ELSTRU
INSTALLATION AND TESTING

For
Windows XP
Windows 7
Windows 8

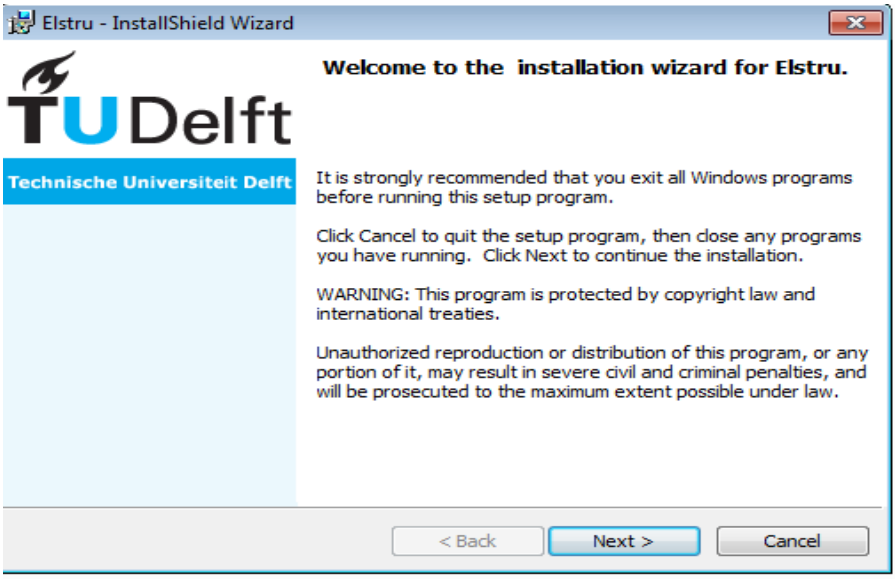
manual revision : 1.0

Software version 1.1

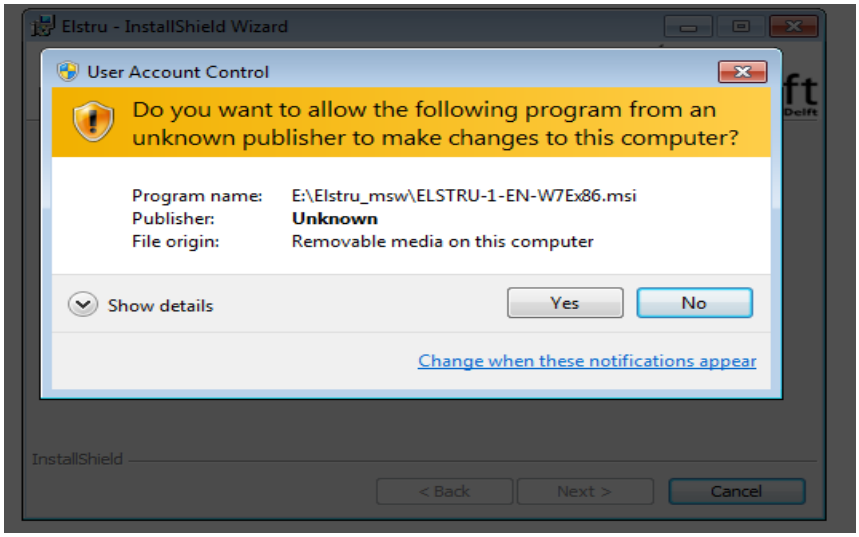
Contents

1.Installation

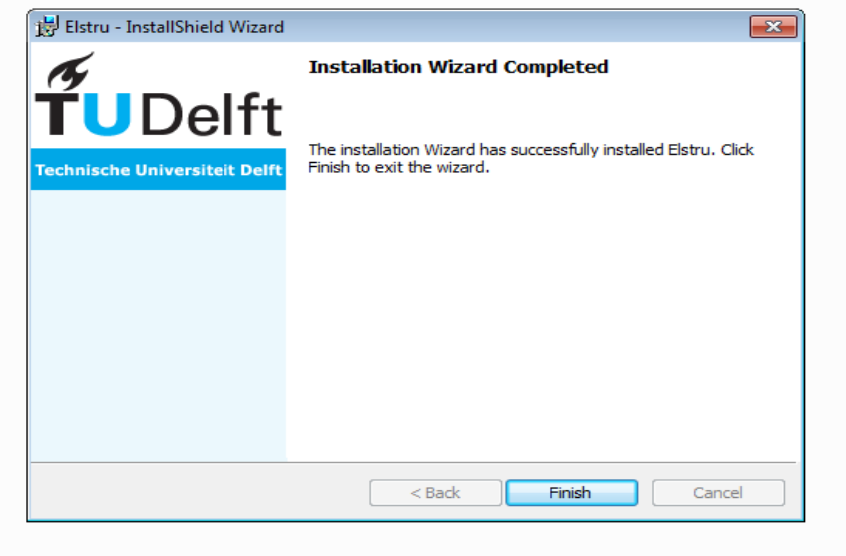
Currently ELSTRU for Microsoft-Windows runs both on 32-bit as on 64 bit versions of XP, 7 & 8.
The Installation package for Elstru can be downloaded as an install-package from our FTP-server :
ftp://nchrem.tnw.tudelft.nl/elstru/ELSTRU-1-EN-W7EX86.msi
Copy this file to the machine where you want to install. Do not use IE,because a bug in IE makes it fail to download this file. Firefox is better suited for the task. After downloading "*double click*" on the ELSTRU-1-EN-W7EX86.msi file.



Click on "Next".



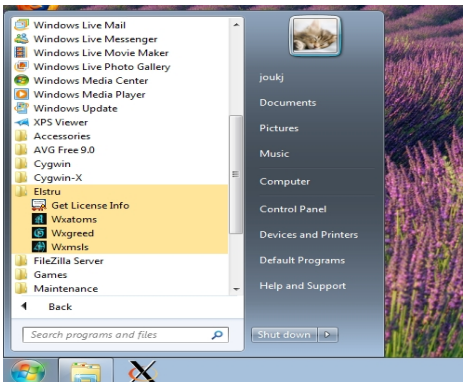
Allow for installation as "admin" user. Finally you should get get following window



