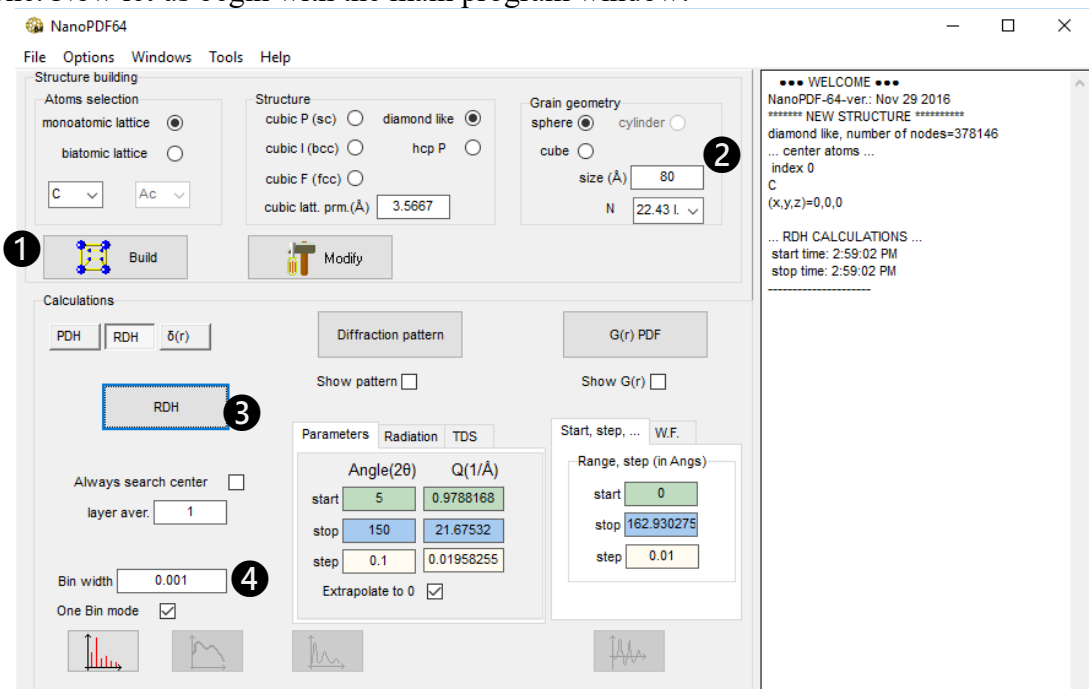
Automated fitting of G(r) in multiple finite size ranges

Example1

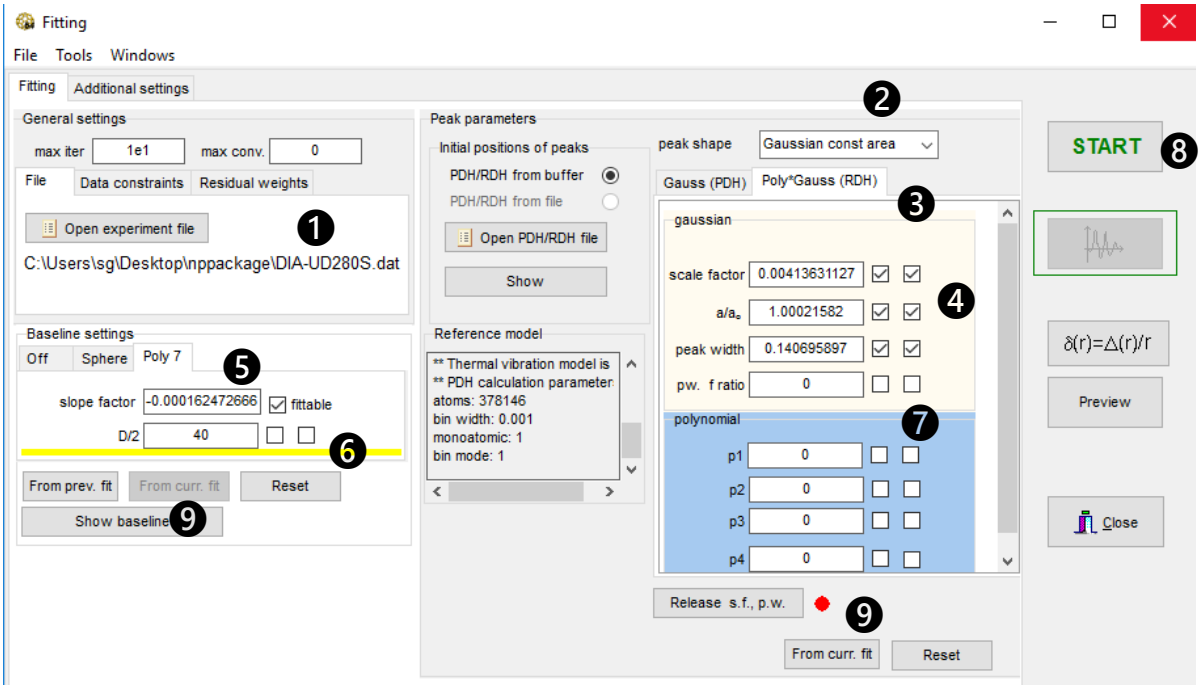
Determination of Δr/r and fwhm(r) from experimental G(r).

