

# General Information

XBroad is public domain program designed for easy-to-use determination of basic microstructural information from XRD powder data. Nowadays, preparation of nanomaterials with controlled particle size and shape has been found to be essential for tailoring the desired materials properties so quick and effective line broadening analysis is an imperative. Although methods implemented in program are considered to be “traditional” ones authors believe that program will provide very fast platform for non-crystallographers working in the field of materials science, as well as for students learning basics of size-strain analysis.

## Hardware and software environment

The program runs on any PC. Operating systems: Windows, Linux and Macintosh (Mac OS)

## Program specification

X-ray, synchrotron or neutron diffraction data can be used. Program requires input experimental data in XY format. The results are stored in merged textual output file `xbroad/dist/logfile.dat`.

## Authors

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## References

# Installing and running the program

## **On PC-Windows platforms**

Unzip xbroad.7z. Run cheby.exe which is located in xbroad/dist

## **On Mac platforms**


Work in progress

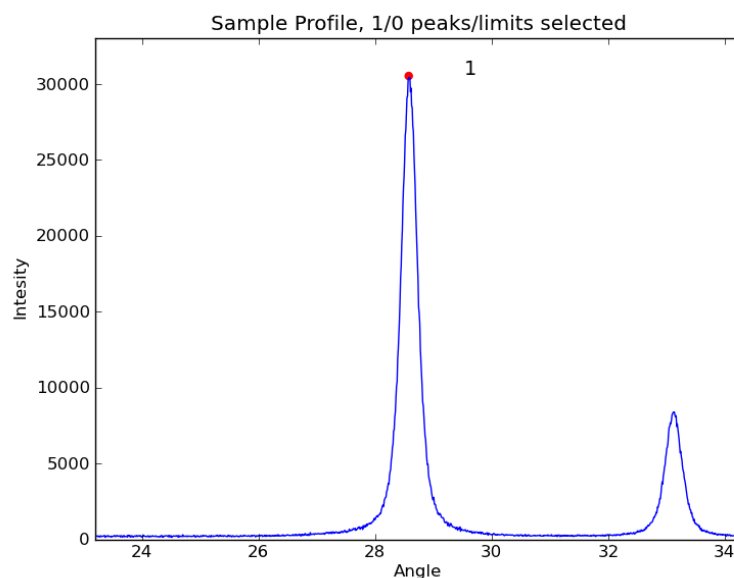
## **Running the program**

The tutorial test data files can be downloaded from: [http://mysite.du.edu/~balzar/s-s\\_rr.htm#Data](http://mysite.du.edu/~balzar/s-s_rr.htm#Data).  
Download following files: lebailsh.xy (instrumental profile) and lebailbr.xy (sample profile).

The original data files should be changed to appropriate format by deleting first two lines, and should be saved in .dat format.

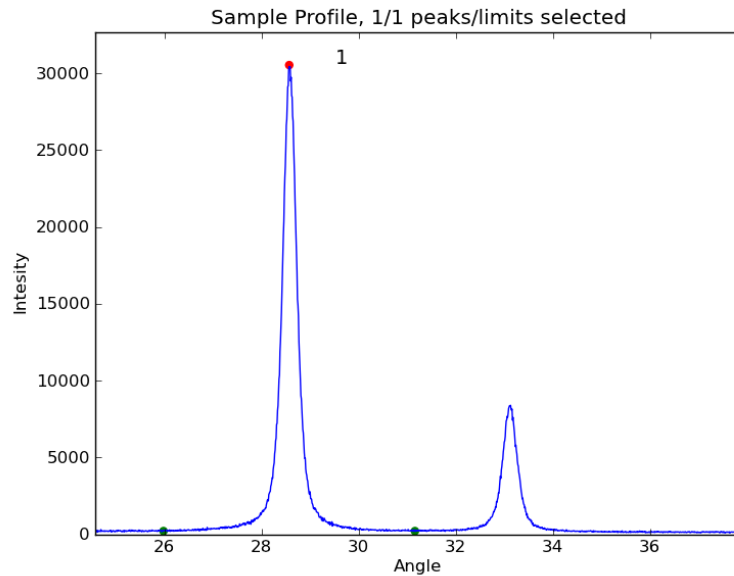
## Step-by-step tutorial on CeO2

1. Press Sample button to load leailbr.dat. Diffraction pattern called *Sample profile* is displayed in new window.
2. Press Instrumental button to load leailsh.dat. Diffraction pattern called *Instrumental profile* is displayed in new window.
3. Make sure that Cu wavelength is selected.
4. Zoom in first peak in *Sample profile* window by pressing . Place the cursor on the maximum intensity of first peak (around 30000 counts) and press A. Red dot should appear at the maximum intensity of chosen peak. Header changes to 1/0 peaks/limits selected, meaning that first peak is successfully selected.