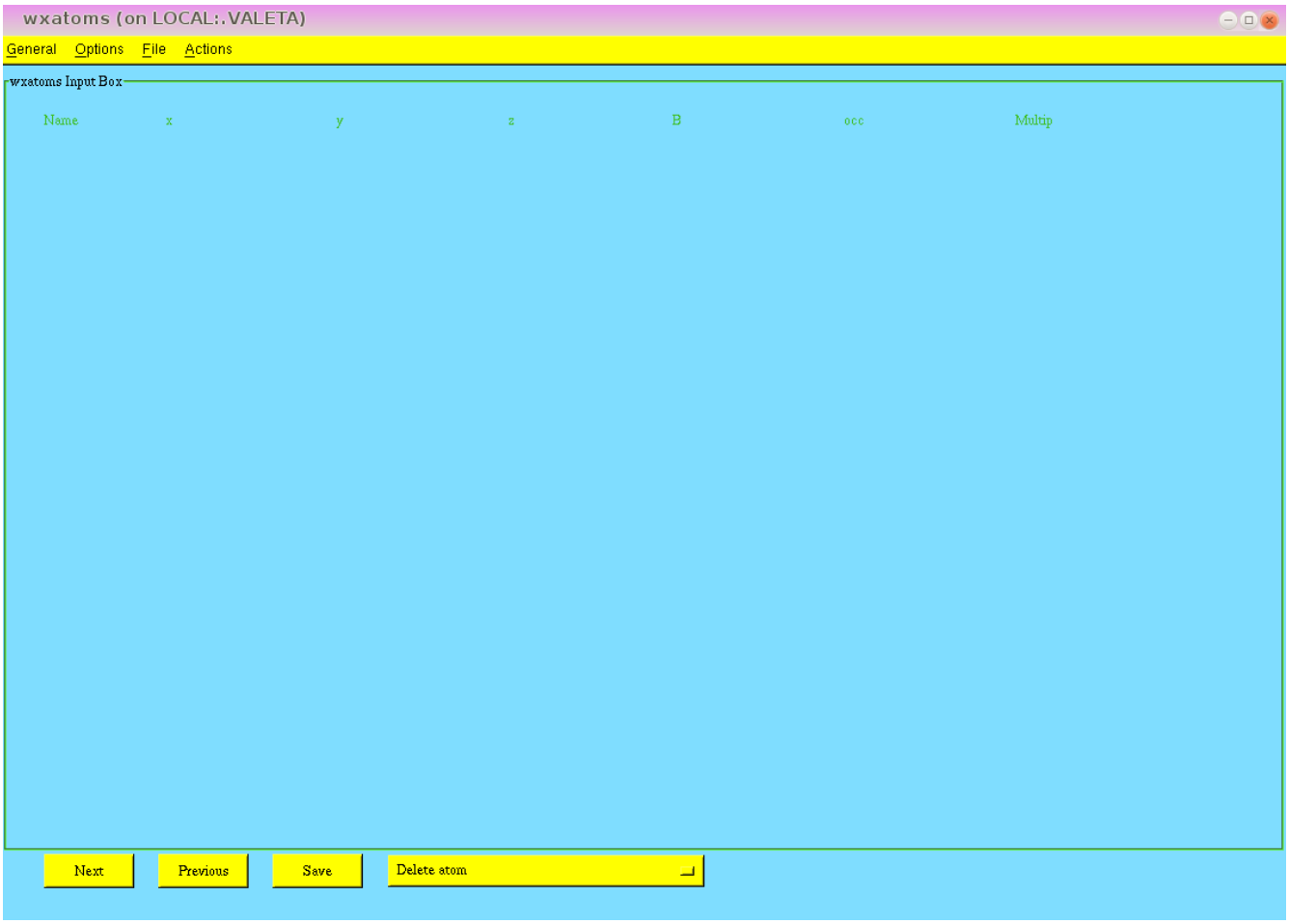
Click on “Finsish” to end the installation. Congratulations you installed your version of Elstru.

2. Testing the installation

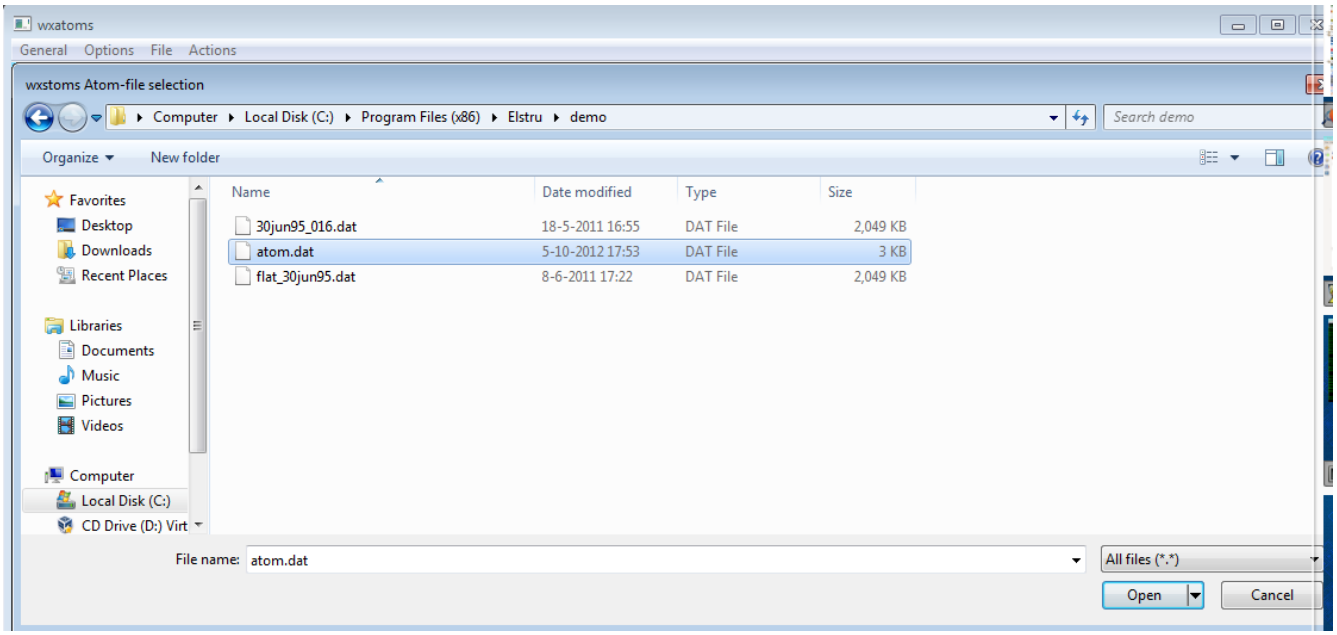
Select from the “Start”-menu: Start->Elstru-wxatoms.