The idea behind the procedure is the following. If the crystal lattice of a nanocrystal is not ideally periodic, and we believe it is not, peaks in G(r) will be slightly shifted from "ideal" positions. Also the peak widths will vary. In a typical G(r) only a few peaks at the very beginning may be resolved. Others heavily overlap and neither their widths nor positions cannot be individually determined. In order to overcome this limitation we divide the available data span into narrow ranges and fit G(r) in every range separately to get an average lattice parameter – *apparent lattice parameter – alp* – and an average peak width inside each range. From such data we try to learn about the actual atomic structure of nanocrystals.

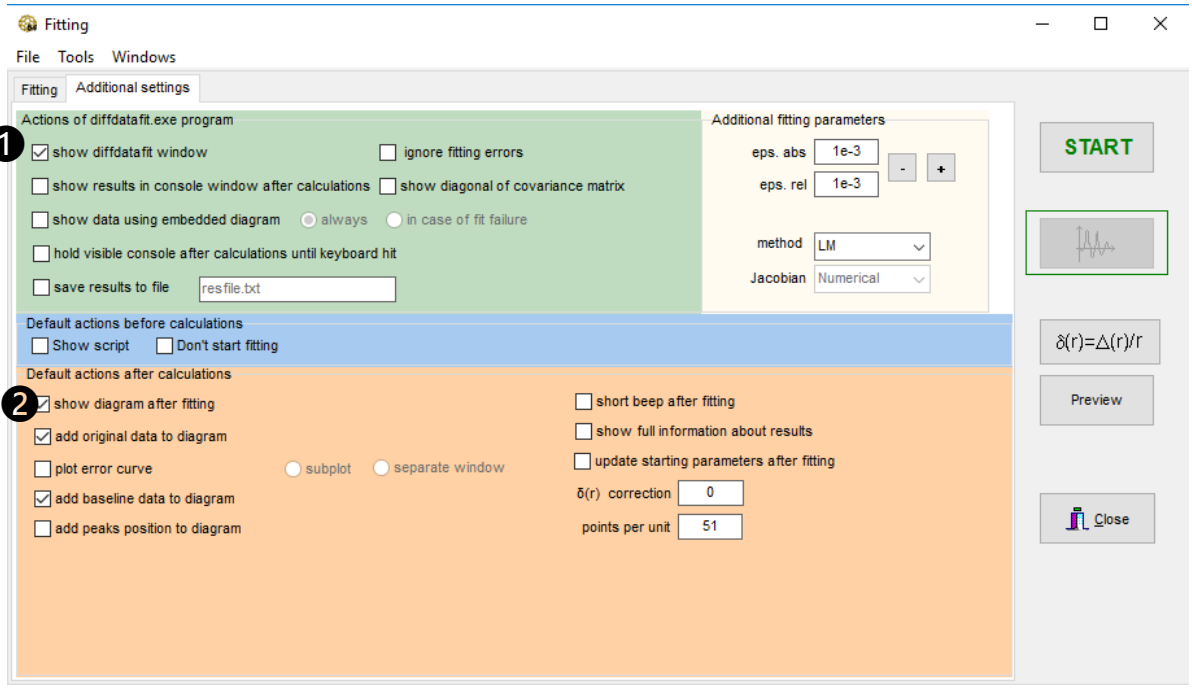
We assume that you have already familiarized yourself with the fitting part by going through the first example. If certain parts of the procedure are not explicitly mentioned they "default" to what you have already done. Now let us begin with the main program window:



Build ❶ diamond sphere of 80A radius ❷ and calculate RDF ❸ for it. Make sure the "bin width" is small – try 0.0001 – and check that you are in "One bin mode" ❹. Than go to **Tools→Fitting**.

