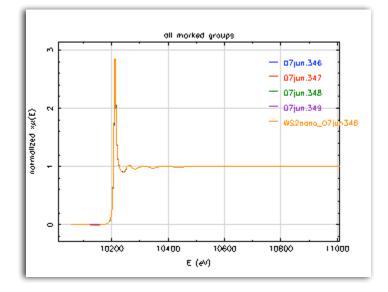
# Modeling bulk and nano WS<sub>2</sub>

Shelly Kelly

#### Read data into Athena

Project       :A/My Documents/XAFS/EXAFSschool2007/WS2nano.prj         Current group       07jun.346         File:       /home/skelly/Xafs/Ni/NiandW/2007.06/07jun.346         Z:       W         Edge:       Importance:         1       Ref 07jun.347         Background removal       Show additional parameters         E0:       10209.54         E0:       10209.54         E0:       10209.54         Friedram       File:         Pre-edge range:       -142.520         Interpret in the step:       1131.85         Pre-edge range:       -142.520         X       to       1131.85         Spline range:       k:       0         E:       0.000       to         Y       Plotting options         E       k.range:         Backward Fourier transform       mu(E)         dr:       0.2         window type:       hanning         R-range:       1         I       y-axis offset:         Plotting parameters       plot multiplier.         plot multiplier.       y-axis offset:	Athena File Edit Group Values Plot Mark Data Merge Analysis -	_ [ ] × Settings Help
File:       /home/skelly/Xafs/Ni/NiandW/2007.06/07jun.346         Z:       W       Edge:       3       Importance:       1         Background removal       Show additional parameters       07jun.347         E0:       10209.54       E shift:       0       Ref 07jun.348         E0:       10209.54       E shift:       0       Ref 07jun.348         Fre-edge range:       142.520       10       3         Normalization range:       150       X       1131.85         Spline range:       k:       0       X       07jun.349         Forward Fourier transform       k:       0       X       07jun.349         K-range:       3       X       to       177.981       X         Phase correction:       no       15.981       X       Plotting options       E       k R       q         R-range:       1       X       to       3       X       pre-edge line       post-edge line       post-edge line       Normalized       Emin: _200       Emix: _800		
Z       W       Edge:       L3       Importance:       Importance: <t< th=""><th>Current group 07jun.346</th><th>☑ 07jun.346</th></t<>	Current group 07jun.346	☑ 07jun.346
Z       W       Edge:       Importance:       I         Background removal       Show additional parameters       Ref 07jun.347         E0:       10209.54       E shift:       Ref 0.7jun.348         K-weight:       I       Edge step:       2.069.4         Pre-edge range:       -142.520       to       -30         Normalization range:       150       X       to       1131.85         Spline range:       k:       0       X       to       11231.830         Forward Fourier transform       k-weight:       1       dk:       1       window type:       hanning         k-range:       3       X       to       15.981       W       E       k range:       1       X       to       3       X         Phase correction:       no       M       3       X       Forward Fourier transform       Pre-edge line       post-edge line       post-edge line       Normalized       E       Normalized       E       Derivative       E       Derivative       E       E       Normalized       E       Derivative       E       E       Normalized       E       Derivative       E       E       Normalized       E       Derivative       E <t< th=""><th>File: /home/skelly/Xafs/Ni/NiandW/2007.06/07jun.346</th><th>E Ref 07jun.346</th></t<>	File: /home/skelly/Xafs/Ni/NiandW/2007.06/07jun.346	E Ref 07jun.346
Background removal       Show additional parameters         E0:       10209.54 X       E shift:       0       Rbkg:       1.0 X         k-weight:       1       Edge step:       2.069 Y       fix step         Pre-edge range:       -142.520 X       to       -30 X         Normalization range:       150 X       to       1131.85 X         Spline range:       k:       0 X       to       177.981 X         E:       0.0000 X       to       1231.830 X       E       k       R       q       kq         Forward Fourier transform       k-weight:       1       dk:       1       window type:       hanning       E       k       R       q       kq         Phase correction:       no       15.981 X       mu(E)       E       k       R       q       stack       ind       PF         R-range:       1       X       to       3       X       indow type:       hanning       E       k R       q       stack       ind       PF         Phase correction:       no       indow type:       hanning       indow       pre-edge line       indow       indow       post-edge line       indow       indow       indow	7' W - Edge: 13 - Importance: 1	🗹 07jun.347
E0:       10209.54 ×       E shift:       0       Rbkg:       1.0 ×         k-weight:       1       Edge step:       2.069.1       fix step         Pre-edge range:       -142.520 ×       to       -30 ×         Normalization range:       150 ×       to       1131.85 ×         Spline range:       k:       0 ×       to       17.981 ×         E:       0.000 ×       to       1231.830 ×       E       k       R       q         K-weight:       1       dk:       1       window type:       hanning       E       k       R       q       kq         Forward Fourier transform       k-weight:       1       dk:       1       window type:       hanning       E       k       R       q       kq         Phase correction:       no       15.981 ×       mu(E)       ©		Ref 07jun.347
Lb. 1000311 (model)       L sinit.       log (kdg.)       p110 (model)	Background removal Show additional parameters	
k-weight: 1 Edge step: 2.069 · • • fix step   Pre-edge range: -142.520 × to -30 ×   Normalization range: 150 × to 1131.85 ×   Spline range: k: 0 × to   E: 0.000 × to 1231.830 ×     Forward Fourier transform   k-weight: 1   k-weight: 1   k-range: 3 × to   15.981 ×   Phase correction: no     Backward Fourier transform   dr: 0.2   window type:   hanning   g   k-range:   1   X   to   Solution   Plotting parameters   plot multiplier:   1   y-axis offset:   0     Mathematical content in the step     R-range:     1   y-axis offset:     0     Ref 07jun.349   WS2nano_07jun346   E   k   R   q   k-range:   1   y-axis offset:     0     Ref 07jun.349   WS2nano_07jun346   E   k   R   q   v   Plotting parameters   plot multiplier:   1     v     Plotting parameters     Plotting parameters     Plotting param	E0: 10209.54 🗙 E shift: 0 Rbkg: 1.0 🔀	
Pre-edge range:       -142.520 × to       -30 ×         Normalization range:       150 × to       1131.85 ×         Spline range:       k:       0 × to       17.981 ×         E:       0.000 × to       1231.830 ×       E       k q kq         Forward Fourier transform       k-weight:       1 dk:       1 window type:       hanning         k-range:       3 × to       15.981 ×       E       k q stack ind PF         Phase correction:       no       mu(E)       E       w mu(E)         Backward Fourier transform       dr.       0.2       window type:       hanning       pre-edge line         R-range:       1 × to       3 ×       O       Derivative       Derivative         plot multiplier:       1 y-axis offset:       0       Derivative       Emin: -200 Emax: 800	k-weight: 1 Edge step: 2.069 🕩 📕 fix step	
Normalization range:       150       X       to       1131.85       X         Spline range:       k:       0       X       to       17.981       X         E:       0.000       X       to       1231.830       X       E       k       R       q       kq         Forward Fourier transform       k-weight:       1       dk:       1       window type:       hanning       E       k       R       q       kq         K-range:       3       X       to       15.981       X       mu(E)       Image:       E       k       R       q       to       background       pre-edge line       post-edge line       post-edge line       Normalized       Image:       Normalized       Image:       Derivative       Image:       Derivative       Image:       Ima	Pre-edge range: -142.520 🗙 to -30 🗴	
E:       0.000       x       to       1231.830       x         Forward Fourier transform       k-weight:       1       dk:       1       window type:       hanning       x         k-range:       3       X       to       15.981       X       E       k       R       q       kq         Phase correction:       no       no       x       mu(E)       x       window type:       hanning       x       x       x       mu(E)       x       window type:       hanning       x	Normalization range: 150 🔀 to 1131.85 🔀	
Forward Fourier transform         k-weight:       1       dk:       1       window type:       hanning       V       Plotting options         k-range:       3       X       to       15.981       X       E       k       R       q         Phase correction:       no       no       E       k       R       q       Multiplice         Backward Fourier transform       dr:       0.2       window type:       hanning       Image:		Ek R q kq
Forward Fourier transform         k-weight:       1       dk:       1       window type:       hanning         k-range:       3       X       to       15.981       X       E       k       R       q       Stack       Ind       PF         Phase correction:       no       no       Image:	E: 0.000 🗙 to 1231.830 🗙	E k D a
k-weight:       1       dk:       1       window type:       hanning       Image: Ima	Forward Fourier transform	
k-range:       3       X       to       15.981       X         Phase correction:       no       window type:       background         Backward Fourier transform       dr.       0.2       window type:       hanning       pre-edge line         R-range:       1       X       to       3       X       Normalized       Image:         Plotting parameters       plot multiplier:       1       y-axis offset:       0       Emin:       -200       Emax:       800	k-weight: 1 dk: 1 window type: hanning 🛋	
Phase correction:       no         Backward Fourier transform       Image: background         dr.       0.2         window type:       hanning         R-range:       1         X       to         Plotting parameters       Derivative         plot multiplier:       1         y-axis offset:       0	k-range: 3 X to 15.981 X	
Backward Fourier transform       Image:	Phase correction: 📕 no	
dr.       0.2       window type:       hanning       Image:       Image:       post-edge line         R-range:       1       X       to       Image:       <	Backward Fourier transform	🔽 background
R-range:       1       X       0       Image: I		📕 pre-edge line
Plotting parameters     Image: Constraint of the second seco		📕 post-edge line
plot multiplier: 1 y-axis offset: 0 Emin: -200 Emax: 800		📕 Normalized 🛛 🕥
Emin200 Emax. joou		🗖 Derivative 📕
nlatting in energy from group 107iup 346' donel	plot multiplier: 1 y-axis offset: 0	Emin: -200 Emax: 800
Morring in consign round and an Januara in double	plotting in energy from group '07jun.346' done!	

