, then refine it.

These brief instructions should be supplemented by the **ORIENTEXPRESS.HLP** file which can be viewed with <https://ehubsoft.herokuapp.com/chmviewer/> The Laue patterns shown here are the X-ray scattering examples provided with the OrientExpress software, not those obtained with our cameras.

## Re-orienting the crystal on new axes

On the OrientExpress main menu, click "**Reorientation**" and enter the crystal orientation eg (1,1,1) that you want either parallel to the beam axis OX, or parallel to the vertical camera axis OZ, then click **calculate**. You will obtain a number of combinations of rotations phiX, phiY, phiZ that will achieve that. Choose the solution most convenient for your goniometer.

Finally you can click on one of these solutions to display the expected Laue diagram, and you can check your new orientation by comparing that with a new measured diagram.

**OrientExpress. Calculation of the angles to reset the crystal.**

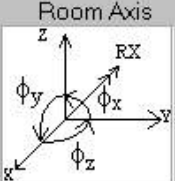
The cell is rhomboedral. Do you want to work with hexagonal directions?

Yes  No

Coordinates of the crystal direction to be reoriented:

Space  Direct  Recipr.

[? Help](#) [Calc.](#)



**Angles of the direction 1 1 1(R) with X,Y,Z room axis: 117.09 30.87 76.31**

Rotation angles to bring this direction:

Parallel to the beam axis (OX) :

Rot.	PhiX	PhiY	PhiZ
1: Z'	-15.41	0.00	-117.09
2: ZY'	0.00	152.54	-59.13
3: YX'	74.59	117.09	0.00
4: YZ'	0.00	13.69	-117.95
5: ZX'	164.59	0.00	117.09
6: ZY''	0.00	-27.46	59.13
7: YX''	-105.41	-117.09	0.00
8: YZ''	0.00	-13.69	62.05

Parallel to the camera axis (OZ) :

Rot.	PhiX	PhiY	PhiZ
1: YZ'	0.00	-76.31	-117.95
2: YX'	74.59	27.09	0.00
3: XY''	59.13	62.54	0.00
4: XZ'	76.31	0.00	-27.95
5: YZ''	0.00	76.31	62.05
6: YX''	-105.41	-27.09	0.00
7: XY'	-59.13	-117.46	0.00
8: XZ''	-76.31	0.00	152.05

Sample reference:

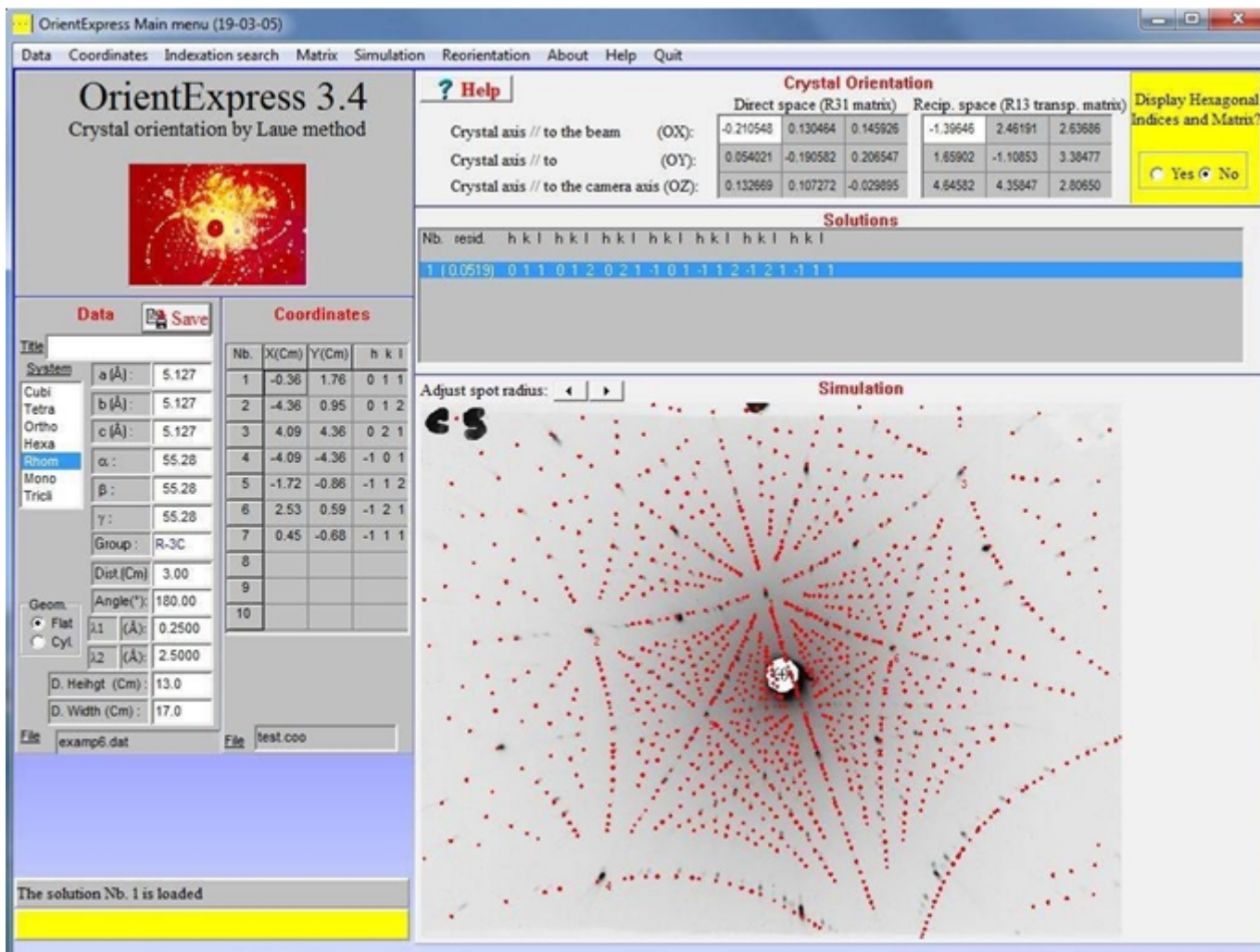
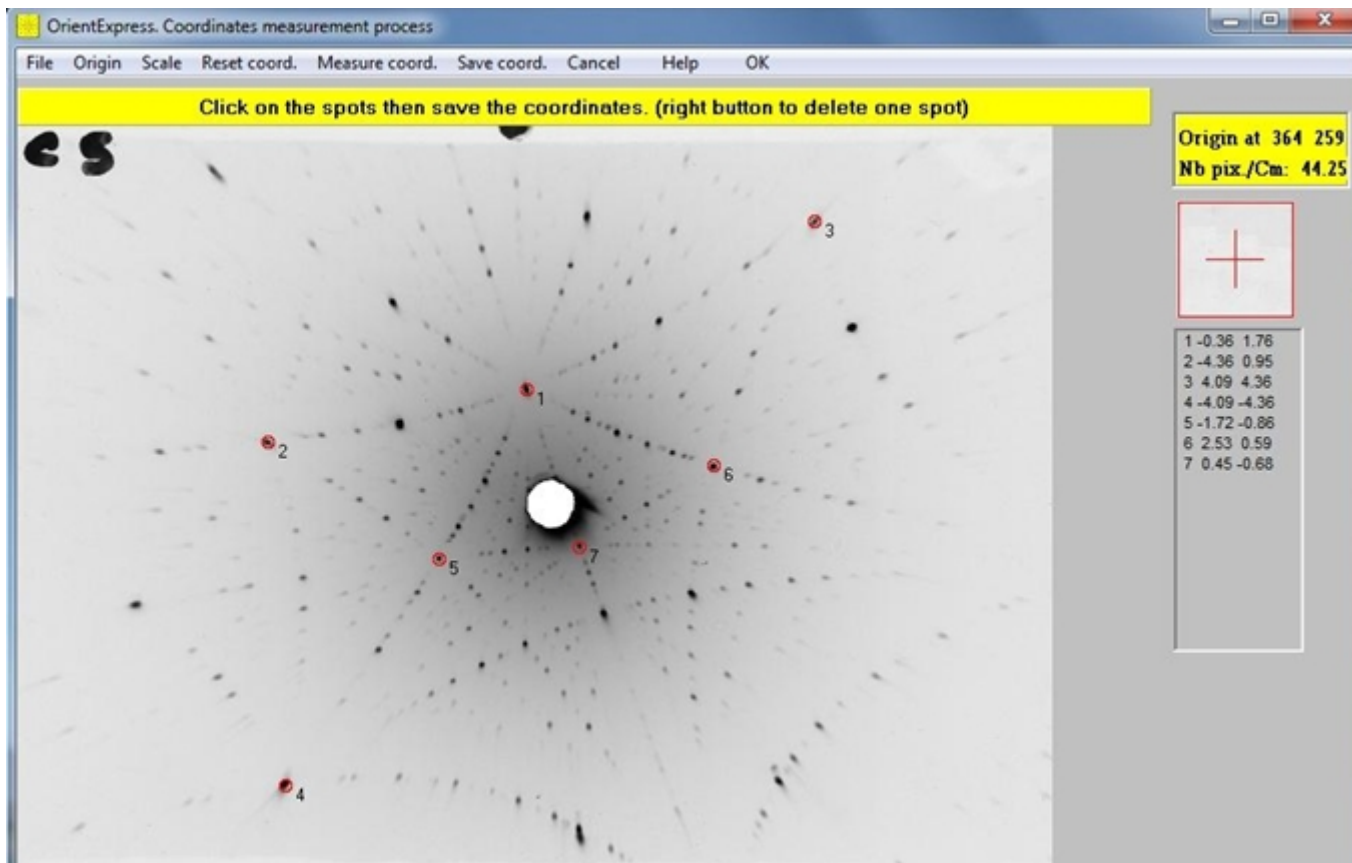
[Click here to print](#)

