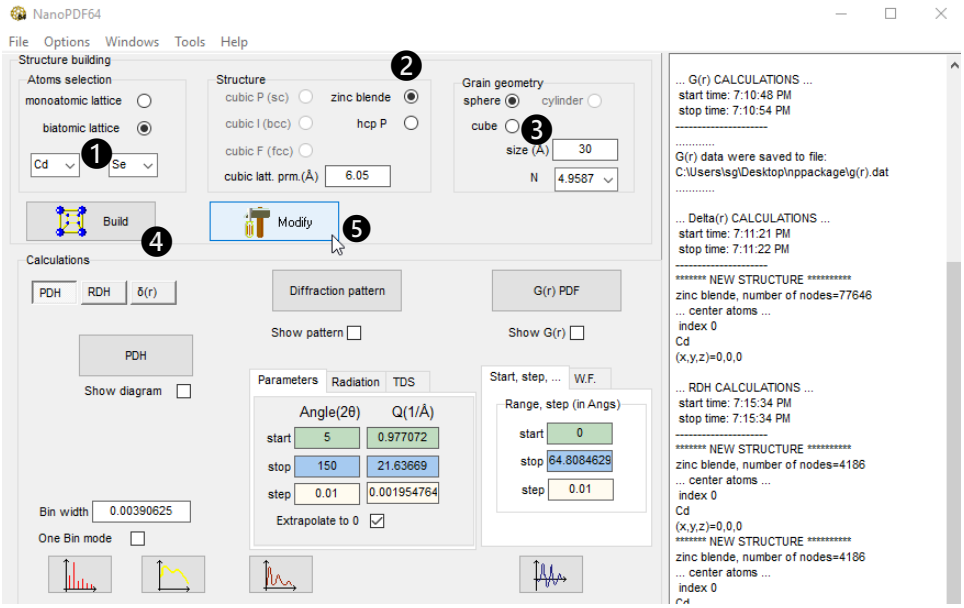
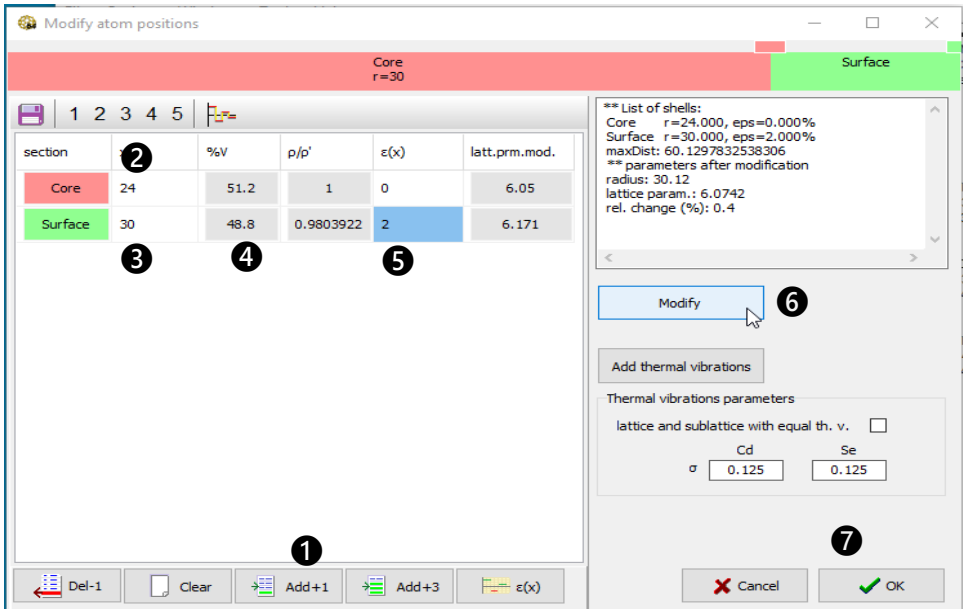
Automated fitting of G(r) in multiple finite size ranges