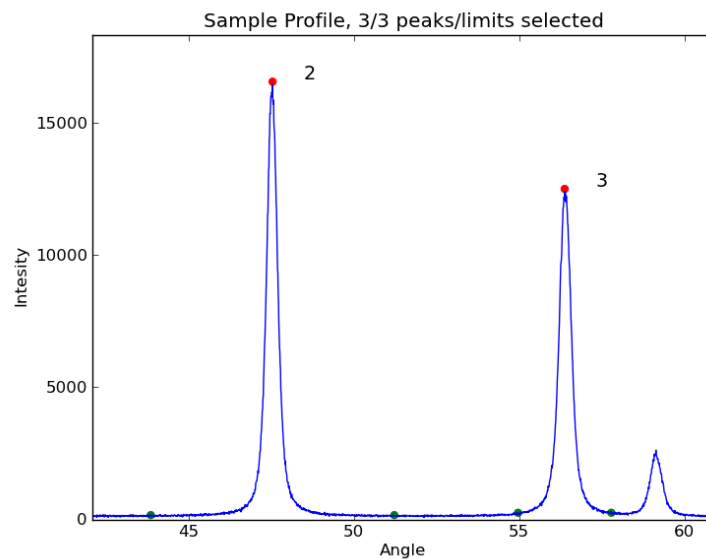



If the dot appears at some place other than maximum intensity (because the program looks for the local maximum in the very near vicinity of the place where the cursor is located) it should be deleted by placing the cursor on it and pressing D.

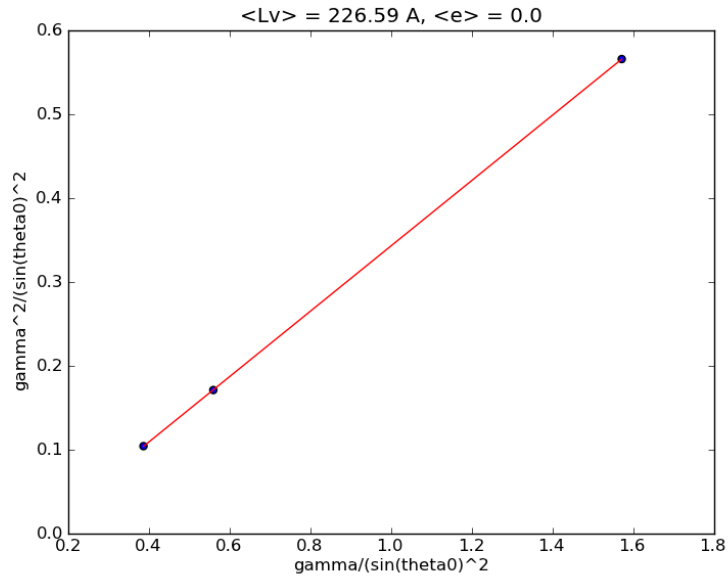
5. Select the limits of the peak by placing the cursor at  $26^\circ 2\theta$  and press W. Green dots appear on the lower angle, and symmetrically, on the higher angle side of the maximum. The limits can be deselected by placing the cursor on the green dot and pressing R. Header changes to *1/1 peaks/limits selected* meaning that both peak position and profile limits are successfully selected.



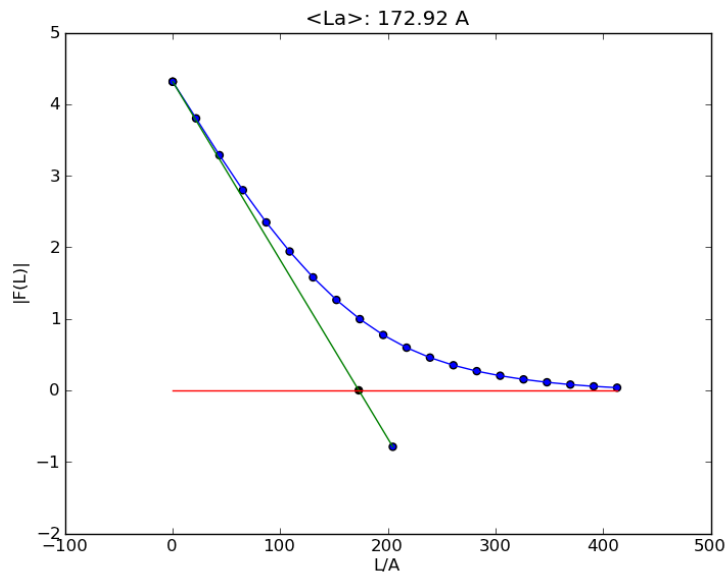
- Zoom in the range between  $44^\circ$  and  $60^\circ$   $2\theta$ . Repeat the same procedure for both peaks. Header changes to *3/3 peaks/limits selected* meaning that all peaks and profile limits are successfully selected.