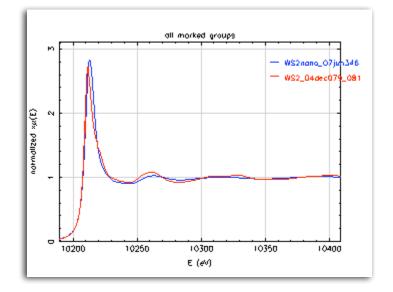
- Read individual files into Athena
  - Align data using the reference spectra
  - Merge data in  $\mu(E)$
  - Overplot merged data and aligned spectra



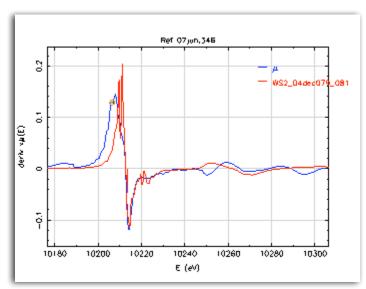
#### Merged Athena project file

Athena 👘	
File Edit Group Values Plot Mark Data Merge Analysis	Settings Help
Project y Documents/XAFS/EXAFSschool2007/WS2-1merged.prj	ANI
Current group Ref 07jun.346	🔽 WS2nano_07jun346 🍵
File: reference channel for 07jun.346	Ref 07jun.346
Z: W - Edge: L3 - Importance: 1	WS2_04dec079_081
Background removal Show additional parameters	
E0: 10206.46 🗙 E shift: 1.52 Rbkg: 1.0 🗴	
k-weight: 1 Edge step: 1.060 🕩 📕 fix step	
Pre-edge range: -142.520 🗙 to -30 🔀	
Normalization range: 150 🗶 to 1131.85 🗶	
Spline range: k: 0 🔀 to 17.981 🗶	E k R g kg
E: 0.000 🗙 to 1231.830 🗙	
Forward Fourier transform	E k R q
k-weight: 1 dk: 1 window type: hanning 🖃	Plotting options
k-range: 3 X to 15.981 X	E k R q Stack Ind PF
Phase correction:	🖬 mu(E) 🛛 🧿
	🔽 background
Backward Fourier transform	pre-edge line
dr: 0.2 window type: hanning 🛏	, ,
R-range: 1 🗙 to 3 🔀	post-edge line
	📕 Normalized 🛛 🖲
Plotting parameters	Derivative
plot multiplier: 1 y-axis offset: 0	Emin: -20 Emax: 200
Saved entire project to C:/Documents and Settings/skelly.PEA/My Documents/XAP	S/EXAFSschool2007/WS2-1me