Example2

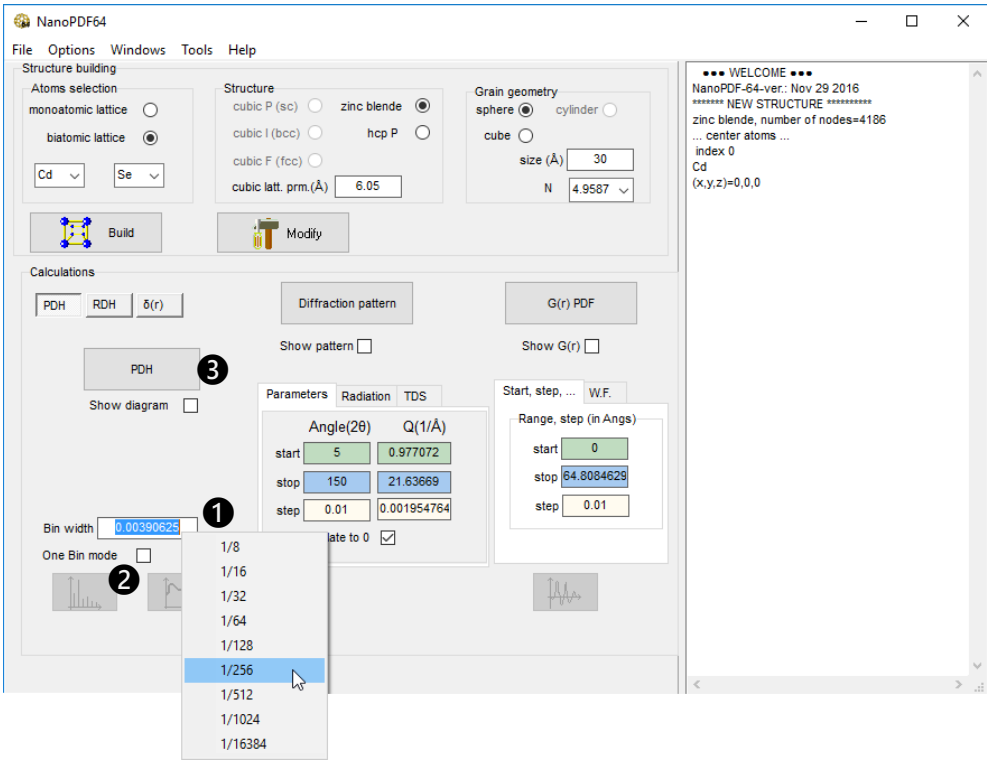
Building a core-shell model and analyzing it's G(r)



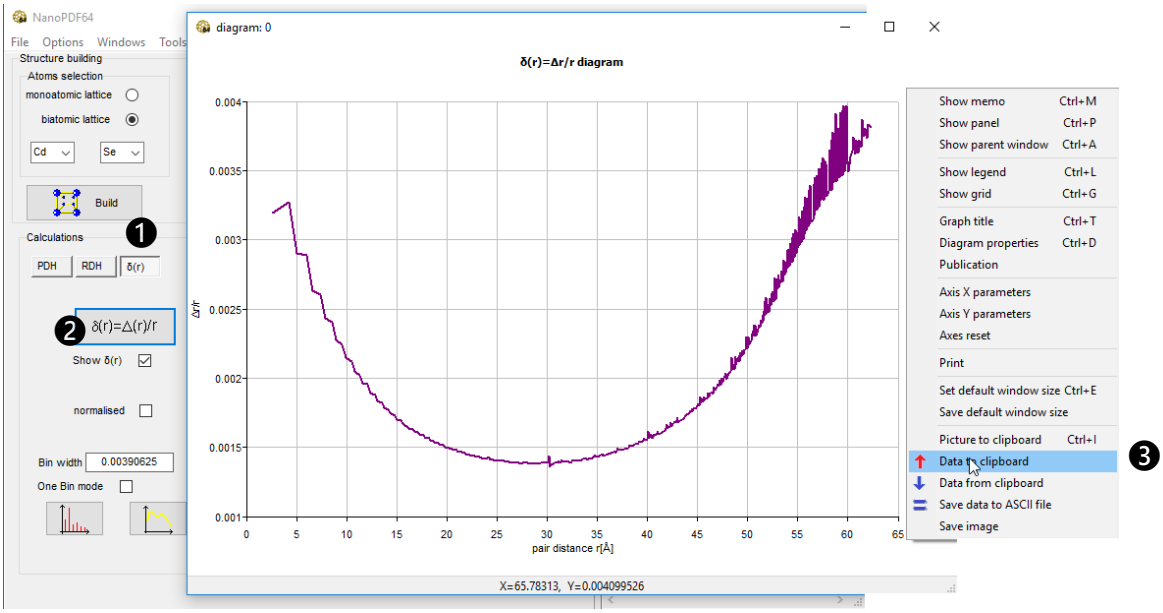
Begin with building a CdSe nanocrystal. Set “biatomic lattice” and select Cd and Se ❶ from the drop lists. Set “zinc blende” ❷ structure and sphere of 30Å radius ❸. Now “Build” ❹ and go to “Modify” ❺
Untill now we’ve had a nanocrystal with perfectly periodic lattice. We are going to split it into core and shell having slightly different lattice parameters.



