Notes on the Configuration, Installation, and Use of the 4Spots ImageJ plug-in

Configuring 4spots

The 4spots plugin will quickly measure the length of two g-vectors, as well as the angle between them. It will further use these values to compute associated d-spacings. This is accomplished through the well-known relation $gd = \lambda L$. For this computation, it is necessary to manually set the value of λL. In this case, λ is the wavelength of your electrons and L is the camera length used when obtaining your SAED data. At this time, the plugin is not completely developed so this value must be hand entered into the code.

1. Open the file 4_Spots.txt in any text editor.
2. Go to line #11 of the plugin and change to value of the variable lambdaL to that of your microscope (see note below).
3. Save the file.

NOTE
The value of λL needs to be in units of pixel·Å using a pixel value consistent with your image digitization for the plugin to operate correctly.

I suggest that λL be computed first in units of mm·Å, this value can then be multiplied by your image digitization in units of pixels/mm (i.e., $dpi \times 1\ in/25.4\ mm$) to obtain the correct units. A correct value of λ for your electron energy may be computed using Wolfram Alpha at the following (rather annoying) URL:
http://www.wolframalpha.com/input/?i=PlanckConstant%2Fsqrt%282+Electronmass+300+keV+%2B+%28300+keV%2FLightspeed%29%5E2%29 .

As an example; I operate with $300\ keV$ electrons and customarily use a $1200\ mm$ camera length for SAED data collection. My images are normally digitized at 600 dpi. My theoretical camera constant is then given by: $\lambda L = (1.97\ \times 10^{-2}\ \text{Å})(1200\ mm) = 23.6\ mm \cdot \text{Å} \times 600\ pix/25.4\ mm = 557\ pix \cdot \text{Å}$. This value might, of course, be better determined by experiment.

This unit combination is then quite useful as it allows measurements on the image to be made in pixels, and $d = \lambda L/g$ then having units of Å.

Installing 4spots

1. First, install ImageJ.
2. Once this is accomplished, copy the file 4_Spots.txt into the directory ImageJ\plugins\Macros.
3. Now, open ImageJ and press Ctrl+Shift+M and the ImageJ macros installer window will open. Navigate to the plugins\Macros directory and click the file 4_Spots. Txt. Then click open to complete the installation. Figure 1 shows what you should see after pressing Ctrl+Shift+M.
4. The installation is now complete, and the plugin is ready for use.