The following window should appear.



wxatoms is the atomic parameter editing program for Elstru.
Select from the top-menu : File->Openfile In the browser window go to c:\Program Files\elstru\demo

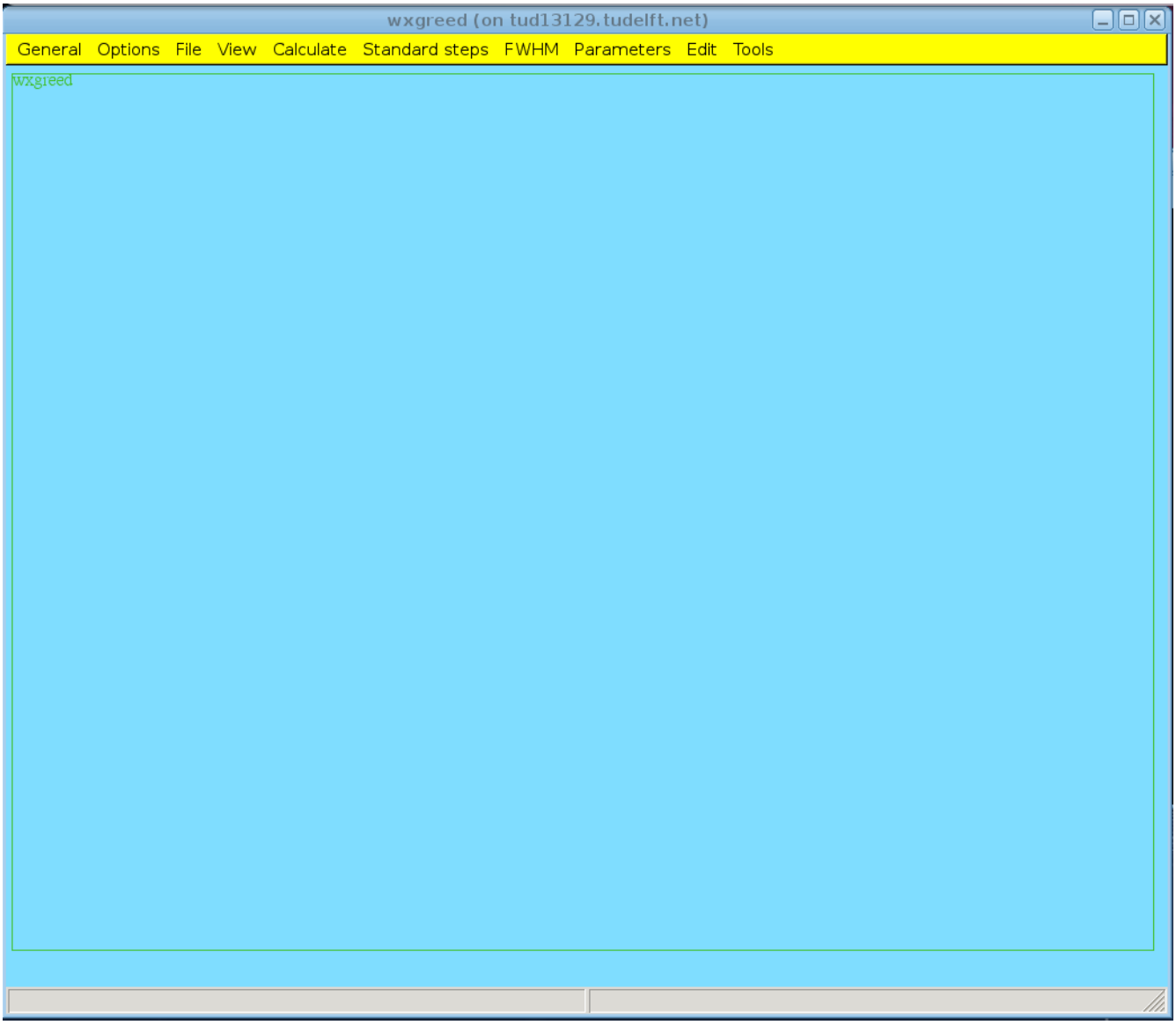


Select the file atom.dat and click on “Open”. The following should be visible:

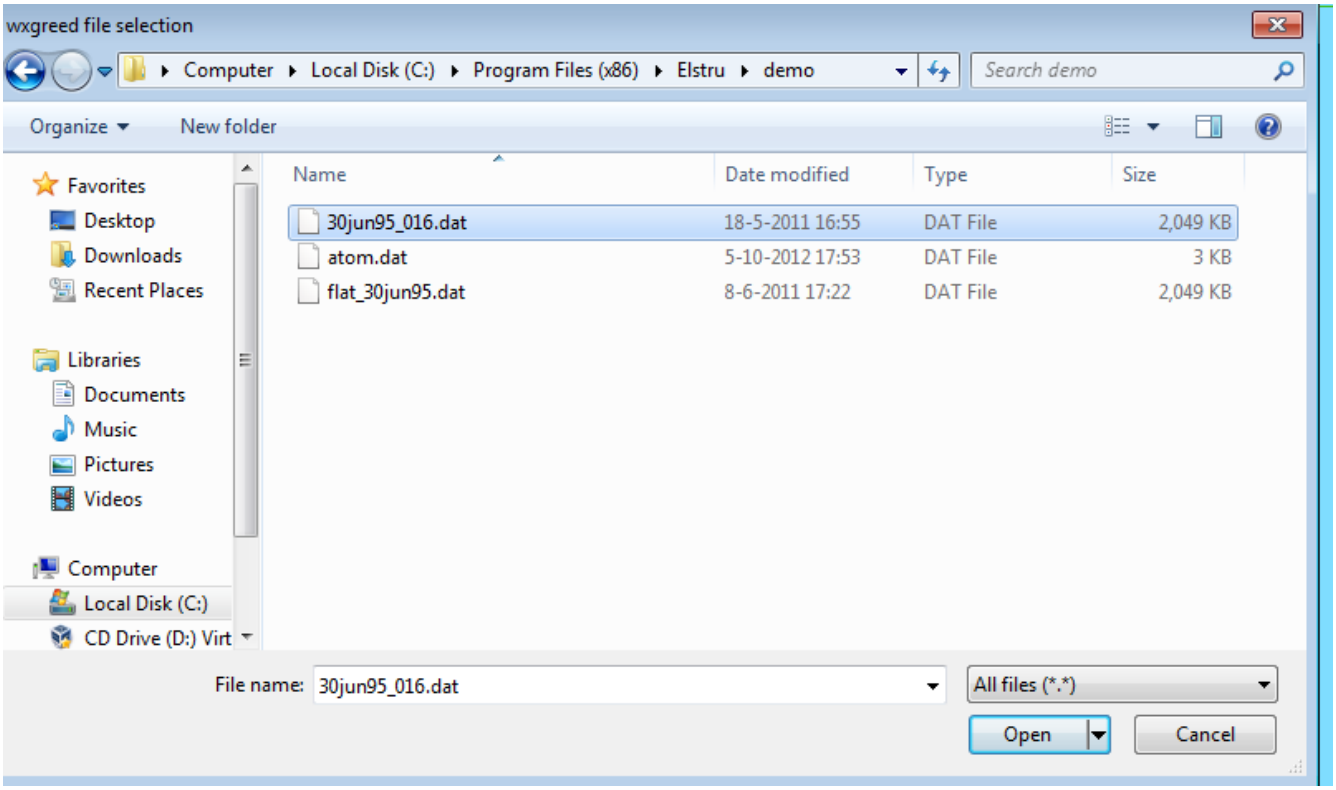
For the demonstration everything is filled in correctly. By selecting *"general->exit"* from the top-menu you can leave the program

Exit the program by clicking on "OK"

The next program to run is the data reduction program (greed=Graphical REduction of Electron Diffractiondata). Select from the "start-menu" Start->Elstru->Wxgreed.
The following window should appear.