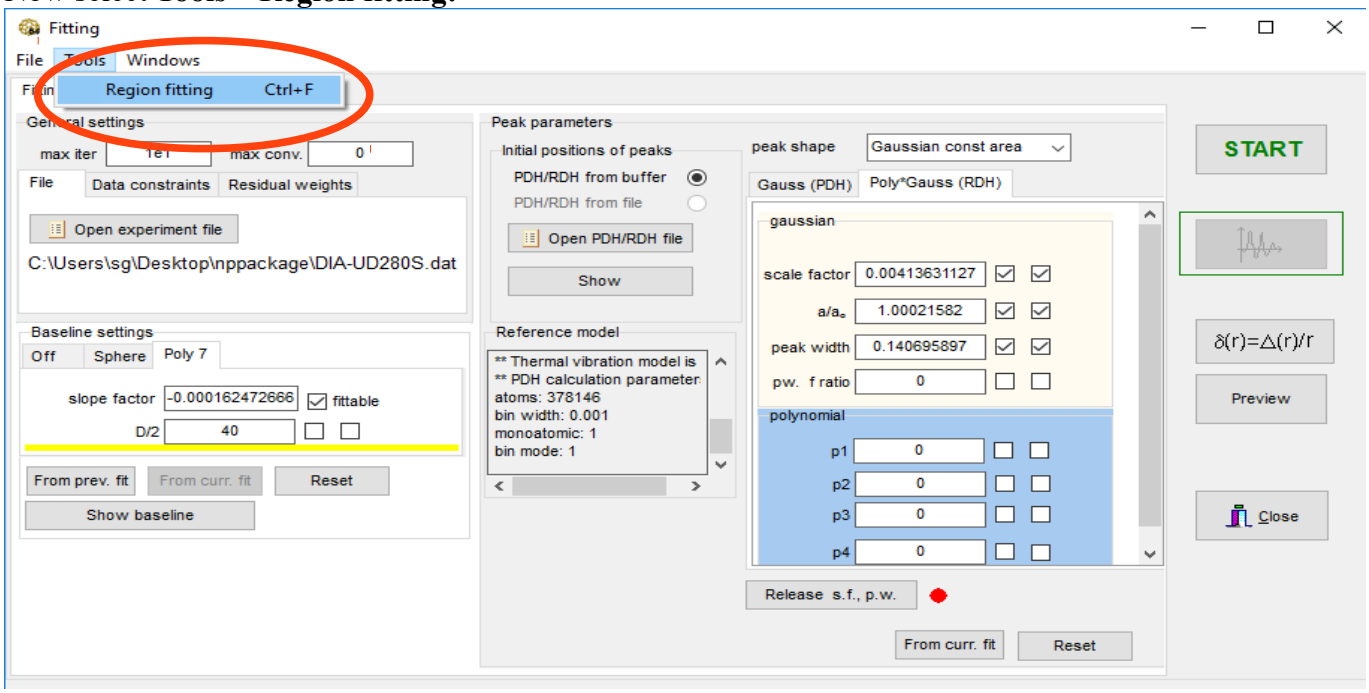


Load experimental G(r) ❶, choose "Gaussian const. area"❷ and "Poly*Gauss(RDH)"❸. Set "scale factor", "a/a_0", "peak width" ❹ and "slope factor"❺ to something reasonable and make those parameters fittable. Also set "D/2" to 40 but don't let it vary❻. Set to zero all the remaining parameters and don't let those to vary❼. If in doubt consult the picture above. Run a fit ❽ to get some reasonable starting parameters. Remember to update the parameters by clicking on **<u>two</u>** "From curr. fit" ❾ buttons.

