

QLaue Notes

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QLaue (<https://sourceforge.net/projects/qlaue/>) allows you to display expected Laue Spot patterns for different crystal structures. It is no longer being updated, and has some rough edges, but it is easy to install on your computer and works.

Current (as of April 2016) Mac and Windows versions are also available from <http://www.physics.utoronto.ca/~phy326/laue/QLaue-0.2-macx-R27.dmg.zip> and <http://www.physics.utoronto.ca/~phy326/laue/QLaue-0.2-WinXP-R27.msi.zip> respectively.

The following notes are based on using the Mac version.

Feel free to add to this file and give to the Advanced Physics Lab Coordinator for posting.

Warnings

- QLaue is not always robust. If you end up in an odd state, it is sometimes best to close the program and start over.
- Just to confuse you, the location of the cursor in the main QLaue image window is given as X and Y values in the coordinate box above the image, even though the image is clearly labeled as being the YZ plane.
- The simulated spot intensities may be helpful, but should not be trusted overmuch.

Sample input files

Example_W_Random_QLaue.xtl

A tungsten sample with a somewhat random orientation and few spots, so it is essentially impossible to identify by simple inspection. This is the data used for the example given within `Laue_Spot_Identify.py`.

To open

From within QLaue

Top Menu : File → Open → `Example_W_Random_QLaue.xtl`
QLaue → Preferences

Tick all boxes, set Anode to W, Tube Voltage to 35 KV.

Parameters

If Example_W_Random_QLaue.xtl is missing, you can also set it up by entering the following from within QLaue. It is best to do in the order given to avoid confusing QLaue.

Laue Controls: Sample Film Distance (mm) → 50

Top Menu: QLaue → Preferences

Tick all boxes, set Anode to W, Tube Voltage to 35 KV.

Crystal --> Set Lattice

Spacegroup: Cubic, Im-3m (229)

Lattice: a --> 3.1652 (make sure b & c automatically change to same value, if not, re-enter 3.1652 into a again)

Unit cell: 74 W

Crystal --> Set Orientation

Primary (X-axis) enter: 2.790937, -0.871863, -1.212029

Secondary (Z-axis) enter: -0.450078, 1.958644, -2.445328

Click OK

(make sure Crystal Orientation: Current crystal shows correct x, z axis values.)

Laue --> Set Image Scale: Pixel size (microns) = 170.45

Example_W001_45kV_18mA_30mm.xtl

This example is based on the Laue image available from this experiment's web page, which is also for the Laue_Spot_Identify.py sample data file Laue_Data.txt.

QLaue How To

Set parameters, from within QLaue

To set X-ray parameters

QLaue Top Menu: QLaue → Preferences → Tick all boxes, set Anode and Tube Voltage to whatever parameters you used, e.g. W, 35 kV.

To set film-crystal distance,

Laue Controls Panel: Sample Film Distance (mm) → whatever distance you used, e.g. 30.

Adjust simulation spots and orientation

To align crystal orientation to a particular hkl direction:

QLaue Top Menu: Crystal --> Set Orientation:

For example, to align crystal 110 direction with beam, and 001 direction with vertical (z) axis, enter:

Primary (X-axis) : H=1, K=1, L=2

Secondary (Z-axis): H=0, K=0, L=1

To adjust crystal orientation by hand:

Click and hold on image window, move pointer as desired, release.

To fine tune crystal orientation:

Use rotations toolbox (tick QLaue Top Menu : Window → Tools → Rotations Toolbox).

View a Laue image from within QLaue**Scan the image**

If the scan does not have sufficient contrast, you can lay a piece of paper over the image on a light table and mark the spots on the paper with a pen, and then scan that.

To import image, from within QLaue

QLaue Top Menu : Laue → Import Image → Select your file and click Open.

Note: The image file must be png or jpg; QLaue cannot input pdf files.

To set scale of image,

QLaue Top Menu : Laue → Measure Scale → Select film rectangle on image.

A Dialog box should appear, for Film Type select “Other”.

Enter the width (in mm) of the film and click OK. (It ignores whatever you enter for height.)

To set beam spot location,

QLaue Top Menu : Laue → Define Origin → Centre the cross-hairs over the centre of beam spot and click.

Print or Save a QLaue Pattern.

The print function in QLaue may not produce very useful output, so it may be better to just use Screen Capture.

- **On a Mac**, press Command-Shift-3 or Command-Shift-4 to save all or a selected part of your screen as a png file on your desktop. For more details and additional options (e.g. saving to the clipboard), see <https://support.apple.com/en-ca/HT201361>.
- **On Windows**, use the PrtScn key or Alt-PrtScn to copy the whole screen or current window to your clipboard.

For more details and for other operating systems, see <http://www.take-a-screenshot.org/>.

Display adjustments

To hide imported image: Unclick QLaue Top Menu : Laue → Show Image

To hide simulated pattern: Laue Controls Panel: Show Simulation.

If some spots are red and some are blue: Unclick Laue Controls Panel: Show Characteristic Intensities, to make all the spots red.