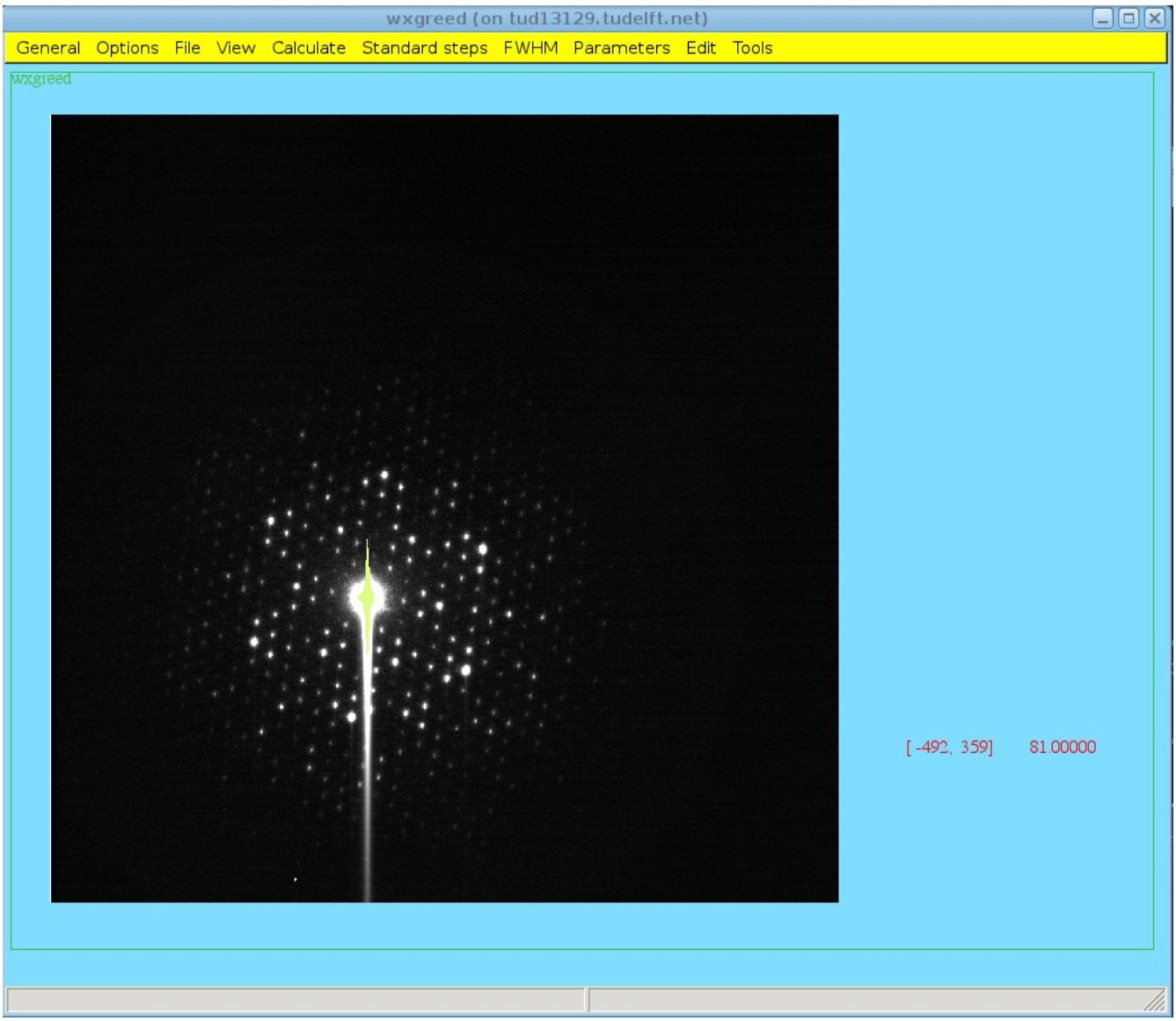


To open the data-file, select “File->Open file” from the menu bar. A file-selection window should pop-up.



Select the file “c:\Program Files\Elstru\demo\30jun95_016.dat” and click on “Open”

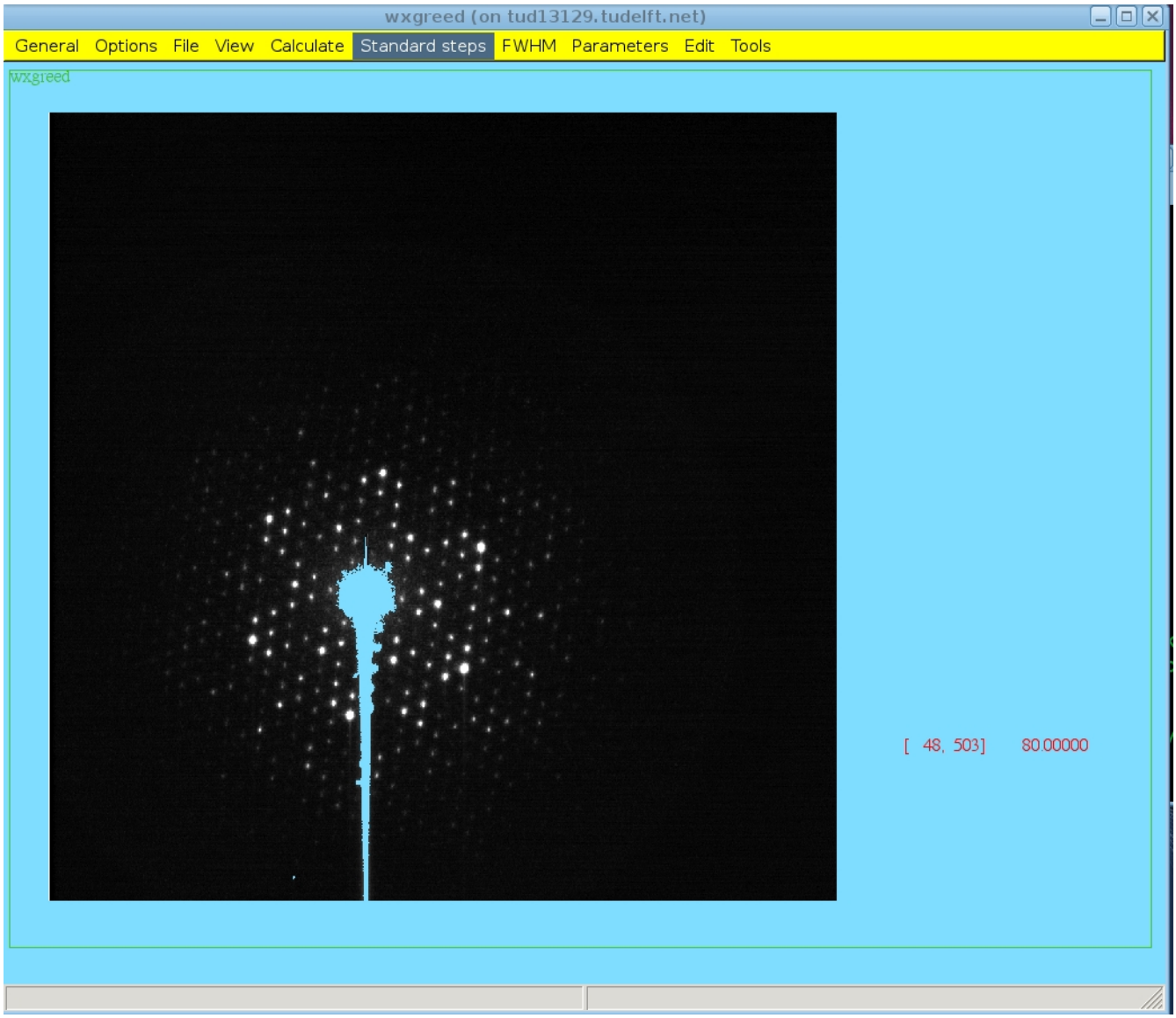
The diffraction patterns should be displayed. This image is taken using an old CCD-camera with no ant-blooming capability. The yellow areas are overexposed and contain no reliable pixel intensities.



