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

Example2

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

ructure building	2		
nonoatomic lattice	cubic P (sc) zinc blende	Grain geometry sphere cylinder	start time: 7:10:48 PM stop time: 7:10:54 PM
Cd v	cubic F (fcc) Cubic Iatt. prm.(Å) 6.05	cube () size (A) 30 N 4.9587 ~	G(r) data were saved to file: C:UsersisglDesktopinppackage\g(r).dat
Build	Modify		Delta(r) CALCULATIONS start time: 7:11:21 PM stop time: 7:11:22 PM
PDH RDH (r)	Diffraction pattern	G(r) PDF	zinc blende, number of nodes=77646
PDH	Show pattern	Show G(r)	index 0 Cd (x,y,z)=0,0,0
Show diagram	Parameters Radiation TDS Angle(28) Q(1/Å) start 5 0.977072 stop 150 21.63669	Start, step, W.F. Range, step (in Angs) start 0 stop 64.8084629	RDH CALCULATIONS start time: 7:15:34 PM stop time: 7:15:34 PM ****** NEW STRUCTURE ******** zinc blende, number of nodes=4186 center atoms
Bin width 0.00390625 One Bin mode	step 0.01 0.001954764 Extrapolate to 0 🗸	step 0.01	index 0 Cd (x,y,z)=0,0,0 ******* NEW STRUCTURE ******
Ìlus È	1m	ÎAA~	zinc blende, number of nodes=4186 center atoms index 0

Begin with building a CdSe nanocrystal. Set "biatomic lattice" and select Cd and Se ① from the drop lists. Set "zinc blende" ② structure and sphere of 30Å radius ③. Now "Build" ④ and go to "Modify" ⑤ 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.

Modify ato	m positions					- 🗆 X
				Core r=30		Surface
1 2	345	₽~-				** List of shells: Core r=24.000, eps=0.000%
section	2	%V	р / р'	ε(x)	latt.prm.mod.	maxDist: 60.1297832538306 ** parameters after modification
Core	24	51.2	1	0	6.05	radius: 30.12 lattice param.: 6.0742
Surface	30	48.8	0.9803922	2	6.171	rel. change (%): 0.4
	6	4	0	6		Modify δ Add thermal vibrations Thermal vibrations parameters lattice and sublattice with equal th. v. Cd Se σ 0.125 0.125 0.125
Del-1	Cle	ar 🔶	Add+1 →	Add+3	=== ε(x)	🗶 Cancel 🗸 OK

Click at Add+1 1 set core to have 24Å radius 2. The shell is up to the max. radius of the model 3. Now core and shell have approximately equal volumes 4. We expand the crystal lattice of the shell by 2% 5, then click on Modify 6 and finally on OK 7



Now we are going to compute Pair Distribution Histogram. Right click on "Bin width" box (1) 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" (2). This also improves accuracy of G(r). Finally do the PDH calculation (3).



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 $\delta(\mathbf{r})$ tab **1** and do the calculation **2**. The diagram shows theoretical i.e. expected $\Delta(\mathbf{r})/\mathbf{r}$ curve. Right click on the diagram and save the data to the Clipboard **3**. We are going to use them later on.



It's time to compute G(r). Start with diffraction pattern. Set start, stop and step **1**. 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 **2** and select Ag radiation **3** or set it manually to something even smaller. Do the diffraction calculation **4**. Then compute G(r) **5**.

File	Options Windows Too	ls Help			
	Open nodes file Open histogram file Open diffraction file Open compared file Open experimental file Open nodes file for $\delta(r)$ Import data	> Ctrl+F3 Ctrl+F4	c) zinc blende () c) hcp P () c) prm (A) 6.05	Grain geometry sphere cube size (Å)	Zinc blende, number of nodes=4186 center atoms index 0 Cd (X, y, 2)=0,0,0 at num: 4186 PDH CALCULATIONS start time: 10:15:13 PM stoptime: 10:15:13 PM
	Save nodes Save PDH, RDH Save diffraction	F2 F3 F4	Diffraction pattern	G(r) PDF	start time: 10:15:13 PM stop time: 10:15:14 PM
	Save G(r) Save delta(r)/r		how pattern 🗌	Show G(r)	G(r) CALCULATIONS start time: 10:15:14 PM stop time: 10:15:14 PM
	Save all Exit	Alt+F7	ameters Radiation TDS	Start, step, W.F. Range, step (in Angs)	at num: 4186
			λ 0.56 Custom ~ S(Q) with s.f.	start 0 stop 65.0462017	PDH CALCULATIONS start time: 10:18:35 PM stop time: 10:18:36 PM
	Bin width 0.00390625 One Bin mode		● Angle(28) ○ Q(1/Å)	step 0.01	Diffraction CALCULATIONS start time: 10:18:36 PM stop time: 10:18:37 PM
	Ì.]	h,	<u> 1440-</u>	G(r) CALCULATIONS start time: 10:18:37 PM stop time: 10:18:37 PM