Double click the rotation number to simulate the diagram

[Return](#)

## Indexing backscattered Laue patterns

For backscattered Laue patterns, the "Angle" in the data file becomes  $180^\circ$  as in the "examp6.dat" file. File "grolland.bmp" is a backscattered pattern from ruby where we have measured 7 spots (first image below) which allow us to find a unique solution (second image below).



## LaueGen - Daresbury Laboratory Laue Software Suite

We recommend [OrientExpress](#) or the ambitious new [ESMERALDA Laue suite](#), and the [Cologne Laue Indexing Program \(CLIP\)](#) is one of the best, along with the [QLaue Indexing Program](#). Or try [WinLaue](#) to simply simulate Laue patterns to become familiar with the technique. Steffen Weber has also programmed a simple interactive [Laue pattern simulator in Java](#).

More experienced crystallographers will also want to use the [Daresbury Laboratory Laue Software Suite](#) ; this software can be downloaded from [EU Open Research Repository](#).

## Calibration of your Laue Camera with a Standard Crystal

The Height and Width of the Laue camera window, required by Orient Express, only correspond approximately to the Laue pattern, but you can measure Distance from the Window to the crystal. To determine the absolute scale of the camera, you must use a standard sample – a small, simple, well crystallised material such as Silicon or the NIST standard Ruby (Al<sub>2</sub>O<sub>3</sub>)  $\mu$ M sphere. For backscattered Laue you can use a large crystal, but for forward or side scattering you should use a small crystal to reduce x-ray absorption. A chip from a Si crystal is fine, but the NIST standard is best. The standard NIST ruby spheres cost \$648 for 3 spheres, and can be purchased on-line from: [https://shop.nist.gov/ccrz\\_ProductDetails?sku=1990&cclcl=en\\_US](https://shop.nist.gov/ccrz_ProductDetails?sku=1990&cclcl=en_US)

Simulate the Laue pattern for the known orientation of your sample, and adjust the dimensions of the pattern manually to correspond approximately with the measured pattern before refinement. See the [OrientExpress](#) manual for further details.

**Please check the latest version of this Neutronoptics Laue Camera manual by downloading:** <https://neutronoptics.com/soft/Manual-NeutronOptics-1CMOS-Laue-Camera.pdf>