Select “Standard Steps->All Steps” from the menu-bar. The following steps will be performed successively:

-Determination of the position of the central beam (origin). This position is marked by a blue cross.

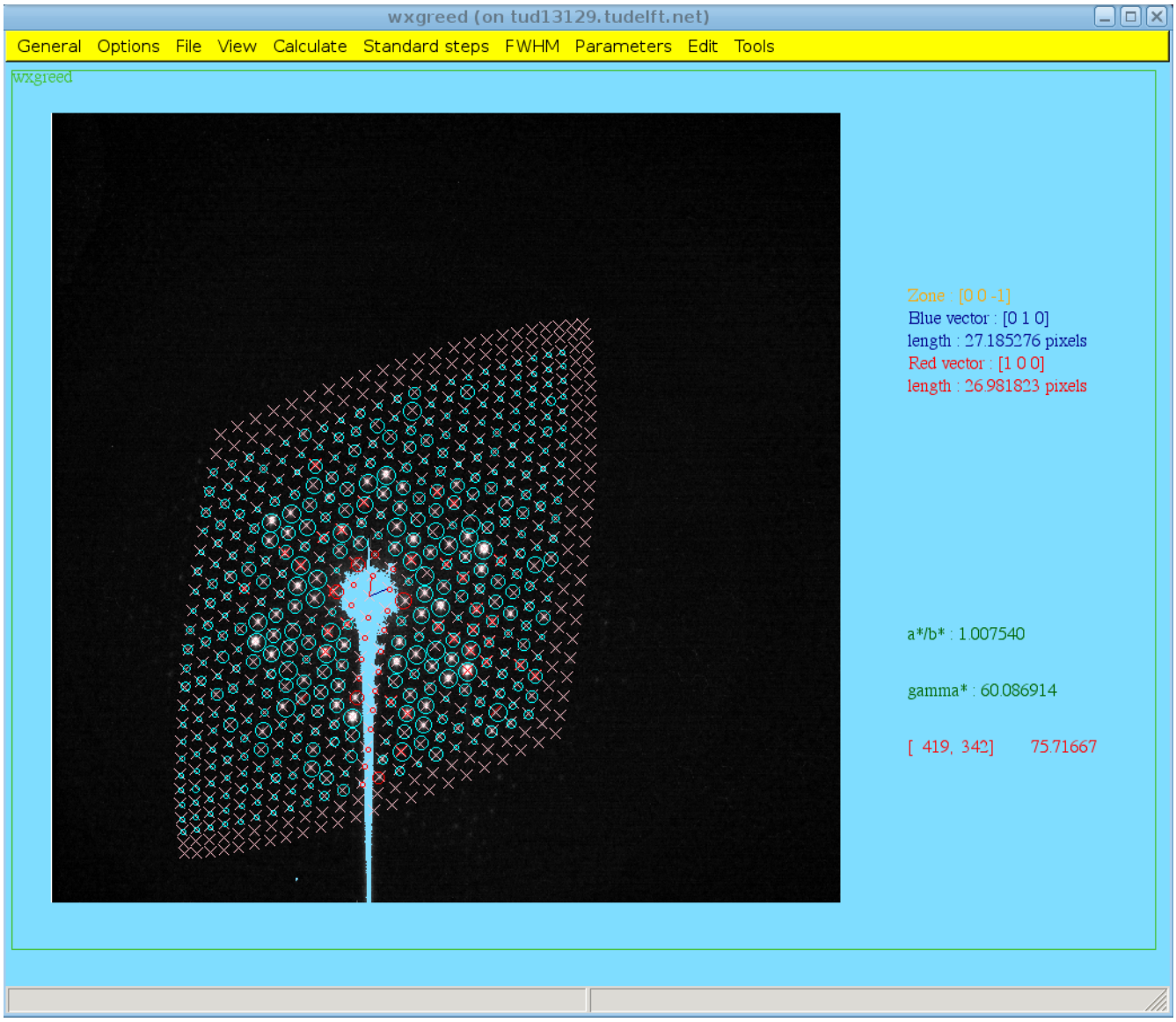
-Determination of the areas which are not to be used, i.e. Due to blooming or over-saturation. These areas are marked blue.



-Correction for the different sensitivity of each pixel on the CCD-chip (Flatfield-correction)
-Search for significant peaks. The are marked by red crosses

-Indexing the peaks. This means that the 2 spanning vectors of the zone (and some correction terms are determined, The vectors are marked red and blue. Than all locations where reflections are expected are marked with pink crosses. For a successful indexing for red cross (found peak) a pink cross should be at the same position. A guess for the actual zone-orientation is given at the right-hand site of the diffraction pattern.