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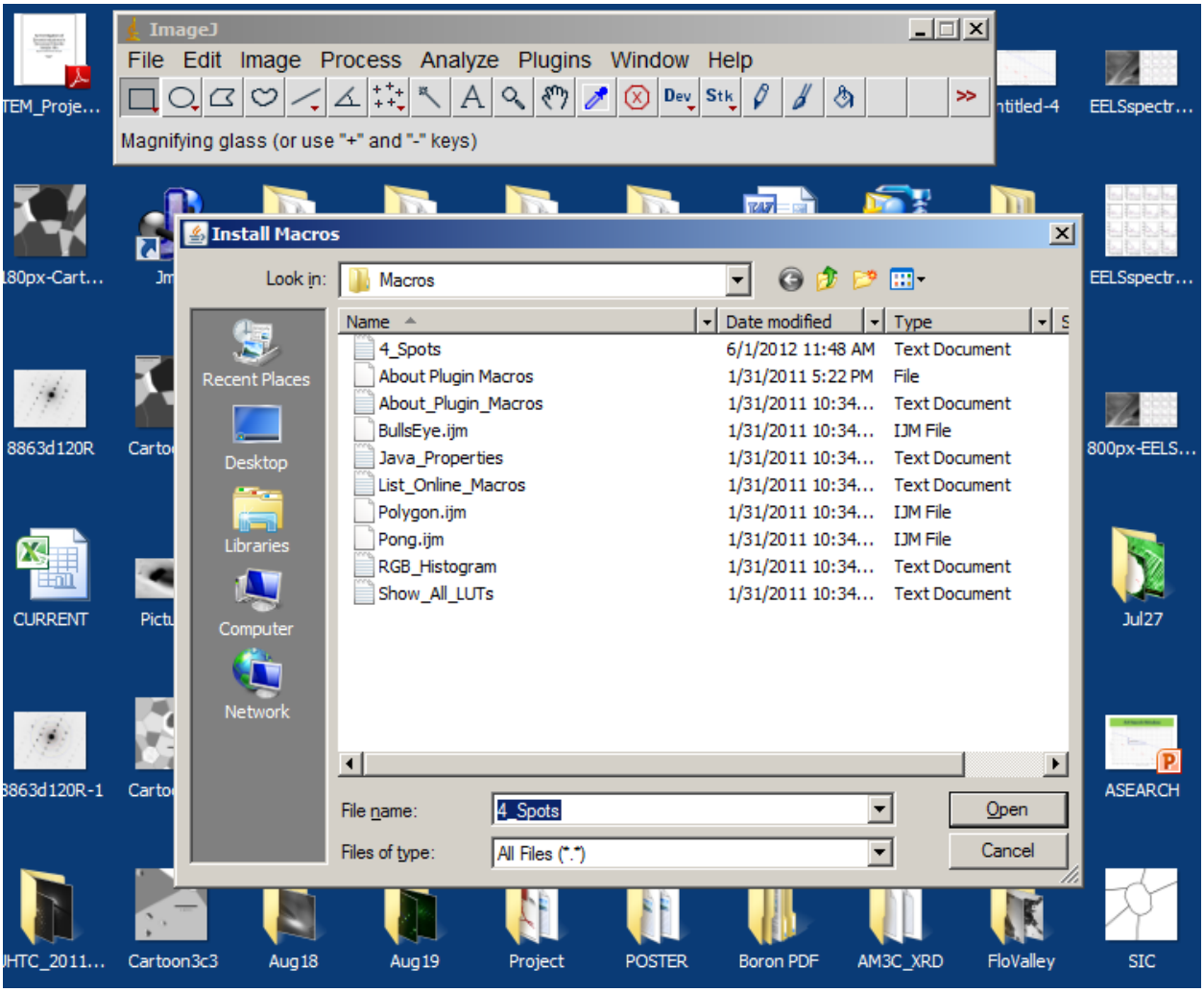

Figure 1: ImageJ Macro Installation Window

Measuring g-vector lengths and d-spacings with 4spots

Now that the plug-in is installed, we are ready to make measurements.

1. In ImageJ, open an SAED data image. Remove any native scaling by selecting Analyze → Set Scale, and click on the "click to remove scale" icon.
2. In the ImageJ menu, go to Plugins → Macros → 4Spots and click (Figure 2).
3. A pop-up will appear asking you to select four diffraction spots (Figure 3).
4. The point picking tool is active, so you need to select four diffraction spots by clicking on them one by one. To obtain valid results, the four chosen spots need to be two symmetric pairs located at 1 g-vector distance from the un-scattered beam. Once four spots are selected, click OK (Figure 4).
5. A results window will now pop up showing two g-vector lengths in pixels, two associated d-spacings in Å, and two supplementary inter-spot angles in degrees (Figure 5).
6. To clear the four chosen spots, click on any other selection tool (rectangle, oval, etc.) and click once in the image. Return to step two if additional measurements are desired.