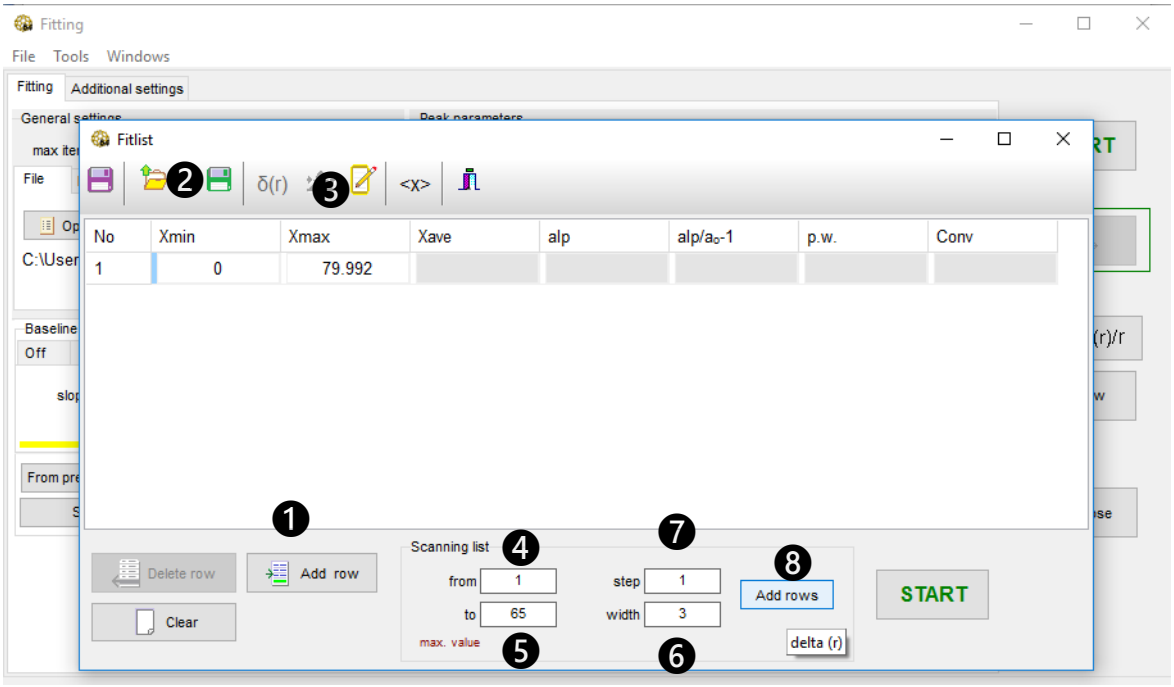


Now we have to decide what to display during the fitting procedure. We are going to make several tens of quick fitting runs in a row and displaying all those console windows makes no sense. Therefore we want to clear the "show diffdatafit window" checkbox. ❶ If you leave "show diagram after fitting" ❷ checked graphical result of every fit will show up and you'll have to close all those windows one by one. On the other hand it'll give you a chance to examine the fit quality. If unchecked, you'll only see numbers. Both situations are described further down in the text.

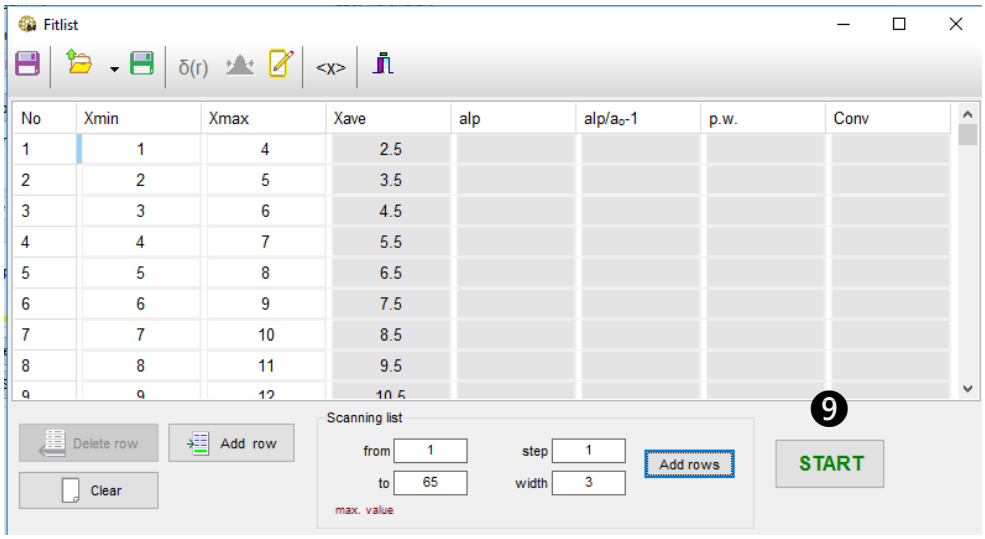
Now select **Tools→Region fitting:**



A window appears to define ranges within which the fits we be executed automatically. They may be defined manually by using “Add row” ❶ and defining “Xmin”❷ and “Xmax”❸ but we will do it in an organized manner.