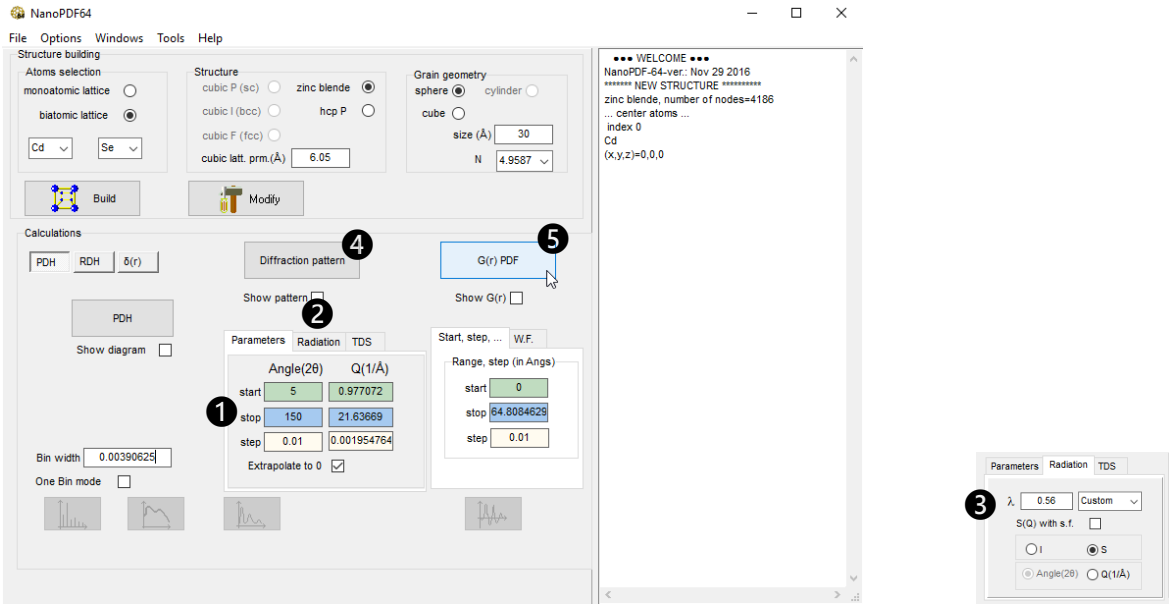
Click at Add+1 ❶ set core to have 24Å radius ❷. The shell is up to the max. radius of the model ❸. Now core and shell have approximately equal volumes ❹. We expand the crystal lattice of the shell by 2% ❺, then click on Modify ❻ and finally on OK ❼



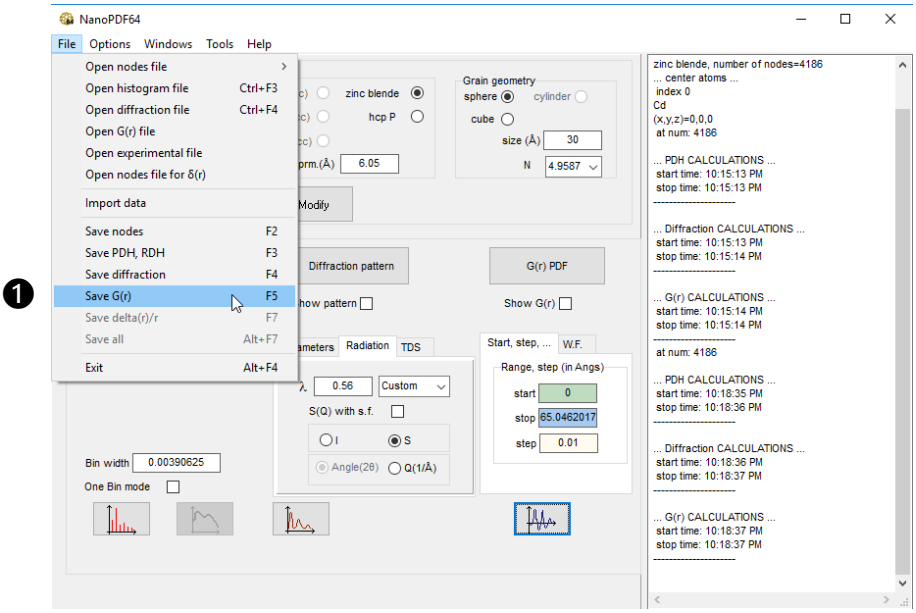
Now we are going to compute Pair Distribution Histogram. Right click on "Bin width" box ❶ to get a list of pre-defined numbers. Using "binary" values speeds up calculations and gives better accuracy when computing G(r). Select 1/256 and clear "One bin mode" ❷. This also improves accuracy of G(r). Finally do the PDH calculation ❸.