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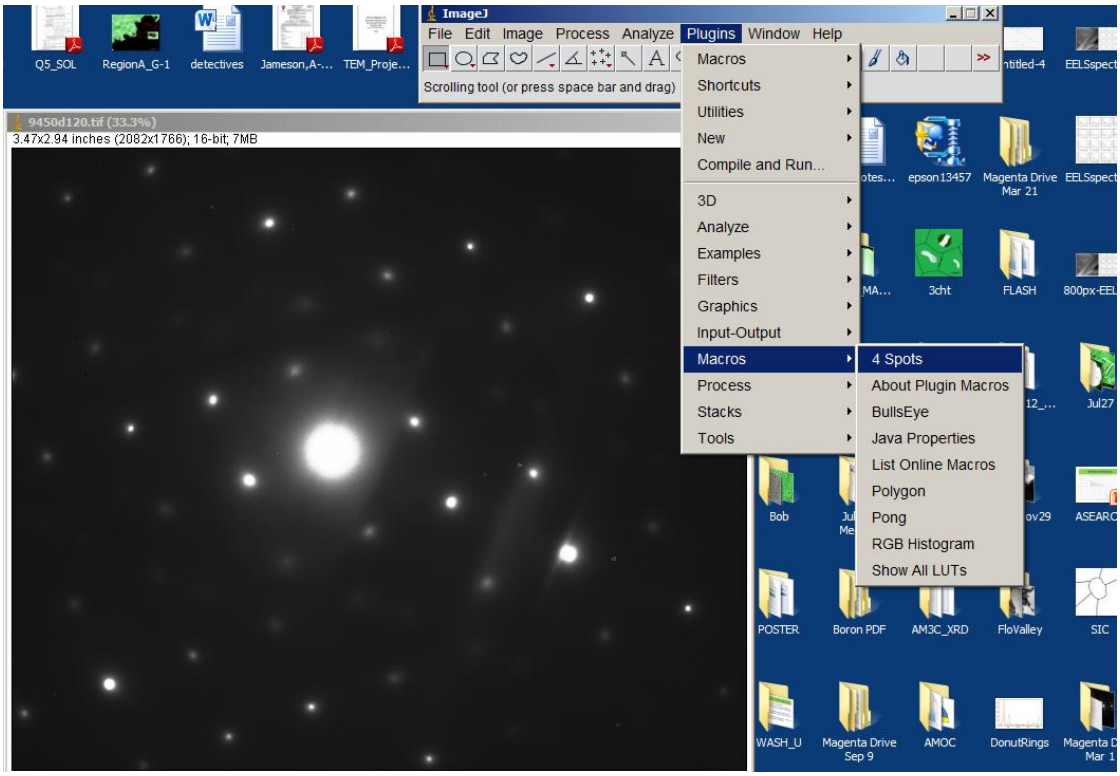