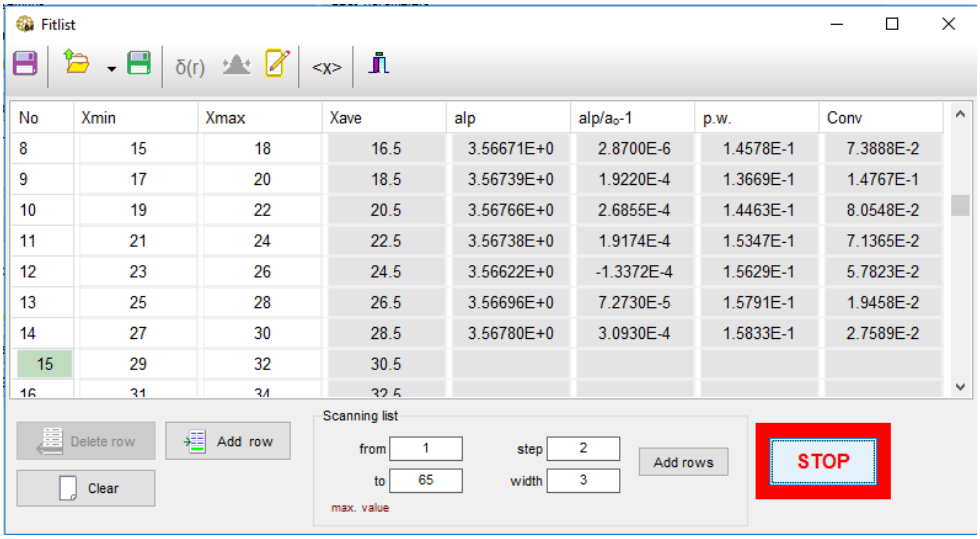


Set the data limits: from 1 ❹to 65Å❺. There are no peaks below 1, and peaks above 65 are so week that least squares get unstable. Now divide all data into a series of ranges 3Å long ❻ shifted by 1Å❼ with respect to each other. Finally press “Add rows” ❽ to execute.