We have just calculated G(r) for the core-shell model. Save it to a file ①. In the "Save As" window which appears select "Syntetic (*.dat)" format, not the "*.gr" format which is the default.

toms selection stelection static of the selection onoatomic lattice of the selection biatomic lattice of the selection of the	vubic P (sc) zinc blende •	Grain geometry sphere cylinder cube size (Å) N 13.223	••• WELCOME ••• W2 2016 •••••• NEW STRUCTURE •••••••• 21to bende, number of nodes=4186 center atoms index 0 Cd (x,y,z)=0.0,0 at num: 4185
Build alculations	T Modify		PDH CALCULATIONS start time: 7:10:30 PM stop time: 7:10:31 PM
	Diffraction pattern	G(r) PDF	Diffraction CALCULATIONS start time: 7:10:31 PM stop time: 7:10:46 PM
RDH	Parameters Radiation TDS	Start, step, W.F. Range, step (in Angs)	G(r) CALCULATIONS start time: 7:10:48 PM stop time: 7:10:54 PM
Always search center	λ 0.561 Ag S(Q) with s.f. 0 I • S	start 0 stop 164.883312 step 0.01	G(r) data were saved to file: C:\Users\sg\Desktop\nppackage\g(r).dat
Bin width 0.001 One Bin mode	Angle(2θ) Ο Q(1/Å)	atop 0.01	Delta(r) CALCULATIONS start time: 7:11:21 PM stop time: 7:11:22 PM
<u>i</u> , 3 <u>></u>	<u>h</u>	Ĵ₩.,	zinc blende, number of nodes=77646 center atoms index 0

Get ready for fitting. Set radius to more than twice of the radius of the model we are going to analyze ①. 70 or 80 is a good choise. Set Bin width to 0.001 ② and activate One bin mode ③. Calculate RDH ④.