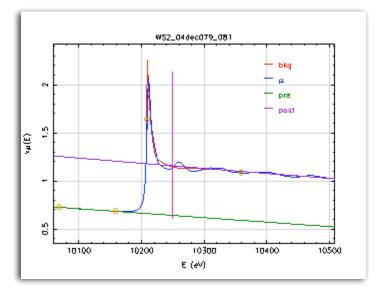
- Keep merged data files together for one project
- Compare  $\chi(k)$  spectra and Fourier Transform

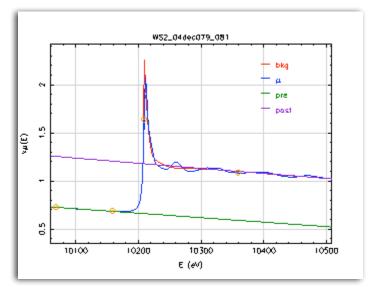


WS2-1merged.prj



Align spectra to a reference spectrum from the nanoparticles





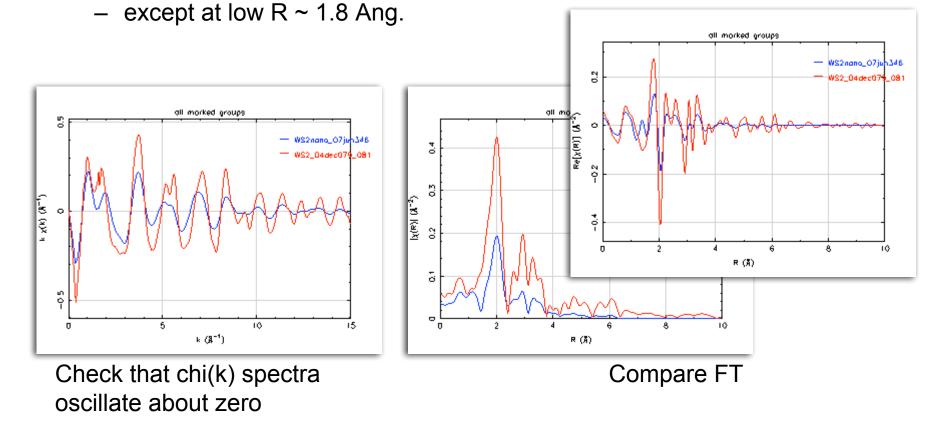
Check the pre-edge and postedge ranges in Athena

Set pre-edge range: -30 to -50 eV

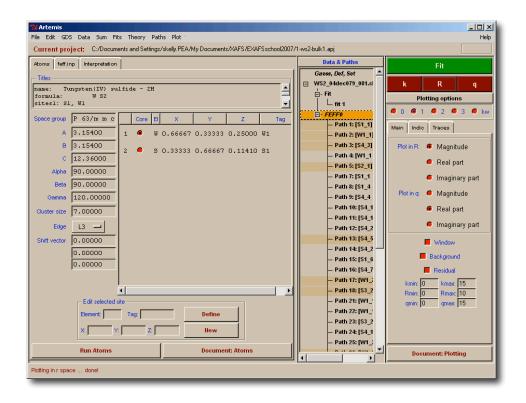
Use IND (indicator) menu to locate  $k_{min}$ =3.3 of FT compared to the edge

#### Comparison of Nanoparticle to Bulk

- Amplitude of nanoparticle  $\chi(k)$  is smaller than amplitude of bulk  $\chi(k)$
- $\chi(k)$  spectra cross zero at the same k for both data sets
  - except for slight shift at low k
- Real part of FT crosses zero at same R for both data sets



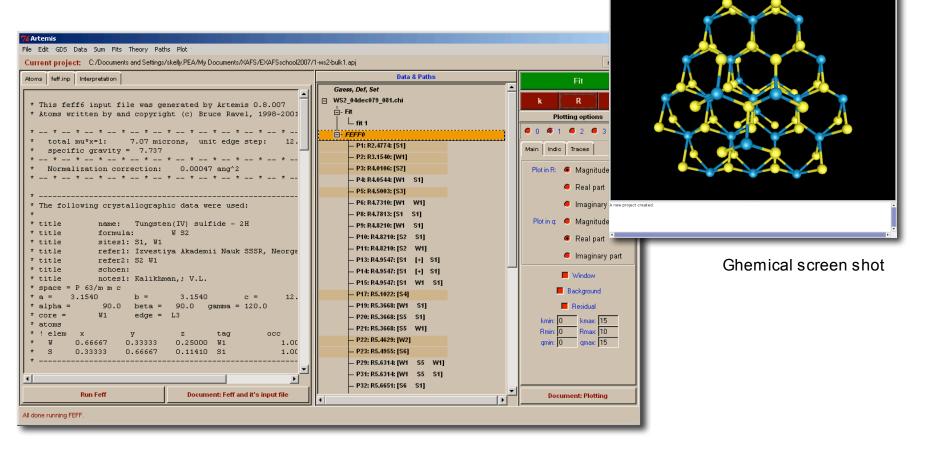
### Get WS<sub>2</sub> theory



- Fill out Atoms page from icsd\_ws2.cif file
- Check edge, Core atom radial button
- Push run atoms button
- Check feff.inp page for reasonable interatomic distances
- Run feff and include all paths in the model