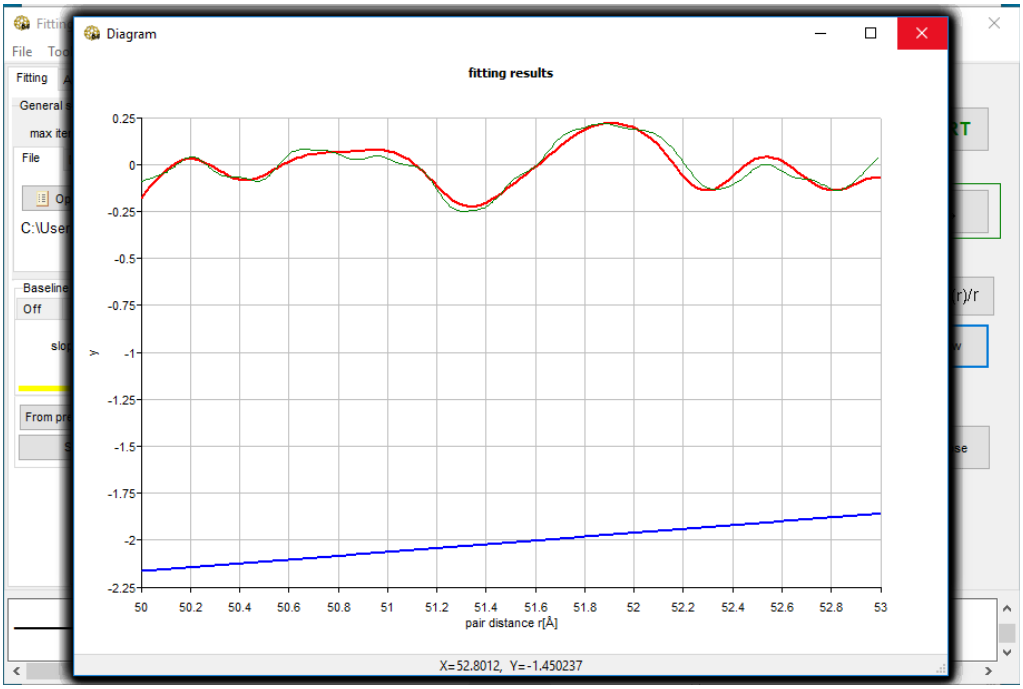


The list gets filled as above. Start fitting ❾

Now depending on the choices you made in “Additional settings” you will either see the list getting filled by the fitted parameters:

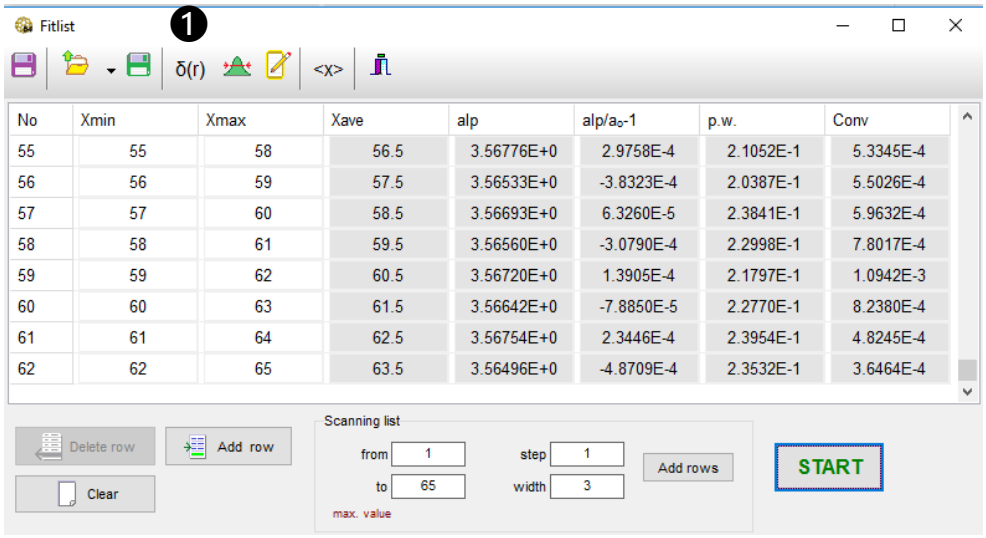


or the graphs of the fitted curves appearing one after another:

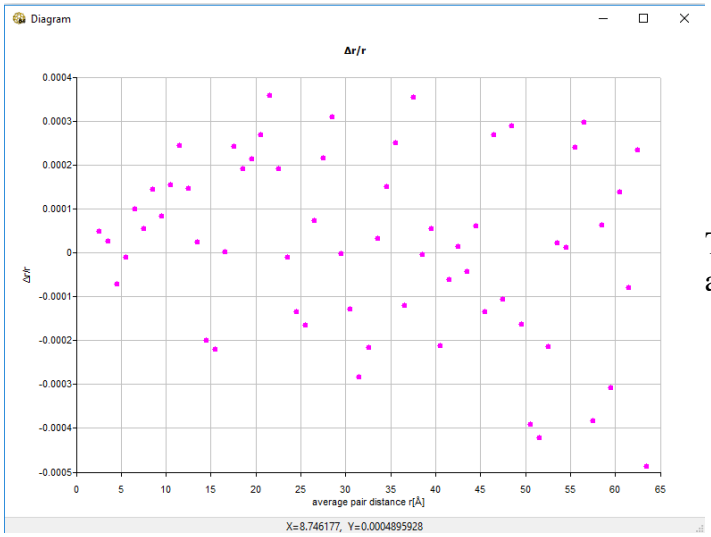


While closing all those windows – 62 in our case – you will have a chance to examine the fit quality.