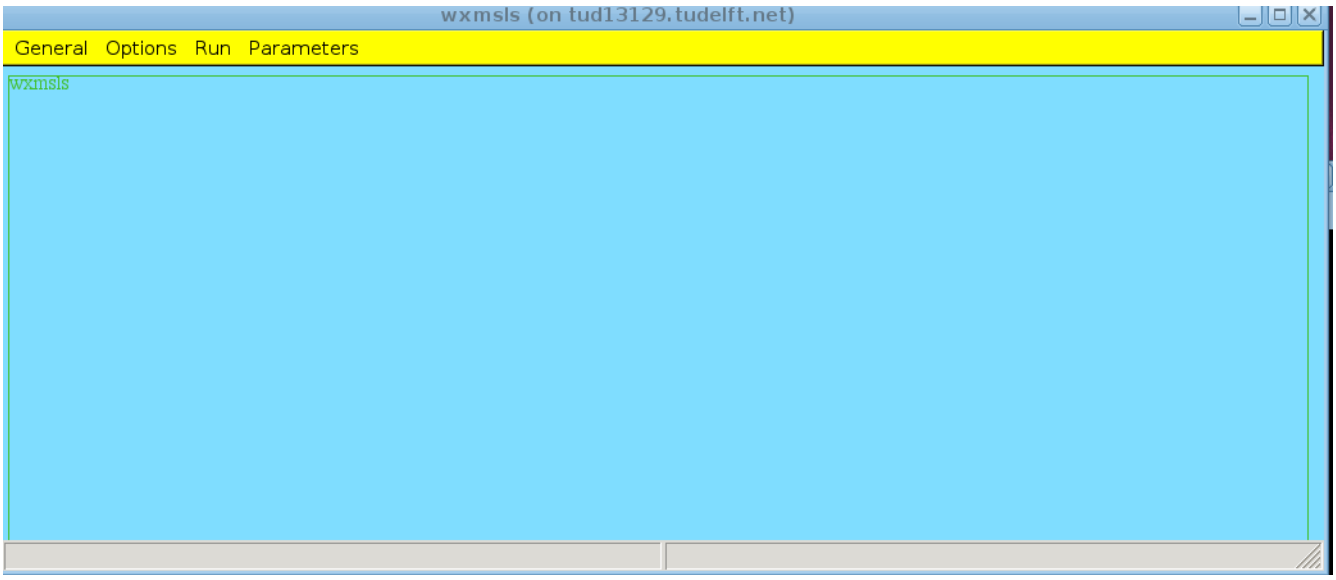
-Determine the integrated indexed intensities by putting blue circles around each reflection position. The integrated intensity is the sum of the intensities of the pixels inside a circle corrected for the background using the pixels on the circles. Reflections in red circles are ignored because they contain pixels in excluded regions of the CCD.



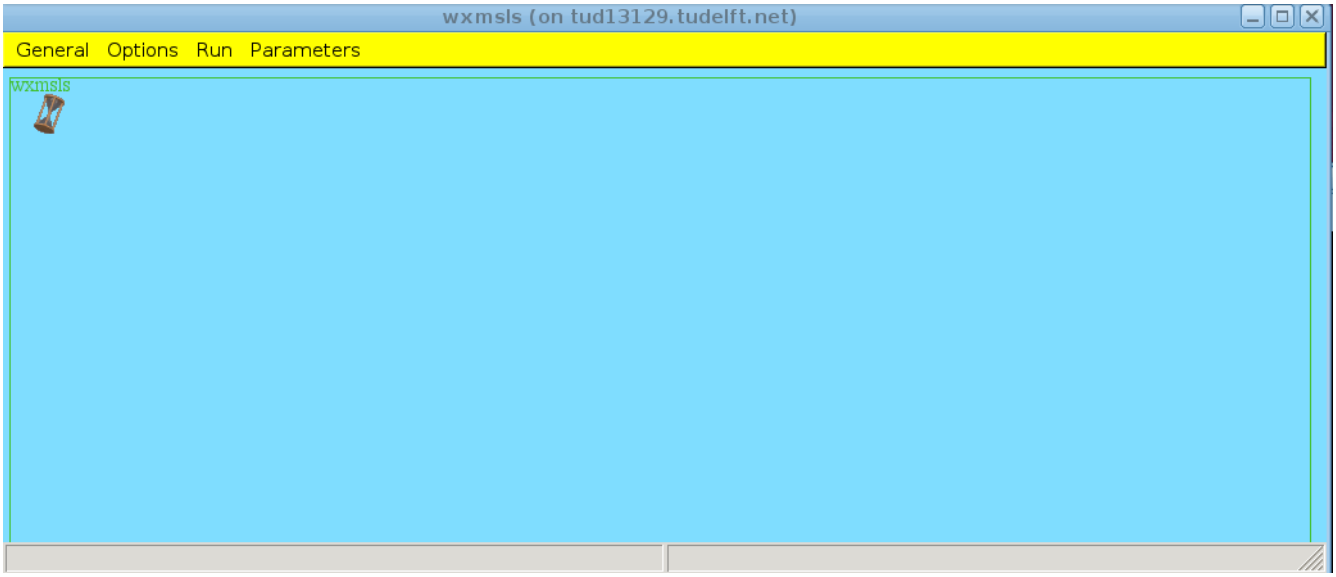
The most important file the program created is call 30jun95_016.ii and contains the indexed integrated intensities.

By selecting *"general->exit"* from the top-menu you can leave the program.

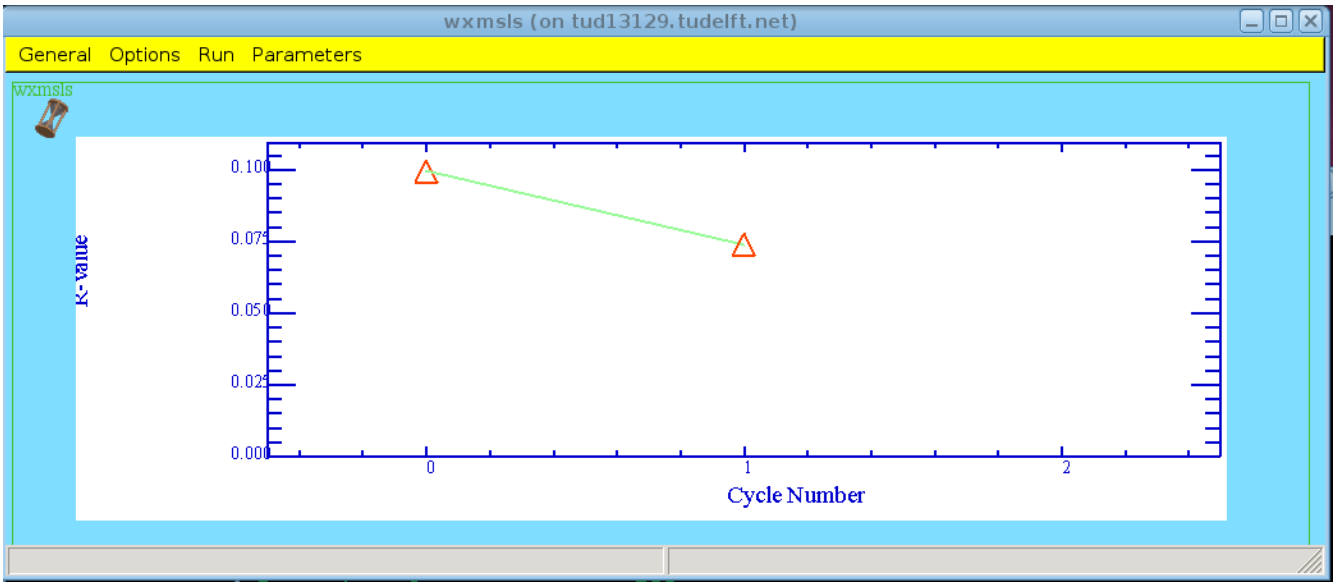
The final program to test is the Least-Squares-Multi-Slice (MSLS) refinement program. To start the program select Start->Elstru->Wxmsls form the “Start-menu”
The following window pops-up.