#### Understand the structure of WS<sub>2</sub>

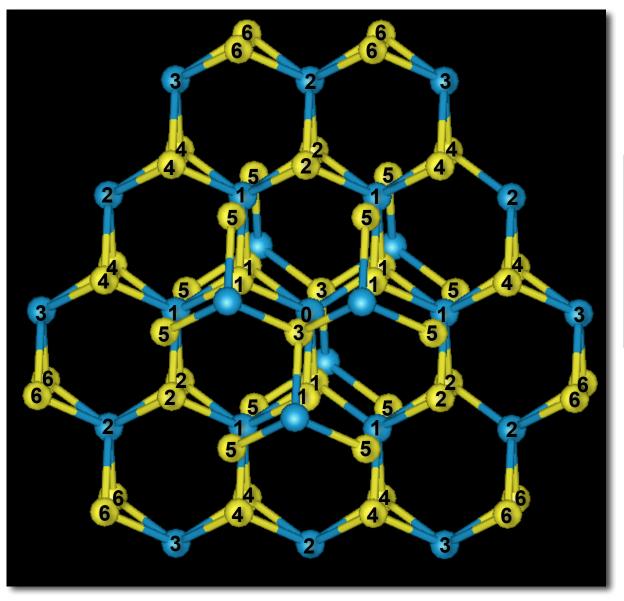
- Make sense of the path names
  - Edit feff.inp tags to decrease the degeneracy of tag names
  - Set preferences to show path number, length and atom type
  - Make ball-n-stick by writing out alc file for ghemical <u>http://www.uku.fi/~thassine/projects/ghemical/</u>



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project view camera #1 view #1

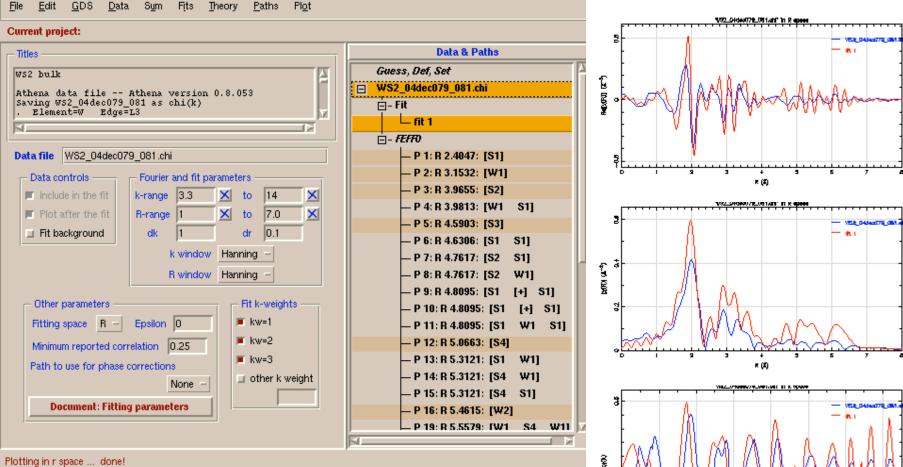
#### Understand the structure of WS<sub>2</sub>



#### **Scattering Paths**

Path	N	R (Å)
W-S1	6	2.48
W-W1	6	3.15
W-S2	6	4.01
W-S4	12	5.10
W-W2	6	5.46
W-S5	12	5.49
W-W3	6	6.31
W-W1-W3	12	6.31
W-W1-W3-W1	6	6.31

#### Compare WS<sub>2</sub> FEFF calculation to WS<sub>2</sub> bulk data



#### Plotting in r space ... done!

- Set e0=0; S 02=1.0; sigma2=0; delr=0
- chi(k) spectra shows difference in background removal and in e0.
- FT crosses zero at the same places and has the same structure.
- FT amplitude is always larger than that of the data
- Notice that the shape of the spectra from 5 to 7 Å is different in the mag of FT but the data look similar in the real part of the FT -Need to use the real part of the FT

ws2-bulk1.apj

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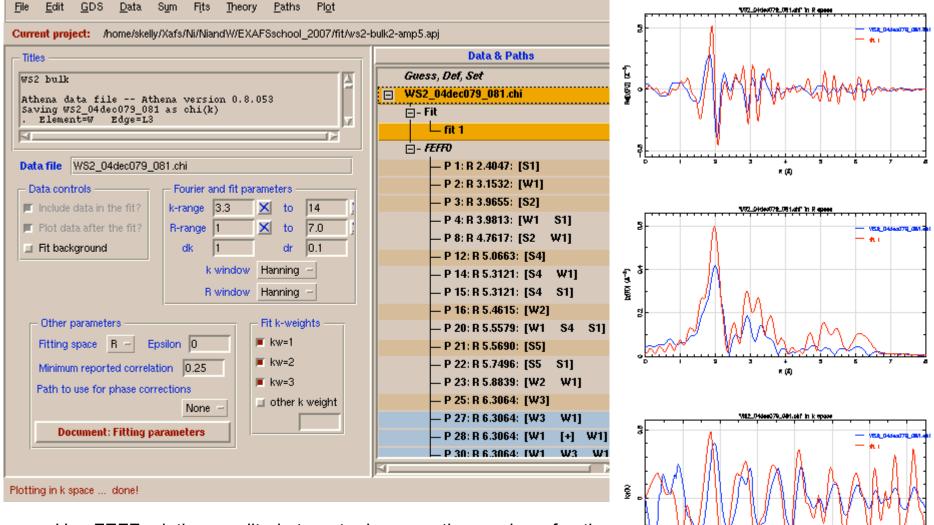
Decisions, Decisions

- Keep all the paths

   go onto the next slide
- Keep only the "big" paths

   skip to slide 27

#### Bulk WS<sub>2</sub>: How many paths can we eliminate?



- Use FEFF relative amplitude term to decrease the number of paths
  - Cutoff at 5%: This keeps all single scattering paths and linear multiple scattering paths.
  - Structure in the data is still present in the model.