Figure 2: Plugins → Macros → 4Spots and click

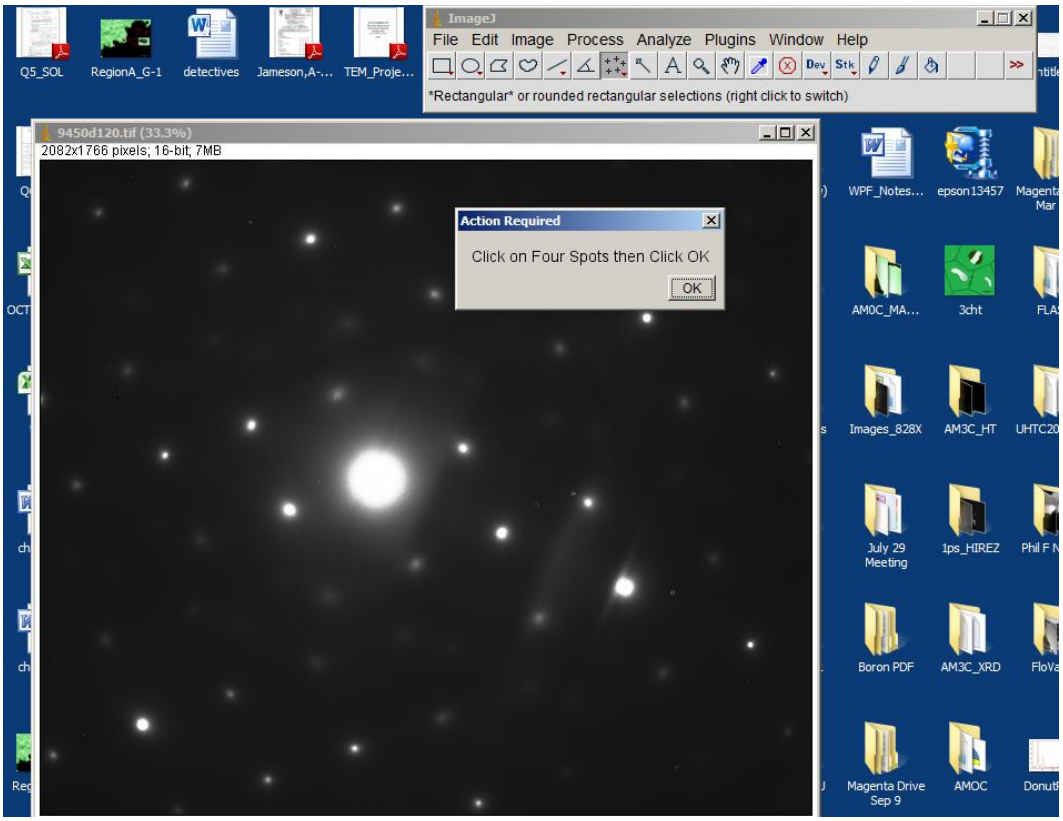

Figure 3: 4 Spots plug-in Selected, awaiting your input!

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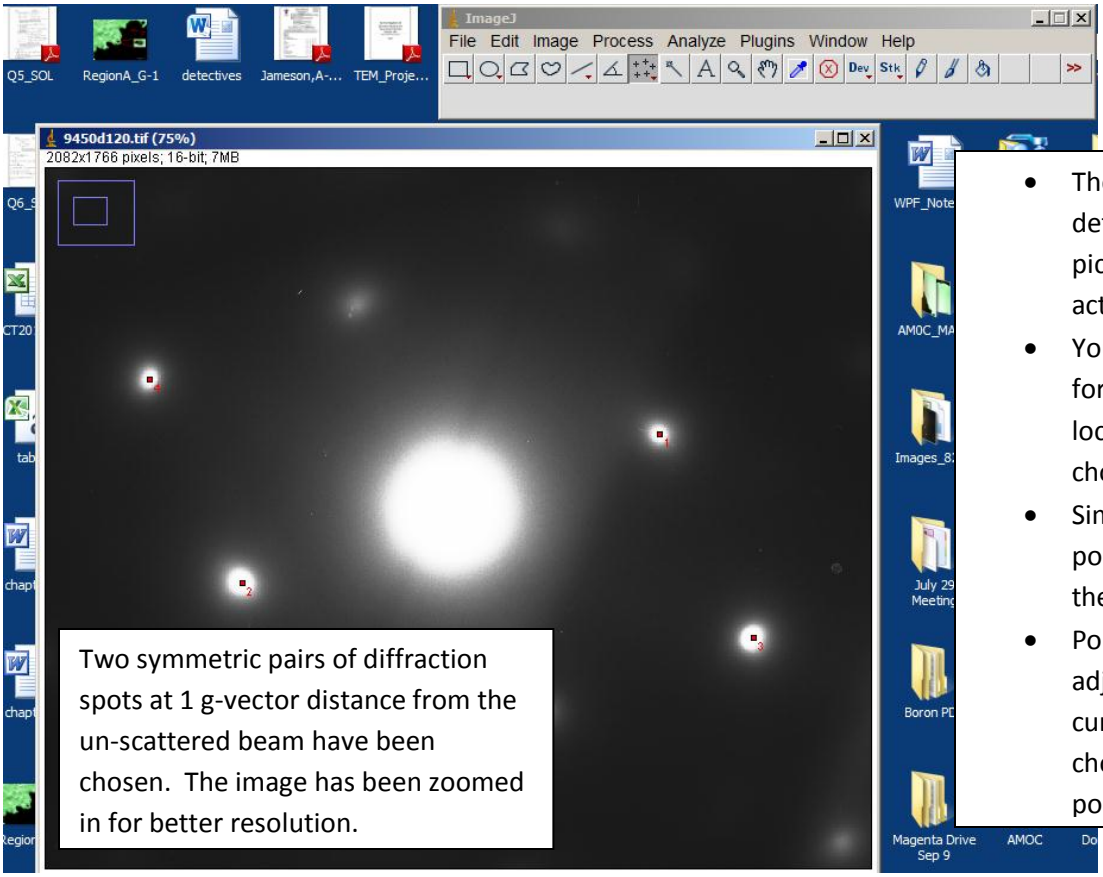