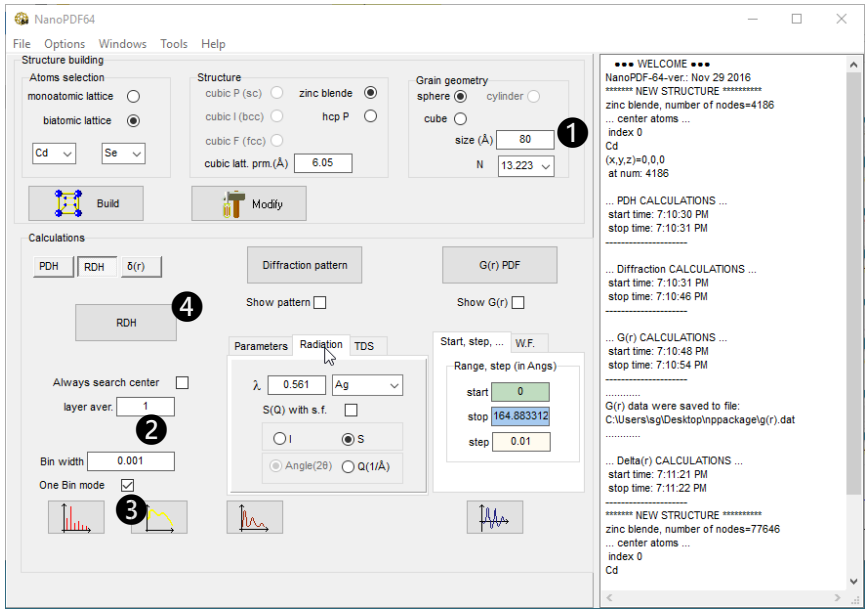
Now we may compare interatomic distances in the "perfect lattice" model – it is still in memory - with those in the core-shell model we have just built. Select the δ(r) tab ❶ and do the calculation ❷. The diagram shows theoretical i.e. expected Δ(r)/r curve. Right click on the diagram and save the data to the Clipboard ❸. We are going to use them later on.



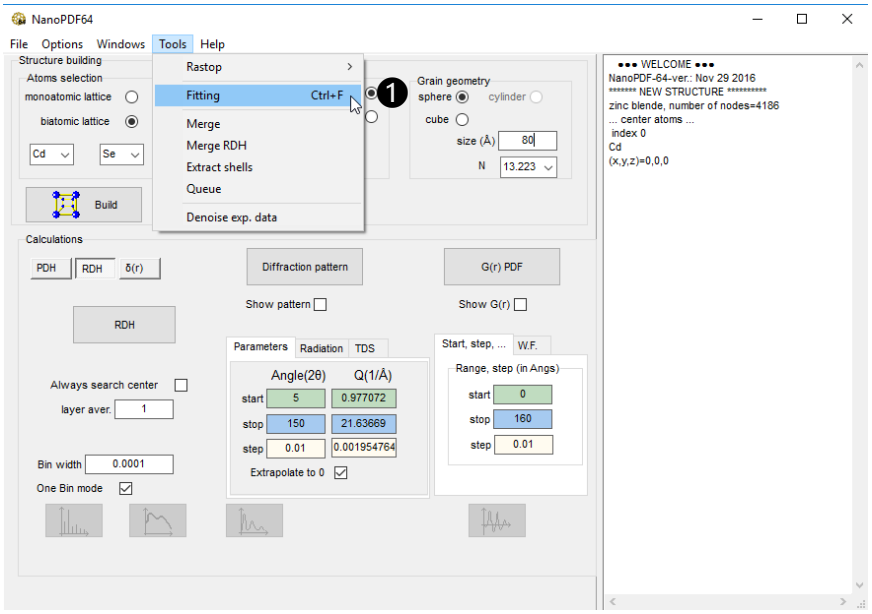
It's time to compute G(r). Start with diffraction pattern. Set start, stop and step ❶. Step in diffraction pattern affects the accuracy of the Fourier transform that will be done in a moment, so set it to 0.01 or less. Go to Radiation tab ❷ and select Ag radiation ❸ or set it manually to something even smaller. Do the diffraction calculation ❹. Then compute G(r) ❺.