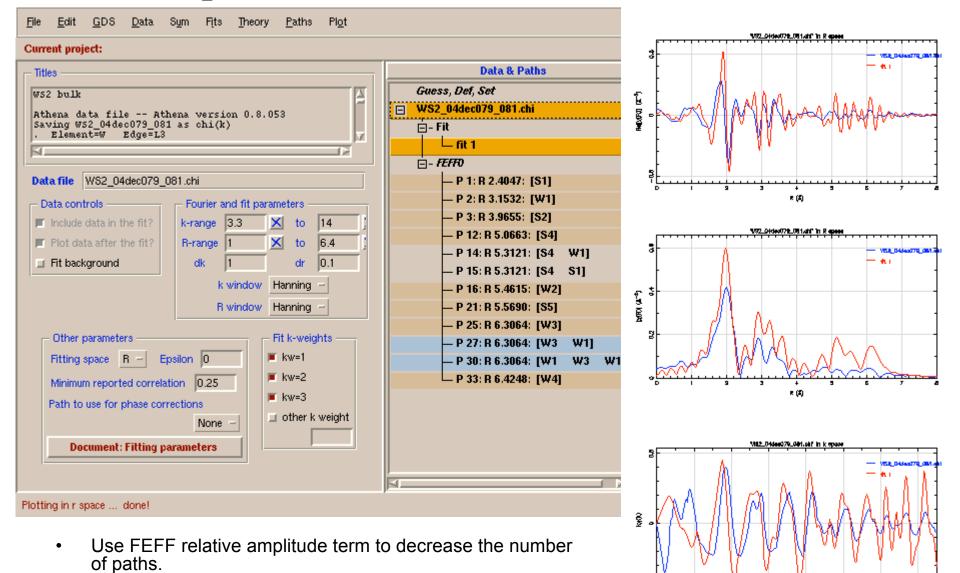
10

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12

ws2-bulk2-amp5.apj

#### Bulk WS<sub>2</sub>: How many paths can we eliminate?



- Cutoff at 10%: This keeps all single scattering paths and linear multiple scattering paths.
- Structure in the data is still present in the model.

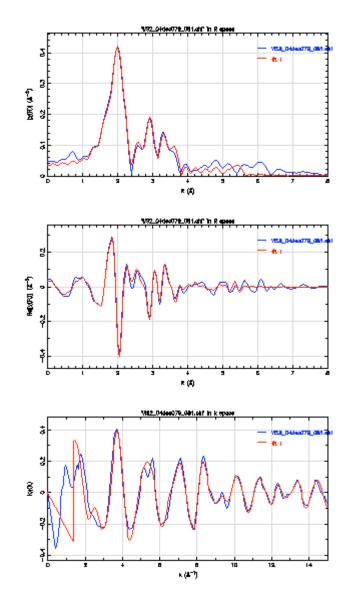
ws2-bulk3-amp10.apj

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#### Bulk WS<sub>2</sub>: Model WS<sub>2</sub> with as few variables as possible

Journal Ifeffit Results Files Echo Properties Messages Results from the last fit Raw log file Save Dismiss Project title Fitting WS2\_04dec079\_081.chi 1 Fit #1 Comment Prepared by Contact 12:37:04 on 9 July, 2007 Started 1 12:37:49 on 9 July, 2007 This fit at . Artemis 0.8.010 using linux, perl 5.008008, Tk 80 Environment . Figure of merit : 1 Independent points 36.401367188 = 9.000000000 = Number of variables Chi-square = 144139.981035478 Reduced Chi-square 5260.320773382 = 0.038557521 R-factor Measurement uncertainty (k) = 0.000161388 Measurement uncertainty (R) = 0.000432548 Number of data sets = 1.000000000 !! WARNING. The following variables had no effect on the fit: !! →> sigs4 !! →> sigw3 11.1 !! Uncertainties could not be estimated. 11 Guess parameters +/- uncertainties (initial guess): (7.3212) 7.3231170 0.0000000 +/enot = s\_02 0.8799000 +/-0.0000000 (0.8797) alpha 0.0000000 (0.0015) 0.0014620 = +/-0.0025010 0.0000000 (0.0025) sigs1 = +/sigs2 = 0.0053490 0.0000000 (0.0054) 2.2804790 0.0000000 sigs4 (2.2805) = +/-0.0025770 0.0000000 (0.0026) sigw1 +/-= -0.0030720 = +/-0.0000000 (-0.0031) sigw2 = -272.3234680 0.0000000 (-272.323! sigw3 Correlations between variables: All other correlations are below 0.25 **51** 

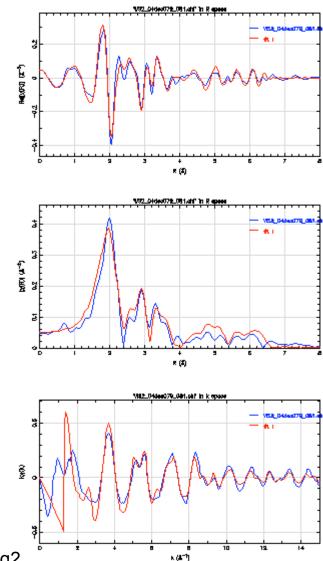
- Model includes e0, alpha\*reff, and 6  $\sigma^2$  terms.
- Model fails at large R because restriction on ∆R is too strong