Figure 4: Four diffraction spots have been chosen, just click OK at this point

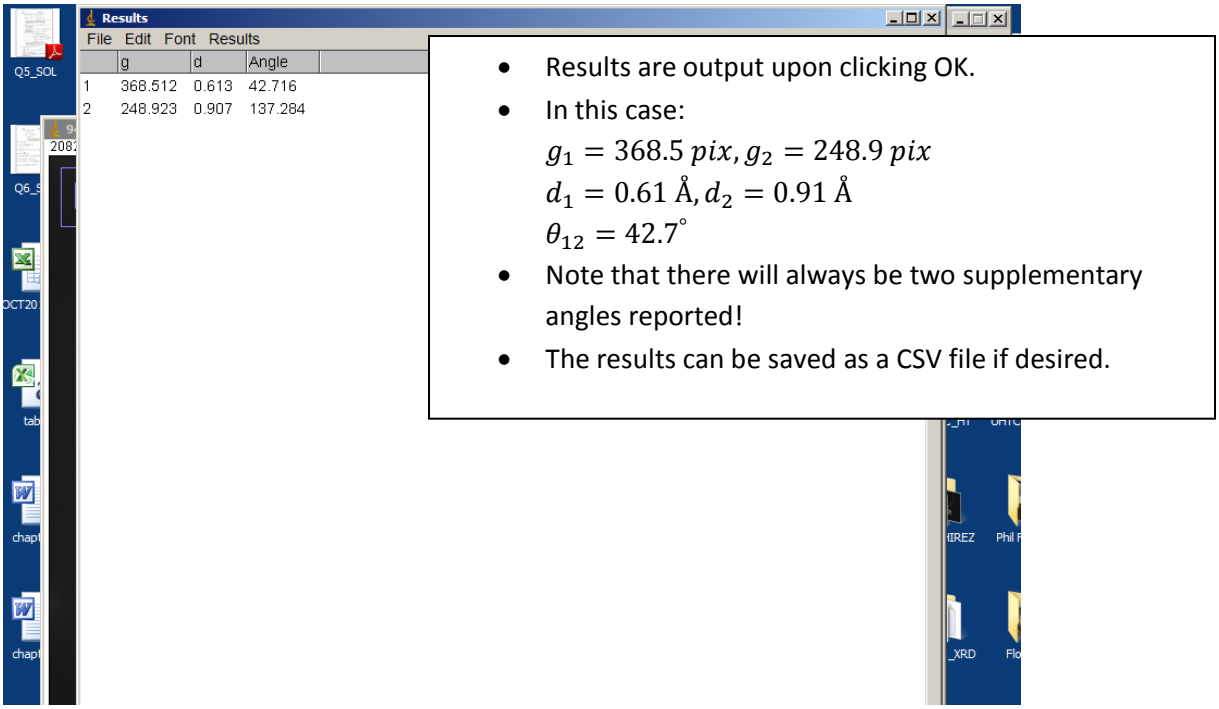

Figure 5: Results

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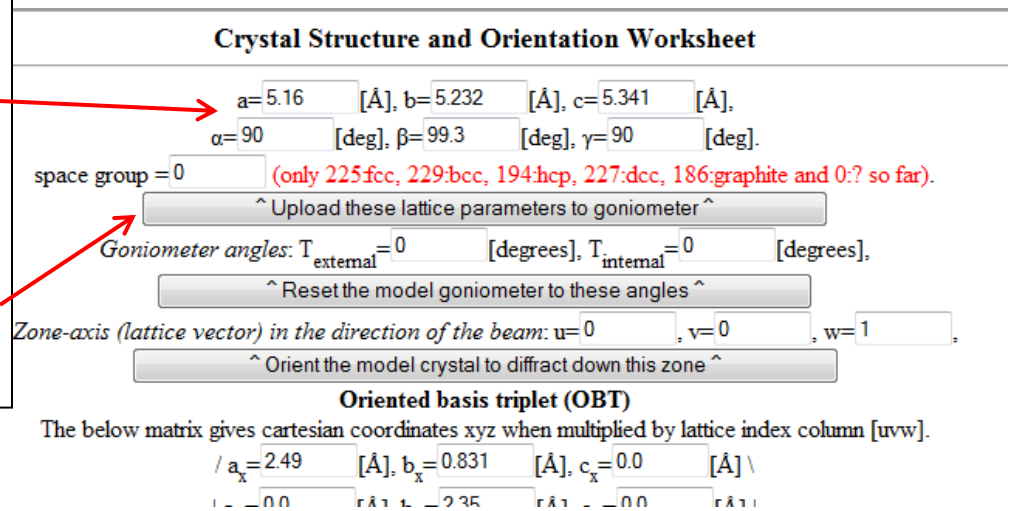
Analyzing the Data

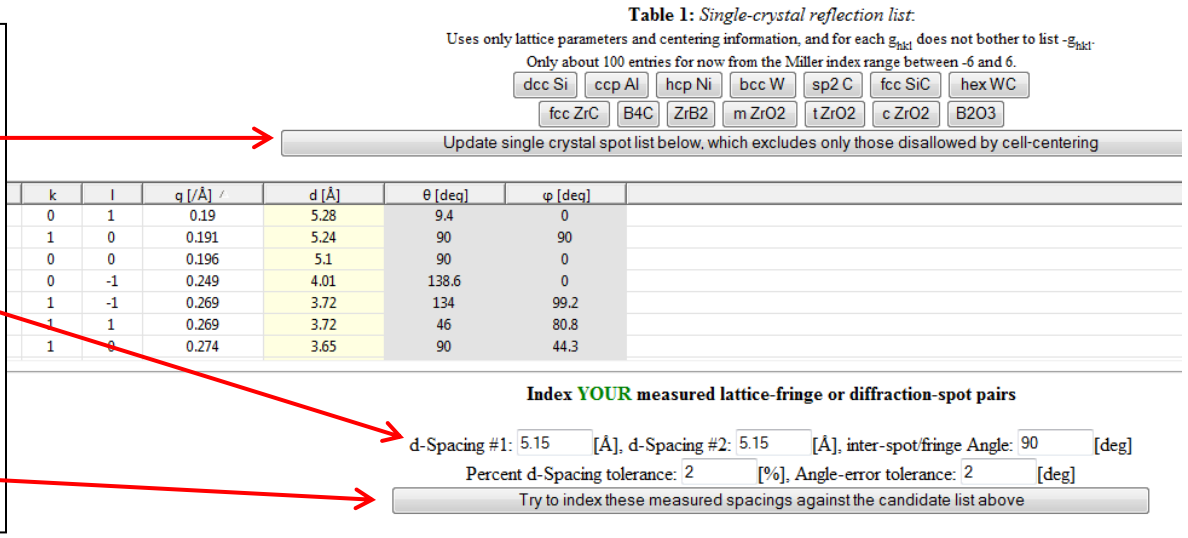
The following notes may be of some use once all required measurements have been obtained.

- The g-vector lengths are a powerful tool since they can be used to compute ratios of d-spacings without any knowledge of the camera constant. If λL can be assumed constant for your microscope, then we have $g_1 d_1 = g_2 d_2 \Rightarrow g_1/g_2 = d_2/d_1$. Candidate phase identifications can then be made using candidate phase d-spacing ratios in combination with θ_{12}.
- If you know your camera constant well enough to produce credible values of d_1 and d_2, then we have a website that may be of some use.
  Navigate to: http://www.umsl.edu/~fraundorfp/nanowrld/newlive/crystal9y.html .
  At this website, you are able to enter lattice parameters (a, b, c, α, β, γ) for any candidate phase. Then, you can use your measured d-spacings and inter-spot angle to rapidly determine whether your diffraction pattern might be indexed with the candidate phase. The following figures show your where to input your data at our website.