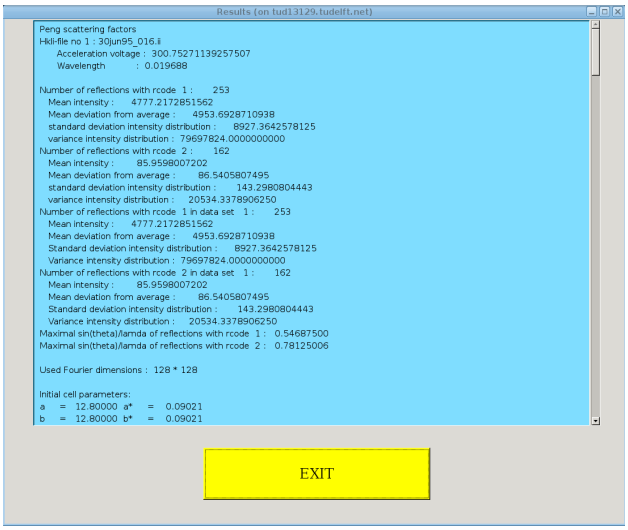
For the testing all parameters are already set to their correct values. So we can start running immediately by selecting “Run->Run MSLS” from the menu bar. An hourglass will tell you that a calculation is in progress.

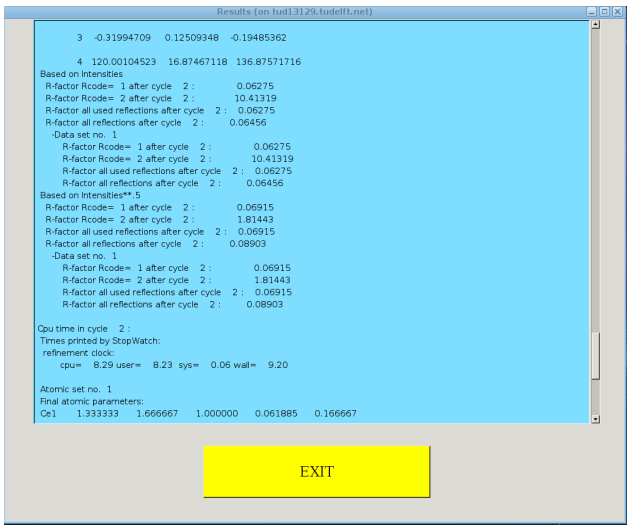


When the first R-values are calculated a graph will appear showing the current status of the R-value.

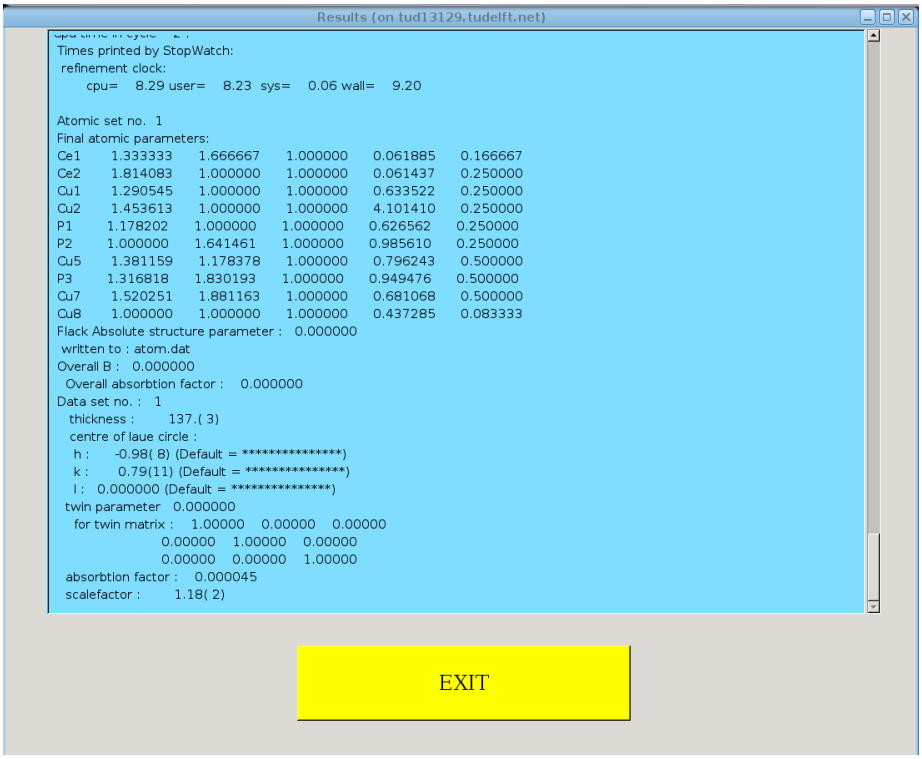


The plot is updated for each refinement cycle. When the refinement is finished a window containing the results pops-up.

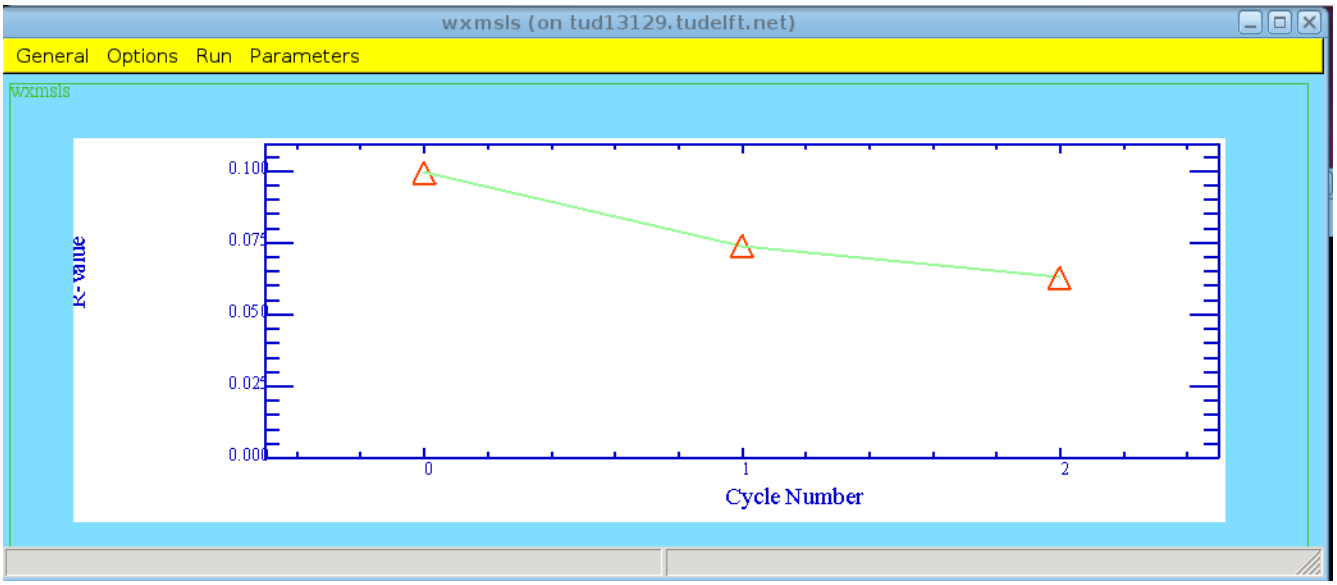




Check now that the values for the crystal thickness, Centre of Lau-circle and scalefactor are close to the values displayed in the sample window below.