ws2-vars.apj

#### Bulk WS<sub>2</sub>: Model WS<sub>2</sub> relaxing constraint on delr

Ifeffit Results Files Messages Echo Journal Properties Results from the last fit Raw log file Save Dismiss Fitting WS2\_04dec079\_081.chi Project title Comment Fit #1 Prepared by Contact 12:41:29 on 9 July, 2007 Started . 12:41:50 on 9 July, 2007 This fit at Artemis 0.8.010 using linux, perl 5.008008, Tk 80 Environment . Figure of merit : 1 Independent points 36.401367188 = 12.000000000 Number of variables = Chi-square = 427344.123 Reduced Chi-square 17513.122093724 0.121995343 R-factor Measurement uncertainty (k) = 0.000161388 Measurement uncertainty (R) = 0.000432548 Number of data sets 1.000000000 (initial guess): Guess parameters +/- uncertainties enot 6.3243200 1.2941090 (6.3327) +/-= s 02 1.3493790 +/-0.1006830 (1.3494) (-0.0038) dels1 = -0.0038970 +/-0.0125000 dels2 0.0020430 +/-0.0390750 (0.0025) = dels4 = 0.0643580 +/-0.0643210 (0.0642) +/dels4w1 = 0.0818160 0.0974970 (0.0817) dels4s1 -0.2643070 +/-0.0680880 (-0.2645) = +/-+/-0.0296260 0.0371610 (0.0297) dels5 = delw1 -0.0107270 0.0106580 (0.0107) -0.0318760 +/-0.0454950 (-0.0320) delw2 = (0.0503) 0.0499580 +/-0.0280620 delw3 = delw4 = -0.2720220+/-0.0573720 (-0.2718) Set parameters: sigs1 = 0.008380 0.009596 sigs2 = 0.005101 sigs4 = 0.005474 sigw1 = 0.005408 sigw2 = = 0.0050282 sigw3 arralations haturaan americhlas:



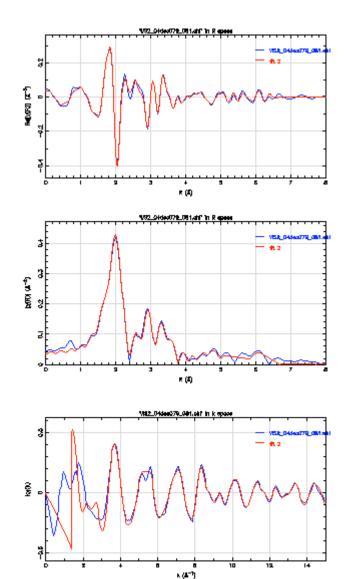
- Model includes e0,10  $\Delta R$  terms, set 6  $\sigma^2$  terms to ~0.005 Ang2.
- Model works fairly well, now that  $\Delta R$  are close, vary all params

ws2-vars2.apj

#### Bulk WS<sub>2</sub>: Model WS<sub>2</sub> relaxing constraint on delr

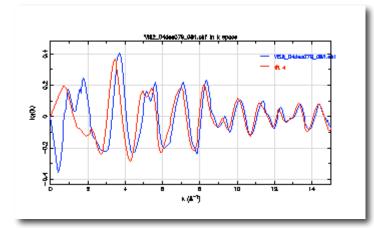
Ifeffit Results	Files Messages	Echo Journal	Properties
Results from	the last fit	Raw log file	- Save Dismiss
Project title Comment Prepared by Contact Started This fit at Environment Figure of mer	: Fit #1 ; ; ; 12:45:38 on ; 12:47:02 on ; Artemis 0.8	9 July, 2007	per1 5.008008, Tk 8
	riables = = = quare = mcertainty (k) = mcertainty (R) =	36.401367188 18.00000000 43315.563177051 2353.931788638 0.011819824 0.000161388 0.000432548 1.000000000	
enot s_02 sigs1 sigs2 sigs4 sigw1 sigw2 sigw3 dels1 dels2 dels4 dels4w1 dels4s1 dels4s1 dels5 delw1 delw2 delw3 delw4	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	4943730         (0.0000)           0449740         (0.8836)           0004100         (0.0025)           0012470         (0.0048)           0063430         (0.0183)           0002810         (0.0026)           0014160         (0.0026)           00033710         (-0.0057)           0120900         (-0.0087)           0413950         (-0.3256)           0838860         (-0.2590)           1254600         (-0.2973)           0030080         (0.0063)           0116360         (0.0112)           0146790         (0.0457)           0224780         (-0.2395)
s_02	between variables and sigs1		

- Model includes e0,10  $\Delta R$  terms, 6  $\sigma^2$  terms.
- Model works fairly well.

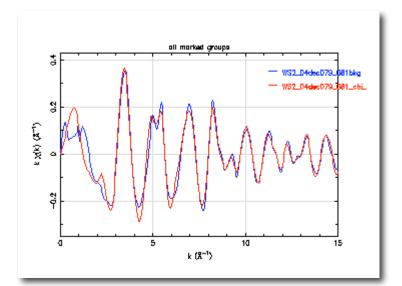


ws2-vars2b.apj

#### Bulk WS<sub>2</sub>: Making a theory for pretty background removal



comparison of data and sum of paths with e0=0. This is done in Artemis.



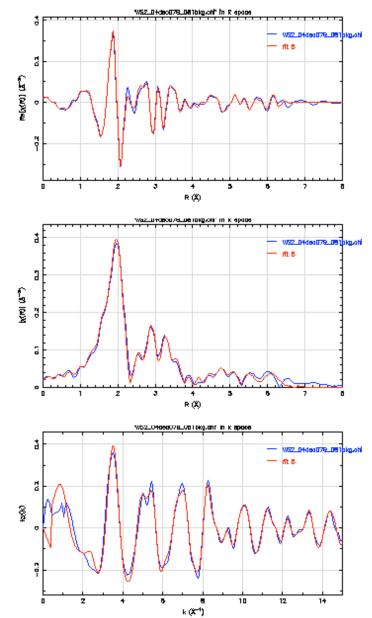
New background removal for the data. This step is done in Athena.