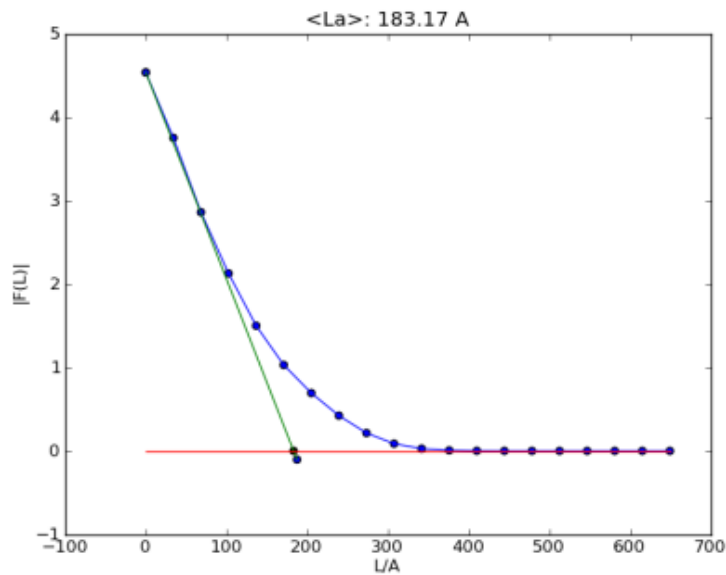
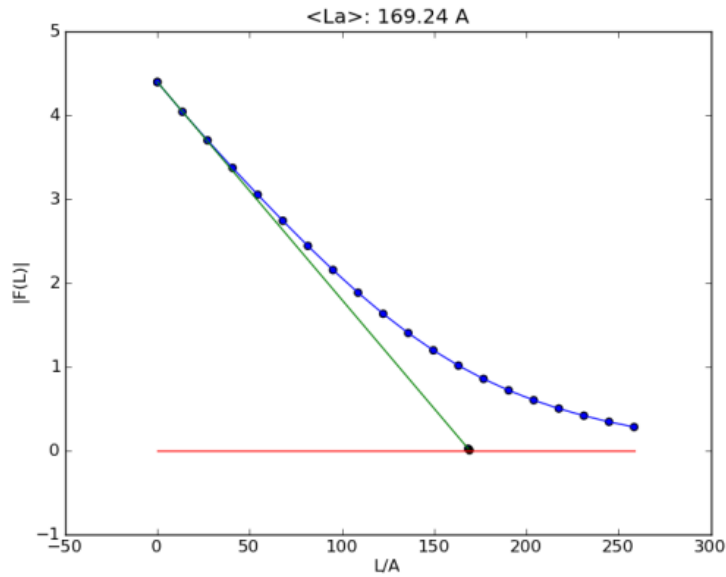
- Switch to *Instrumental profile* window. Repeat the same procedure for peak selection as described at Ad.4. for the same three peaks chosen in *Sample profile*. Header changes to *1 peak selected*. Program sets limits automatically in the case for Instrumental profile.
- Click button *Williamson Hall plot*, graphical result appears in new window. At the top of the screen numerical results for volume-weighted column length  $\langle L \rangle_v$  and approximate upper limit of the lattice strains  $e$  are displayed. The result can be saved in different graphic formats by clicking  (or, alternatively, pressing S on the keyboard).



9. Click *Warren-Averbach-Bertaut* button, but firstly select peak no. 1. from the pull-down menu right to the button. New window appears displaying a  $F(L)$  vs.  $L$  plot. User has to draw the tangent at the first point ( $F(0)$ ) in the following way: click somewhere in the middle of the screen. Program draws the line whose ending point user can freely move by clicking on it until the best visual tangent is observed. At the top of the screen numerical result for area-weighted column length  $\langle L \rangle_A$  is displayed.



10. Repeat the procedure for peaks nos. 2. and 3.



11. Finally, open `xbroad/dist/logfile.dat` and check the results ☺. Note that output file is created after the program is closed.

**Important note about peak selection in *Sample profile*:**

While choosing peaks and limits, user should be careful that there is no peak overlap present.

**Important note about peak selection in *Instrumental profile*:**

In this example, instrumental standard material is  $\text{CeO}_2$  - same as the sample, however, very often the same material cannot be used since it is hard to always obtain satisfactorily narrow lines. In that case suitable certified standard reference material is used and user should select instrumental

peak with  $2\theta$  closest to the one of chosen sample peak. This is necessary because of the angle dependence of instrumental broadening. Also, choose only the peaks which do not overlap with any neighbouring peaks.

**Important note on deconvolution:**

Due to overestimation of the background or overlapping of the adjacent lines the “hook effect” can appear. The obtained value of  $F(0)$  is less than it should be. User is invited to carefully inspect the graphical result of the WAB method in order to note possible appearance of “hook effect” and therefore disregard selected diffraction maximum from further analysis.