File Options Windows Structure building Ratop Alorns selection Ratop biatomic lattice Fitting Cd Se Merge Sitze (Å) Oueue Denoise exp. data Colculations PDH RDH Always search center Isyer aver. Isyer aver. Istrat Stop Uneue One Bin mode Image Image <th>🚱 NanoPDF64</th> <th></th> <th></th> <th>- 🗆</th> <th>×</th>	🚱 NanoPDF64			- 🗆	×
Alores selection Fitting Ctrl = Fitting Grain geometry monodomic lattice Fitting Ctrl = Fitting Size (A) 60 biatomic lattice Merge Merge RDH Size (A) 60 Cd Se Extract shells 0 N 13.22.3 Queue Denoise exp. data G(r) PDF G(r) PDF Cd Calculations Denoise exp. data Show pattern G(r) PDF RDH RDH Diffraction pattern G(r) PDF Alvays search center Show pattern Start, step W/F. layer aver 1 Sign 150 216.83669 step 0.01 0.001954.768 Start, step W/F. Bin width 0.001 Merge Extrapolate to 0 Merge Extrapolate to 0	File Options Windows Tools	Help		••• WELCOME •••	
monoatomic lattice Fitting Ctrl+F sphere © cylinder intermediation biatomic lattice Merge RDH size (Å) @ 0 intermediation intermediation Cd Se Biatomic lattice asize (Å) @ 0 N 13.223 intermediation Cd Queue Denoise exp. data G(r) PDF Show pattern Show pattern Show G(r) Show G(r) RDH RDH Diffraction pattern Show G(r) Shart, step, W.F. Range, step (m Angs) atrix 5 0.977072 start 0 start 0 Stop 150 21.63869 start 0 start 0 Bin width 0.0001 One Bin mode Image Image Image Image Image	Atoms selection		Grain geometry	NanoPDF-64-ver.: Nov 29 2016	
biatomic lattice Merge Merge RDH Extract shells Queue Denoise exp. data Calculations PDH RDH RDH Always search center Iayer aver. 1 Bin width 0.0001 One Bin mode Image Roll Image Roll Calculations PDH RDH Parameters Radiation TSD Start, step, W.F. Angle(26) Q(1/A) start 0 stop 100 0001 0001 001 001 Image Roll Image Roll <td>monoatomic lattice O Fitt</td> <td>ing Ctrl+F</td> <td>sphere cylinder</td> <td>zinc blende, number of nodes=4186</td> <td></td>	monoatomic lattice O Fitt	ing Ctrl+F	sphere cylinder	zinc blende, number of nodes=4186	
Cd Se Merge RDH Extract shells Queue size (Å) @ 0 N [13:223] Cd Cd Cd N [13:223] Build Denoise exp. data Calculations PDH RDH RDH Diffraction pattern Show pattern One Bin mode Diffraction pattern Diffraction pattern Diffractin pattern <	biatomic lattice Me	rge	cube 🔿	center atoms	
Extract shells Queue Denoise exp. data Calculations PDH PDH PDH RDH Always search center layer aver. 1 Bin width 0.001 One Bin mode Image: Image: N 13223 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 (x,yz)=0.0.0 </td <td>Cd Se Me</td> <td>rge RDH</td> <td>size (Å) 80</td> <td>Cd</td> <td></td>	Cd Se Me	rge RDH	size (Å) 80	Cd	
Queue Denoise exp. data Calculations PDH RDH 0(r) RDH Diffraction pattern G(r) PDF Show pattern Bin width 0.0001 One Bin mode Image: State pattern Image: State patter	Extr	ract shells	N 13.223 🗸	(x,y,z)=0,0,0	
Build Denoise exp. data Calculations PDH RDH Bin width 0.0001 One Bin mode Image: Calculation to the parameters Bin width 0.001 Image: Calculation to the parameters Bin width 0.001 Image: Calculation to the parameters Show pattern Show pattern Show G(r) Show G(r) Show G(r) Show G(r) Show G(r) Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show pattern Bin width 0.001 Calculation to the pattern Show pattern Show pattern Show pattern Show pattern Show pattern Show patte	Qu	eue			
Calculations PDH RDH RDH Bin width 0.0001 Bin width 0.0001 Cone Bin mode	Build	noise exp. data			
PDH RDH bitfraction pattern G(r) PDF RDH Show pattern Show G(r) RDH Parameters Radiation TDS Always search center Angle(20) Q(1/Å) layer aver. 1 Bin width 0.0001 One Bin mode Image: 100	Calculations				
RDH Show pattern Show G(r) Always search center Angle(28) Q(1/Å) layer aver. 1 Bin width 0.0001 One Bin mode Image: State to 0	PDH RDH $\delta(r)$	Diffraction pattern	G(r) PDF		
Always search center Angle(26) Q(1/Å) Start, step, W/F. layer aver. 1 5 0.977072 start 0 start 5 0.977072 start 0 stop 160 Bin width 0.0001 0.001954764 Extrapolate to 0 001 step 0.01 One Bin mode Image: Step in Market in	RDH	Show pattern	Show G(r)		
Always search center Angle(28) Q(1/Å) Range. step (n Angs) layer aver. 1 Start 5 0.977072 stop 150 21.83868 stop 160 Bin width 0.0001 0.001954764 step 0.01 One Bin mode Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Bin width 0.0001 Extrapolate to 0 Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Always search center Image: Alwa		Parameters Radiation TDS	Start, step, W.F.		
Alvays search center Image: Search center layer aver. 1 start 5 stop 150 stop 150 stop 150 stop 100 stop 100 stop 100 stop 160 stop 160 stop 100 Max 100		Angle(20) Q(1/Å)	Range, step (in Angs)		
layer aver. 1 stop 150 21.638689 stop 160 Bin width 0.0001 0.001954764 Extrapolate to 0 0.01 One Bin mode ✓ ✓	Always search center	start 5 0.977072	start 0		
Bin width 0.0001 0.001954764 step 0.01 One Bin mode Image: Step	layer aver. 1	stop 150 21.63669	stop 160		
Bin width 0.0001 Extrapolate to 0			step 0.01		
	Bin width 0.0001	step 0.01 0.001004104			
Inter Inc. Inc.	One Bin mode	Extrapolate to 0			
		Im.	Î44a		
2					