Close the window by pressing the “EXIT” button. Check now that the R-value graph is similar to the one displayed here.

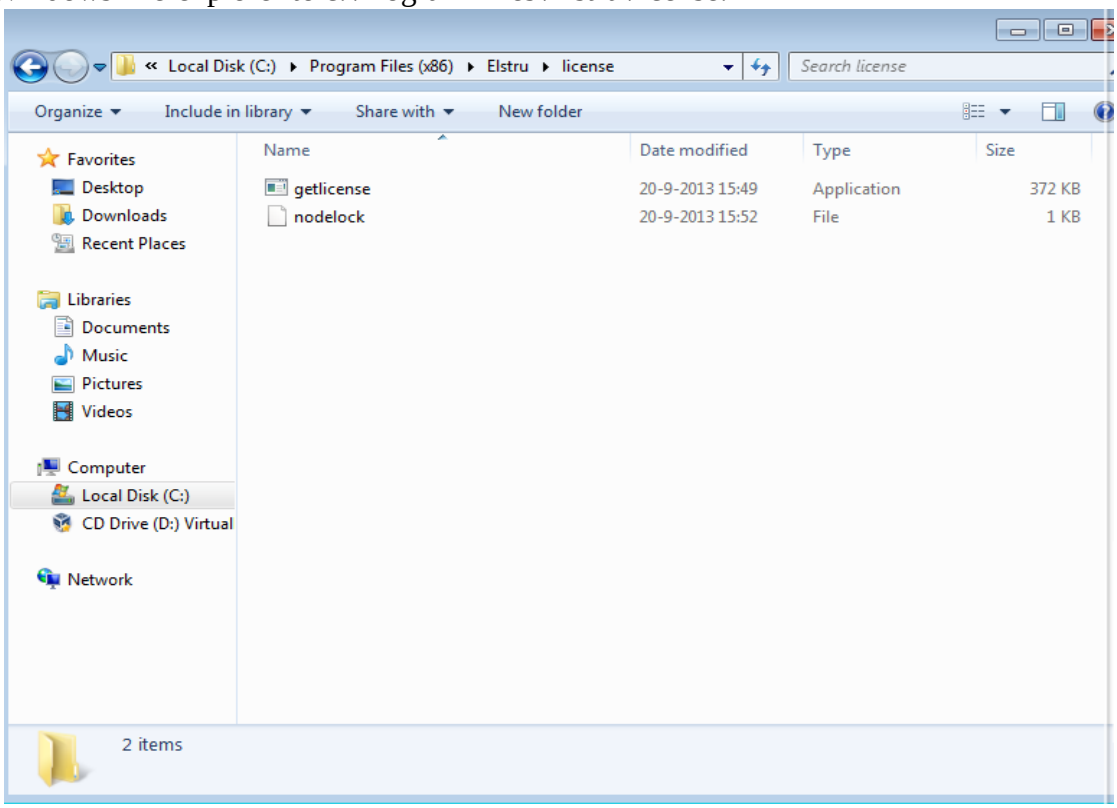


Close the program by selecting “general->exit” from the menu bar.
If everything did run correctly, I can congratulate you with a working version of ELSTRU.

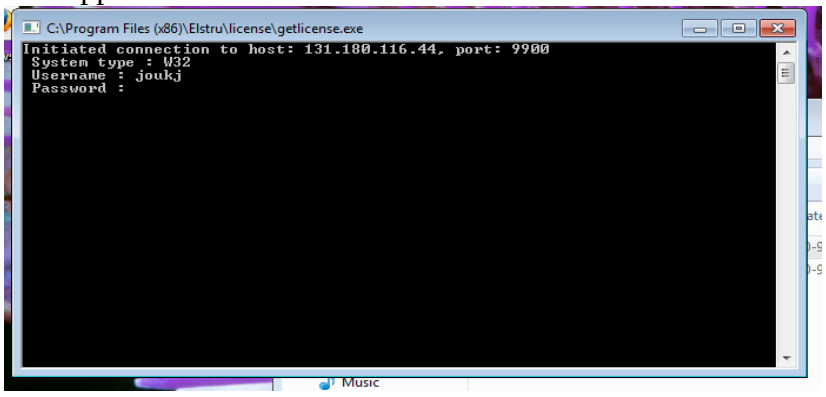
3. Obtain a license

Without a license the programs operate in Demo-mode with a lot of options disabled. This chapter describes how to obtain a license.
Contact Jouk Jansen (joukj@hrem.nano.tudelft.nl) for the license conditions. Once you have a agreed on the license conditions you will be provided with a username/password which is coupled to your E-mail address.
Once you got the username/password you can generate your machine-dependent license file, nodelock, in the following way. Note that this procedure can only used if the computer is connected to the internet and if your fire-wall accepts out-going traffic. If you are not able to run this procedure contact Jouk Jansen (joukj@hrem.nano.tudelft.nl), who will help you with a *manual* generation/installation of the license.

Set the Windows-file-explorer to c:\Program Files\Elstru\license:



Run the program GETLICENSE by 'double-clicking on it. A window in which you can fill in your username/password will appear:



The program now send all the needed information to Delft (see the licinfo.txt file to see what is actually sent). Within a working day an E-mail should be returned containing a nodelock file. This file can be placed in one of the following locations and should be renamed to nodelock

c:\Program Files\elstru\ (For an installation of all users on the machine (32bit windows))
c:\Program Files (x86)\elstru\ (For an installation of all users on the machine (64bit windows))
c:\Documents and Settings \<username>\ (=the home directory of the user using ELSTRU)

Once yo have done this all the programs of the ELSTRU package should be functioning with all the available options.

4. asking questions and making remarks

The ELSTRU software and documentation improves by your comments. So, do not hesitate to ask what is not clear and make comments on what you (dis)like about the software and the documentation. Please, send your questions and remarks to Jouk Jansen (joukj@hrem.nano.tudelft.nl).