- Re-run fit but set all variables to best fit values, except e0 set to zero.
- Artemis file ws2-vars2c.apj used to generate theory
- Save fit in chi(k) to disk and read into Athena

#### Bulk WS<sub>2</sub>: Making a theory for pretty background removal

Results from the last fit       Raw log file       Save       Dismiss         Project title : Fitting WS2_04dec079_081.chi Commant :: Fit #1 Prepared by :: Contact :: started :: 12:45:38 on 9 July, 2007 This fit at :: 12:57:50 on 9 July, 2007 Environment :: Artemis 0.8.010 using linux, perl 5.008008, Tk 81 Figure of merit : 5         Transment :: Artemis 0.8.010 using linux, perl 5.008008, Tk 81 Figure of variables = 18.00000000 Chi-square = 47831.822404141 Reduced Chi-square = 2593.862423273 Refactor = 0.01413526 Measurement uncertainty (k) = 0.000161333 Mumber of data sets = 1.00000000         Guess parameters +/- uncertainties (initial guess): enot = 0.7533200 +/- 0.5887570 (0.0000) s_02 = 0.03453420 +/- 0.0014430 (guessed : sigs1 = 0.0024360 +/- 0.0014430 (guessed : sigs2 = 0.0046840 +/- 0.0014430 (guessed : sigs4 = 0.0139540 +/- 0.0014430 (guessed : sigs4 = 0.0139540 +/- 0.0012120 (guessed : sigw3 = 0.0064500 +/- 0.002360 (guessed : dels4 = -0.051810 +/- 0.012120 (guessed : dels4 = -0.051810 +/- 0.0122500 (guessed : dels4 = -0.051810 +/- 0.0123500 (guessed : dels4 = -0.051800 +/- 0.0123500 (guessed : dels4 = -0.0231690 +/- 0.0141730 (guessed : dels4 = -0.2316960 +/- 0.002300 (guessed : delw4 = -0.2316960 +/- 0.002300 (guessed : delw4 = -0.2316960 +/- 0.0043700 (guessed : delw4 = -0.2316960 +/- 0.0043700 (guessed : delw4 = -0.2316960 +/- 0.0043700 (guessed : delw4 = -0.2316960 +/- 0.0689500 (guessed : delw4 = -0.23	Ifeffit Results Files I	vlessages Ec	ho Journal	Properties	
Comment : Fit #1 Prepared by : Contact : Started : 12:45:38 on 9 July, 2007 This fit at : 12:57:50 on 9 July, 2007 Environment : Artemis 0.8.010 using linux, perl 5.008008, Tk 8 Figure of merit : 5 	Results from the last fi	t J	Raw log file	- Save	Dismiss
Contact : Started : 12:45:38 on 9 July, 2007 This fit at : 12:57:50 on 9 July, 2007 Environment : Artemis 0.8.010 using linux, perl 5.008008, Tk 8 Figure of merit : 5 			dec079_081.ch	i	A
This fit at : 12:57:50 on 9 Julý, 2007 Environment : Artemis 0.8.010 using linux, perl 5.008008, Tk 8 Figure of merit : 5 	Contact :				
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<pre>Independent points = 36.401367188 Wumber of variables = 18.00000000 Chi-square = 47831.822404141 Reduced Chi-square = 2599.362423279 R-factor = 0.014139526 Measurement uncertainty (k) = 0.000161333 Measurement uncertainty (R) = 0.000432403 Wumber of data sets = 1.000000000  Guess parameters +/- uncertainties (initial guess): enot = 0.7593290 +/- 0.5887570 (0.0000)  Guess parameters +/- uncertainties (initial guess): enot = 0.7593290 +/- 0.0490590 (guessed : sigs1 = 0.0024960 +/- 0.0004350 (guessed : sigs2 = 0.046840 +/- 0.0104350 (guessed : sigs4 = 0.0199540 +/- 0.0104350 (guessed : sigs4 = 0.0199540 +/- 0.0002960 (guessed : sigw1 = 0.0026180 +/- 0.0012120 (guessed : sigw2 = 0.0034940 +/- 0.0012120 (guessed : sigw3 = 0.0049650 +/- 0.002520 (guessed : dels1 = -0.0049650 +/- 0.0038900 (guessed : dels2 = -0.091610 +/- 0.0132500 (guessed : dels4 = -0.0510810 +/- 0.125700 (guessed : dels4 = -0.0510810 +/- 0.0132500 (guessed : dels4 = -0.0384190 +/- 0.0132500 (guessed : dels4 = -0.0384190 +/- 0.0032500 (guessed : dels4 = -0.0384190 +/- 0.0032500 (guessed : delw1 = -0.0384190 +/- 0.0032500 (guessed : delw3 = 0.0437020 +/- 0.038500 (guessed : delw4 = -0.2316960 +/- 0.0251520 (guessed : delw4 = -0.2316960 +/- 0.0689500 (guessed : delw4 = -0.</pre>		emis 0.8.01	0 using linux	, perl 5.00800	8, Tk 8
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$\begin{array}{rcrcr} R-factor &= & 0.014139526\\ \text{Measurement uncertainty (k) = } & 0.000161333\\ \text{Measurement uncertainty (k) = } & 0.000432403\\ \text{Fumber of data sets = } &= & 1.00000000\\ \hline \\ \text{Guess parameters +/- uncertainties (initial guess): \\ enot &= & 0.7593290 &+/- & 0.5887570 & (0.0000)\\ \text{s_02 = } & 0.8759420 &+/- & 0.0490590 & (guessed i sigs1 = & 0.0024960 &+/- & 0.0004350 & (guessed i sigs2 = & 0.0046840 &+/- & 0.0014430 & (guessed i sigs4 = & 0.0199540 &+/- & 0.0106960 & (guessed i sigw1 = & 0.0026180 &+/- & 0.0012120 & (guessed i sigw3 = & 0.0049650 &+/- & 0.002120 & (guessed i dels1 = & -0.0034940 &+/- & 0.002120 & (guessed i dels2 = & -0.0091610 &+/- & 0.002520 & (guessed i dels4 = & -0.0510810 &+/- & 0.0921570 & (guessed i dels4 = & -0.0510810 &+/- & 0.0921570 & (guessed i dels4 = & -0.0878950 &+/- & 0.1257000 & (guessed i dels4 = & -0.0878950 &+/- & 0.1257000 & (guessed i dels4 = & -0.065900 &+/- & 0.0032300 & (guessed i dels4 = & -0.0878950 &+/- & 0.1436630 & (guessed i delw1 = & 0.0025170 & (guessed i delw1 = & 0.0025170 & (guessed i delw1 = & 0.00384190 &+/- & 0.0141730 & (guessed i delw3 = & 0.0127130 &+/- & 0.0125120 & (guessed i delw3 = & 0.0437020 &+/- & 0.0251520 & (guessed i delw3 = & 0.0437020 &+/- & 0.0251520 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 = & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 &= & -0.2316960 &+/- & 0.0689500 & (guessed i delw4 &= & -0.2316$	Chi-square	= 4	7831.82240414	i	
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<pre>sigw2 = 0.0034940 +/- 0.0012120 (guessed : sigw3 = 0.0064500 +/- 0.0020520 (guessed : dels1 = -0.0049650 +/- 0.0036900 (guessed : dels2 = 0.0091610 +/- 0.0132500 (guessed : dels4 = -0.0510810 +/- 0.0132500 (guessed : dels4 = -0.0878950 +/- 0.1257000 (guessed : dels4s1 = -0.4542400 +/- 0.1436630 (guessed : dels5 = 0.0384190 +/- 0.1066450 (guessed : delw1 = 0.0065900 +/- 0.0032300 (guessed : delw2 = 0.0127130 +/- 0.0141730 (guessed : delw3 = 0.0437020 +/- 0.0251520 (guessed : delw4 = -0.2316960 +/- 0.0689500 (guessed : delw4 = -0.2316960 +/- 0.0689500 (guessed : s 02 and sigs1&gt; 0.8144</pre>	sigs4 =	0.0199540	+/- 0	.0106960 (g	wessed :
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s 02 and sigs1> 0.8144					
s 02 and sigs1> 0.8144					
	s_02 and sigs1	>	0.8144		
		`			2