Go to Tools \rightarrow Fitting **1**

eneral settings	Deak parameters				
max iter 1e1 max conv. 0 lie Data constraints Residual weights 1) Open experiment file :\Users\sg\Desktop\nppackage\g(r).dat	PDH/RDH from buffer PDH/RDH from buffer PDH/RDH from file Dopen PDH/RDH file Show	peak shape Gauss (PDH) gaussian scale factor	Gaussian const area v Poly*Gauss (RDH)	^ [START
Aseline settings Iff S 3 Poly 7 slope factor 0.000147543465 ffttable D2 30 0 rom prev. ft From 2 Reset Show baseline	Reference model Thermal vibration model is Thermal vibration model is Thermal vibration model is Thermal vibration marameter atoms: 51878 bin width: 0.0001 mmonastomic. 0 bin mode: 1	a/a。 peak width pw. f ratio polynomial p1 p2 p3 p3	0.995212315	~	$\delta(r) = \Delta(r)/r$ Preview Preview
		Release s.f.,	p.w. • From curr. fit Reset		

Open (1) the G(r) you calculated a moment before for the core-shell model.

Set D/2 to 30 (2) and make it not fittable. Make Slope factor (3), scale factor, a/a_0 and peak width (4) fittable. Set to 0 and deactivate all other parameters (5).

🚳 Fitlist Х _ - 🗄 δ(r) 🖄 🖉 8 6 <u>,</u> <χ> ٨ No Xmin Xmax Xave alp alp/a₀-1 p.w. Conv 2 5 3.5 1 2 3 6 4.5 7 3 5.5 4 5 8 6.5 4 5 6 9 7.5 6 7 10 8.5 7 8 11 9.5 8 9 12 10.5 ÷ 11.5 q 10 13 Scanning list Delete row > Add row from 2 step 1 Add rows 1 START 4 55 to 3 width Clear B 0 max. value

Run a fit \bigcirc to get some starting parameters than go to Tools \rightarrow Region fitting \bigcirc .

In the Fitlist window select "from 2 to 55" **1**. 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" **2**, click on Add rows **3** than Start fitting **4**.

Fitlist \times 0 8 δ(r) 🖄 📝 Þ - 💾 <u>,</u> <x> No Xmin Xmax Xave alp/a₀-1 Conv ~ alp p.w. 45 46.5 6.02557E+0 -4.0382E-3 1.5605E-1 7.1113E-3 44 48 45 46 49 47.5 6.02732E+0 -3.7486E-3 1.4869E-1 7.0919E-3 47 50 48.5 6.02989E+0 -3.3245E-3 1.5069E-1 3.7335E-3 46 47 48 51 49.5 6.02961E+0 -3.3703E-3 1.5392E-1 2.3808E-3 48 49 52 50.5 6.03186E+0 -2.9980E-3 1.5652E-1 2.2978E-3 49 50 53 51.5 6.03403E+0 -2.6391E-3 1.4292E-1 1.4607E-3 9.9957E-4 50 51 54 52.5 6.03564E+0 -2.3741E-3 1.4780E-1 8.6896E-4 51 52 55 53.5 6.03636E+0 -2.2545E-3 1.4766E-1 Scanning list Add row Delete row from 2 1 step STAR' Add rows 55 3 to width Clear max, value

Once the fitting is finished, and the list is filled with numbers click on " $\delta(r)$ " (1) button.

We now see the $\Delta r/r$ 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" **2**



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 $\delta(r)$ curve appear flat, the lattice of the analyzed nanoparticles could be considered perfectly periodic. But most likely the experimental $\delta(r)$ 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 $\delta(r)$ -s and compare those to experimental $\delta(r)$ data.