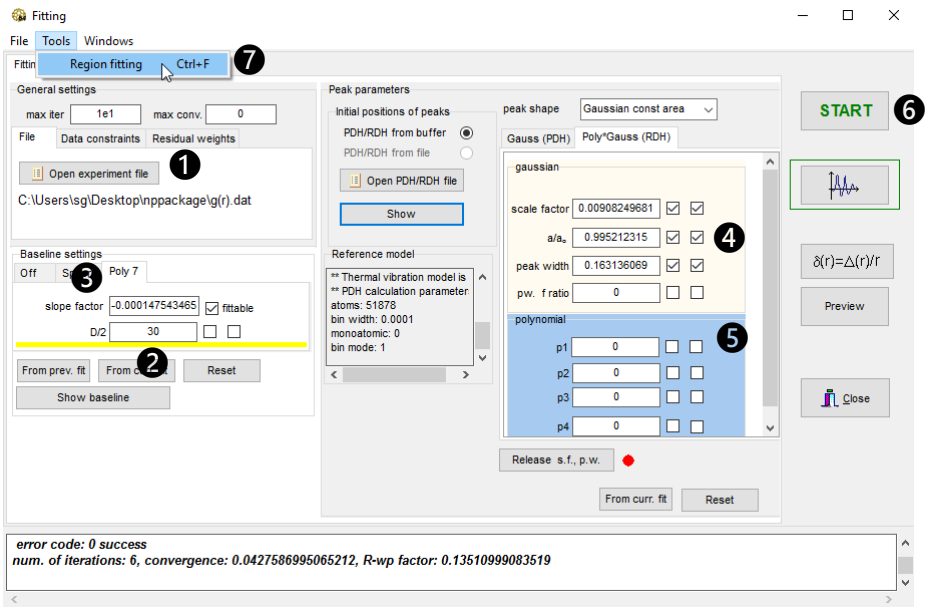
We have just calculated G(r) for the core-shell model. Save it to a file ❶. In the “Save As” window which appears select “Syntetic (*.dat)” format, not the “ *.gr ” format which is the default.



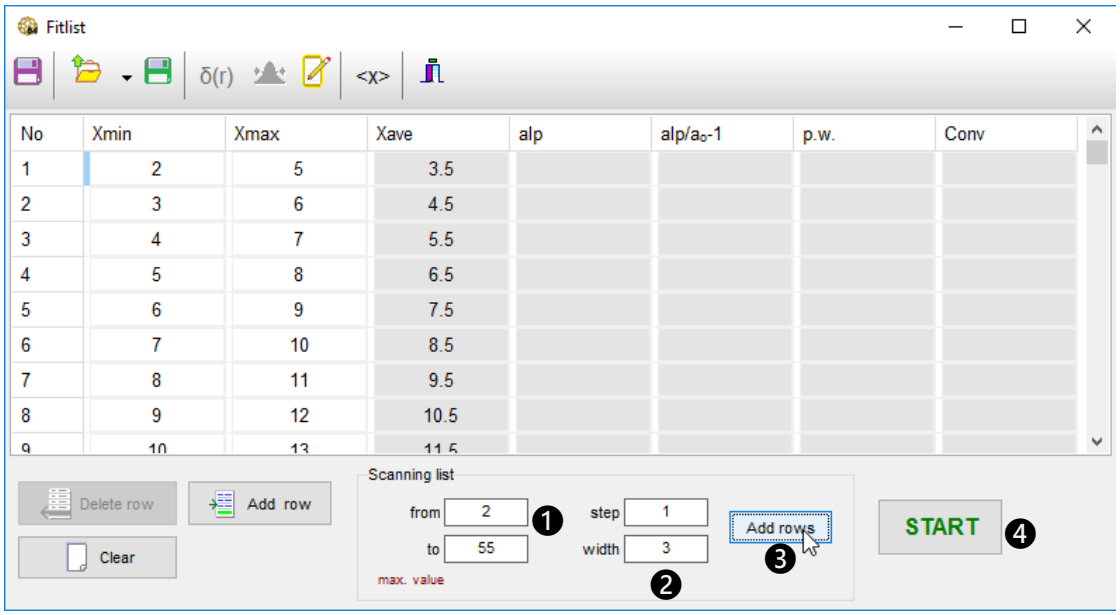
Get ready for fitting. Set radius to more than twice of the radius of the model we are going to analyze ❶. 70 or 80 is a good choise. Set Bin width to 0.001 ❷ and activate One bin mode ❸. Calculate RDH ❹.