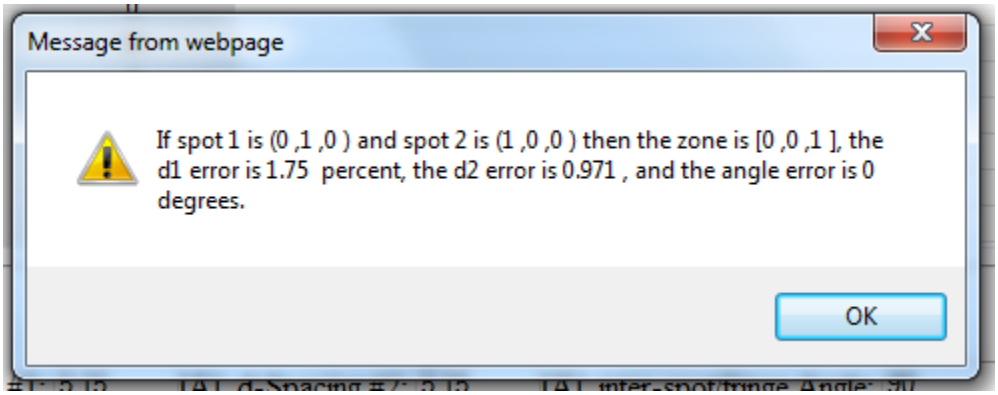
- Scroll down to here first.
- Enter candidate lattice parameters.
- Leave space group = 0.
- Click the upload bar.



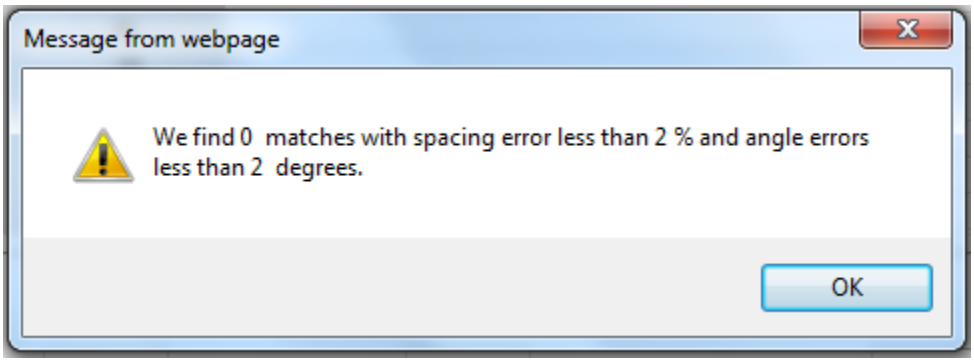
- Then, scroll down to here.
- Click the update bar.
- Enter your values of d_1, d_2, & θ_{12}
- Enter acceptable tolerance values.
- Click the try to index bar.



The results of your trial indexing will then appear as one of the two following popups:



The popup suggests candidate Miller indices along with the zone axis.



The popup indicates that there are no possible indexings.

At this point, it is important to remember that NO means NO, but YES means MAYBE with diffraction analysis. The Miller indices and zone axis are suggestions, not guarantees! Final indexing of the diffraction pattern will require confirmation. One possible method would be to use WebEMAPS to generate a model diffraction pattern for comparison with your possible indexing. Additional measurements and trial indexings will generally be required to completely index any SAED pattern. You should also note that the website will often suggest many possible indexings for your two spots.

Any complaints or comments about 4Spots should be sent to Bob Collins by email at rwcq58@mail.umsl.edu. Bob appreciates any and all feedback on ways in which the plugin can be improved in terms of functionality and ease of use. These instructions are, likewise, a work in progress. Any questions can also be directed to Bob Collins.

-BC

July 5, 2012