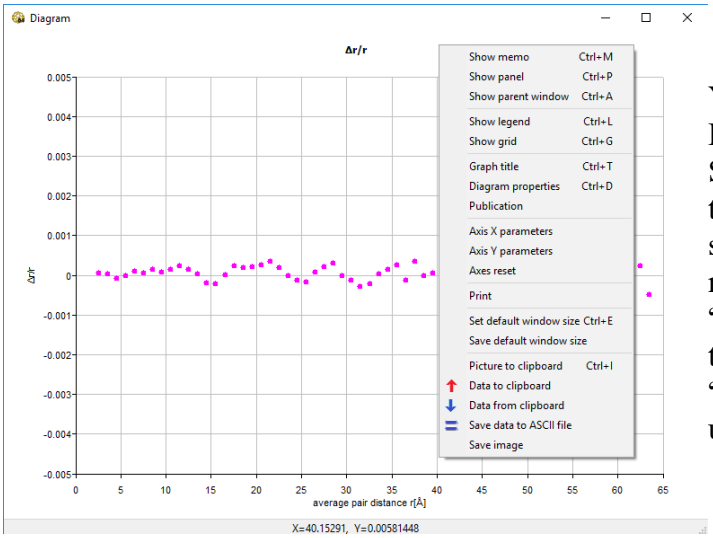
Underneath you will still find the fit results.



Press δ(r) ❶ button to see the how the fitted lattice parameters deviate from the initial value.

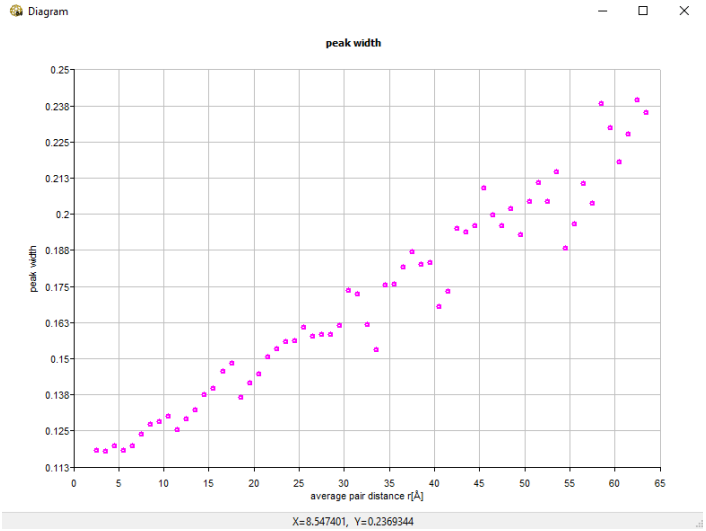


The values look quite scattered but the scatter is actually below 0.1%. It's just statistical noise.



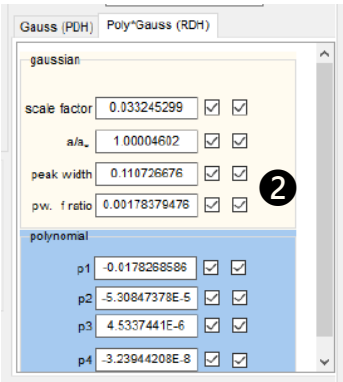
You may change the Y-scale to see it better. Click Righ mouse button on the graph. A menu appears. Select "Axis Y parameters", and change the limits to: min: -0.005 max: 0.005 step : 0.001. Now you see that the line is essentially flat. Other useful menu items are: "Data to clipboard" and "Save data to ASCII". This is the way to export the data from the plot to external file.
"Save image" and "Picture to clipboard" let you use the graph as-is.

The “Width” ❶ button will display width vs. distance plot. The width is not a half-maximum width but actually the “σ” parameter of the Gaussian function.