Go to Tools→ Fitting ❶

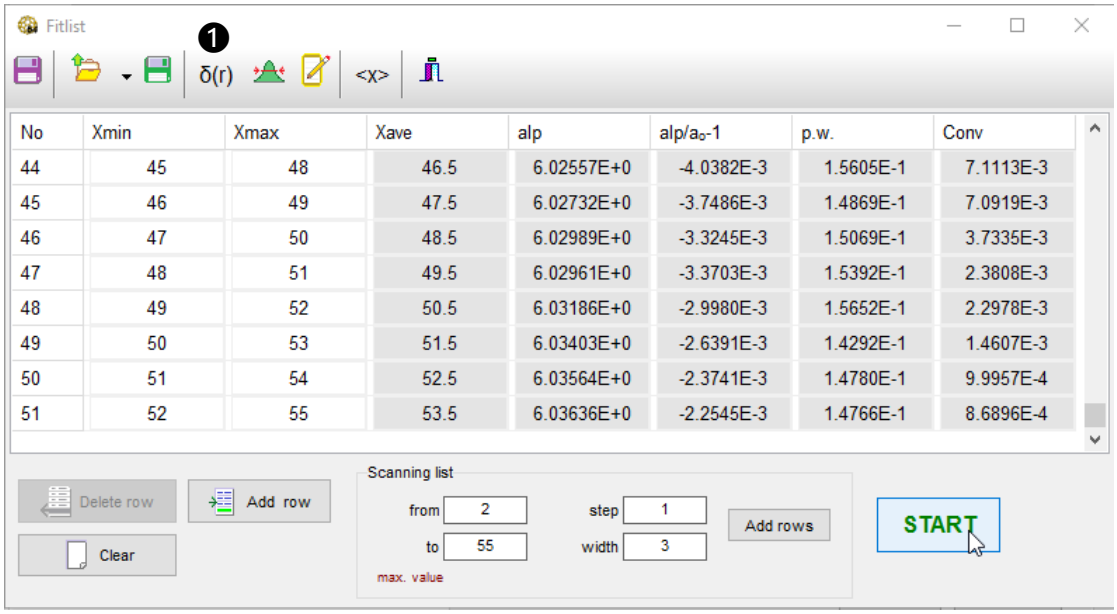


Open ❶ the G(r) you calculated a moment before for the core-shell model.
Set D/2 to 30 ❷ and make it not fittable . Make Slope factor ❸ , scale factor, a/a_0 and peak width ❹ fittable. Set to 0 and deactivate all other parameters ❺.
Run a fit ❻ to get some starting parameters than go to Tools→Region fitting ❼.