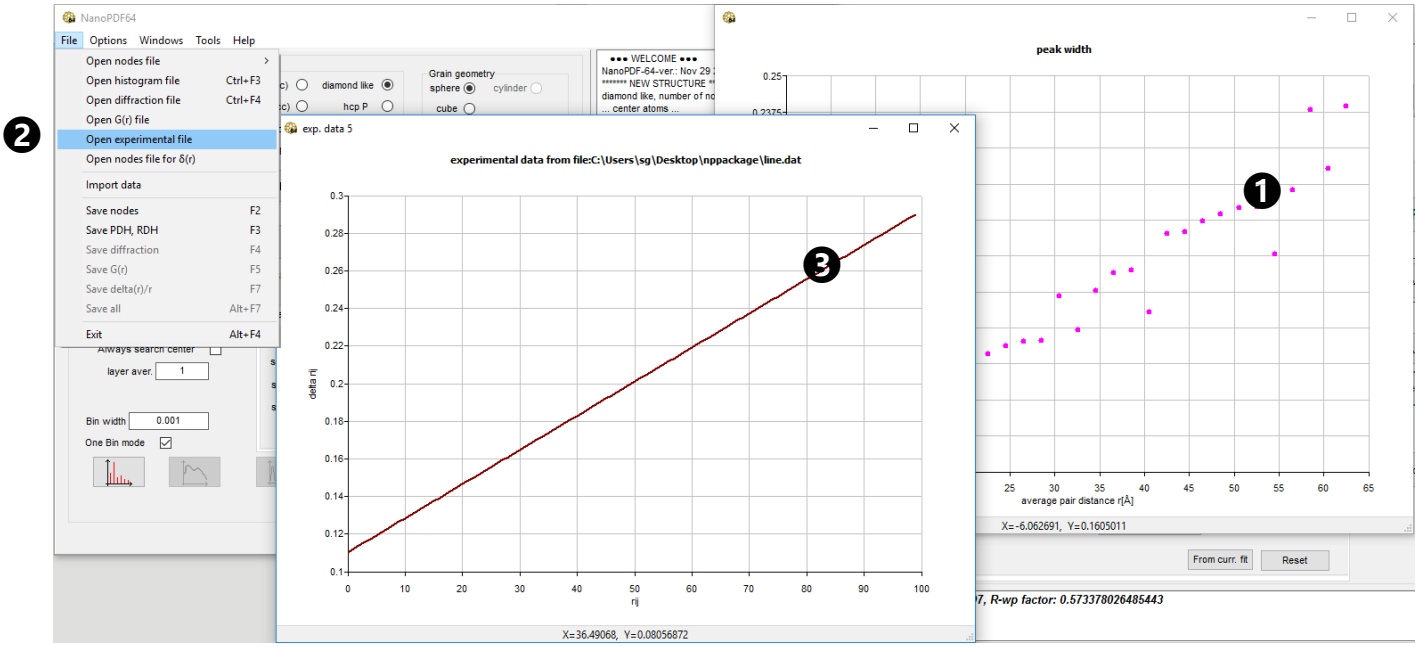
The dependence looks linear.

We may now compare it to what was obtained in the first fitting example during fitting the entire G(r) curve at once:

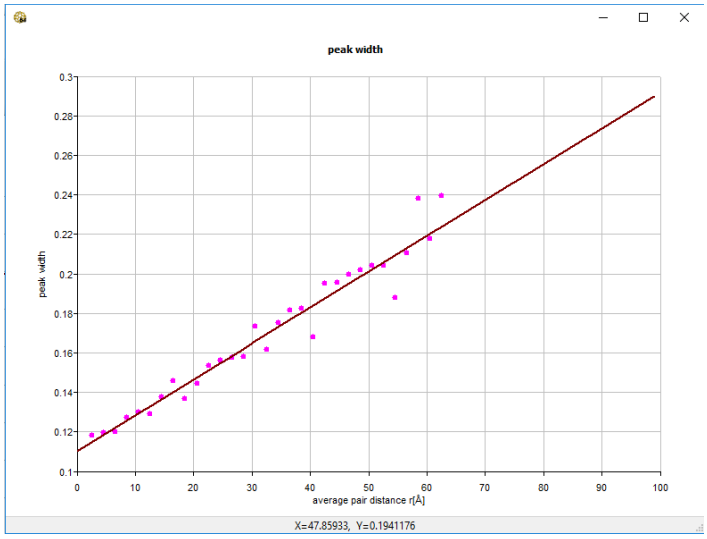


The procedure gave linear dependence with intercept 0.1107 and slope 0.001838 ❷
A data file with exactly such line: “line.dat” is placed inside the NanoPDF64 directory.

In order to overlay it on top of the fit results do the following:
Move the plot of “peak width” ❶ aside, but don’t close it. Don’t close other windows either.
Move them away to dig out the main window of NanoPDF64. Select **File→Open experimental file** ❷ and load “line.dat”.



Plot of the line appears. ❸
Press and hold Shift on the keyboard. Pick the line ❸ with the mouse, drag it to plot ❶ and drop it there. A combined plot appears:



This operation actually copies the data, not just the line!!!

The results of the complete G(r) fitting and of the scanning of G(r) by small ranges appear to be quite similar!