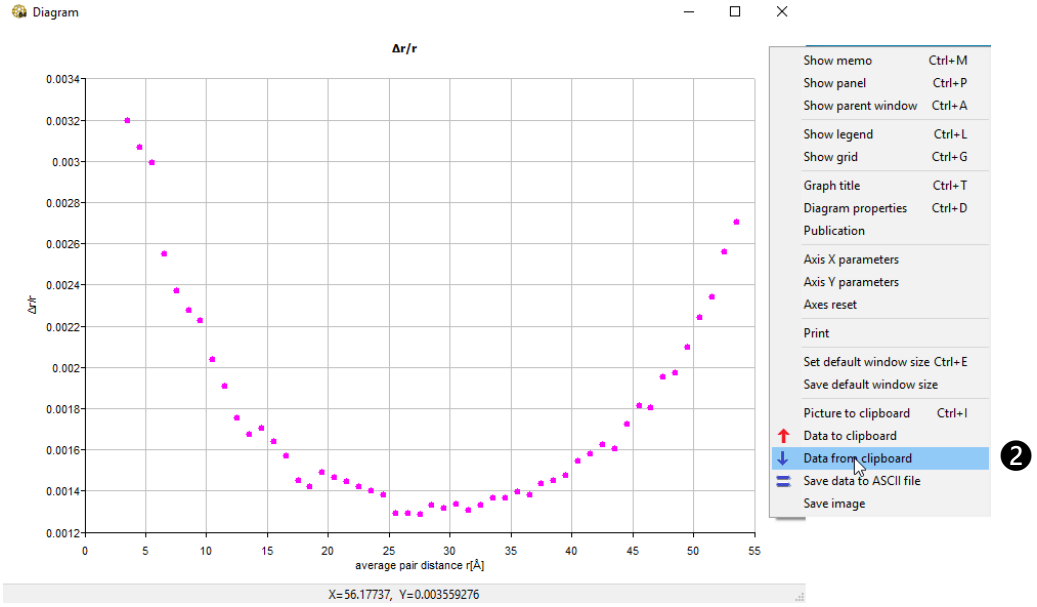


In the Fitlist window select “from 2 to 55” ❶. The model is 60 in diameter, but we don't want to go to where the peaks are very weak. Set “step 1 and width 3” ❷, click on Add rows ❸ than Start fitting ❹.

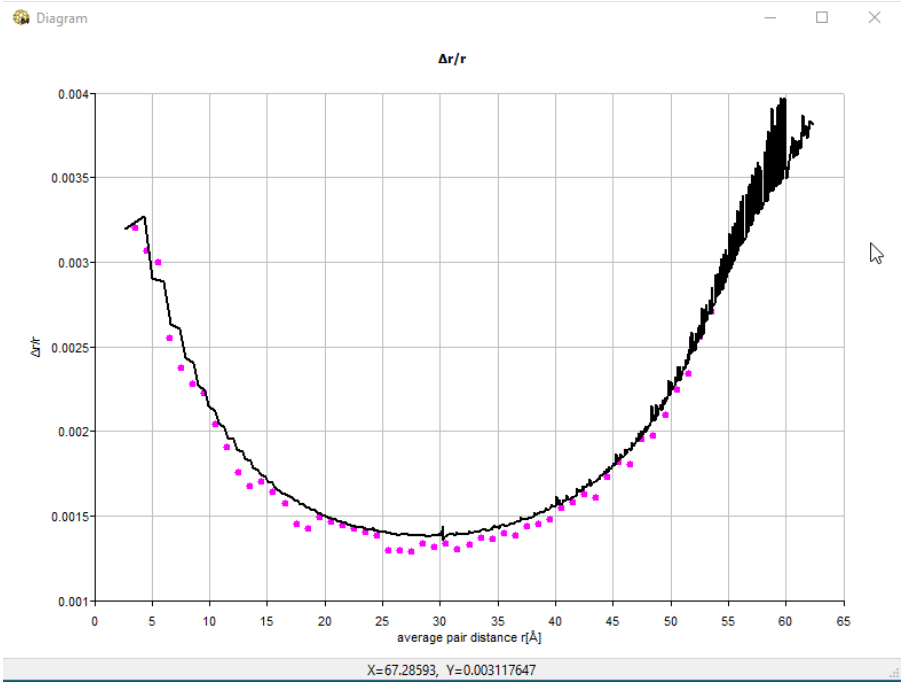
Once the fitting is finished, and the list is filled with numbers click on “δ(r)” ❶ button.



We now see the Δr/r diagram for the core-shell model. It is determined by scanning of calculated G(r).



We may now compare it to the theoretical curve we calculated earlier and saved to Clipboard. Right click on the diagram and select “Data from clipboard” ❷



The diagram now shows nearly perfect match between the “theoretical” data obtained by comparing atomistic models and the “measured” data obtained from G(r).

One may apply the procedure of “scanning” of G(r) to the true **experimental** G(r). Should the obtained δ(r) curve appear flat, the lattice of the analyzed nanoparticles could be considered perfectly periodic. But most likely the experimental δ(r) will not be flat. That will be the evidence of non uniform structure of the crystal lattice of the measured nanoparticles. Using NanoPDF64 one may build core-shell models with multiple shells and various lattice deformations inside the shells, calculate theoretical δ(r)-s and compare those to experimental δ(r) data.