- Beautiful background
- too Many ∆R values highly unsatisfactory.....

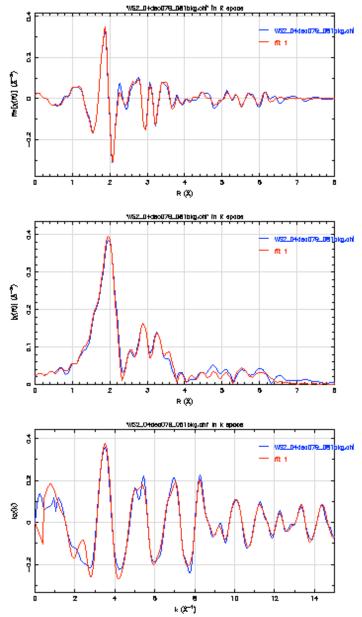


ws2-vars2d.apj

#### **Bulk WS<sub>2</sub>**: Reformulate $\Delta R$ list in terms of unit cell parameters

Ifeffit Results	Files Messages	Echo Journal	Properties	
Results from the	e last fit	Raw log fil	e – Save	Dismiss
Project title Comment Prepared by Contact Started This fit at Environment Figure of merit	: Fit #1 : : 13:06:29 or : 13:08:07 or : Artemis 0.8	204dec079_081bk 19 July, 2007 19 July, 2007 1010 using linu	-	08, Tk 81
				-
Independent poin Number of varial Chi-square Reduced Chi-squa R-factor Measurement unco Measurement unco Mumber of data s	bles = = are = ertainty (k) = ertainty (R) =	36.4013671 12.0000000 59713.3305621 2447.1551164 0.0176502 0.0001613 0.0004324 1.0000000	00 77 87 77 33 03	
Guess parameters enot s_02 sigs1 sigs2 sigs4 sigs5 sigw1 sigw2 sigw3 da dc ds1z	= 0.7683 = 0.8816 = 0.0025 = 0.1438 = 0.0322 = 0.0322 = 0.0033 = 0.0033 = 0.0052 = 0.0072 = 0.4114 = 0.0051	830       +/-         1770       +/-         1410       +/-         1530       +/-         1650       +/-         1650       +/-         1620       +/-         1640       +/-         1650       +/-         1660       +/-         1600       +/-         1600       +/-         1600       +/-         340       +/-	0.5653740       ()         0.0486940       ()         0.0004250       ()         0.0014840       ()         4.4316550       ()         0.0073520       ()         0.0012840       ()         0.0012440       ()         0.0012440       ()         0.0012860       ()         0.1255630       ()         0.0012720       ()	0.6649) 0.8834) 0.0026) 0.0052) 0.0050) 0.0027) 0.0027) 0.0034) 0.0035) 0.0055) 0.0070) 0.4994) 0.0060)
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N				×

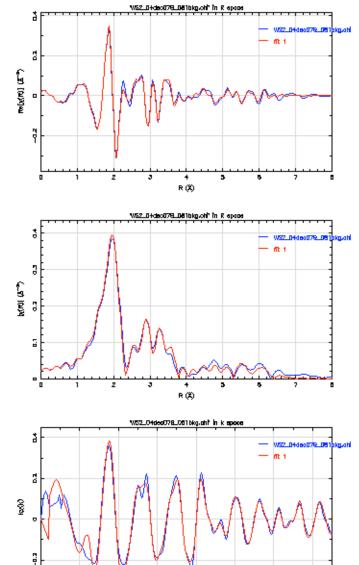
MS paths do not contribute because of large sigma values



ws2-bulk-uc2.apj

#### **Bulk WS**<sub>2</sub>: Reformulate $\Delta R$ list in terms of unit cell parameters

Ifeffit Results	Files Messag	ges   E	cho   Journal	Properties	
Results from th	e last fit		Raw log file	- Sav	e Dismiss
Project title Comment Prepared by Contact Started This fit at Environment Figure of merit	: Fit #1 : : 13:14:12 : 13:15:01 : Artemis : 1	- 2 on 9 1 on 9 0.8.01	dec079_081bkg July, 2007 July, 2007 0 using linux	, perl 5.008	·
Independent poi Number of varia Chi-square Reduced Chi-squ R-factor Measurement unc Measurement unc Number of data	nts bles are ertainty (k) ertainty (R)	= = 6 = =	36.40136718 10.00000000 0719.76416421 2299.87196242 0.01794487 0.00016133 0.00043240 1.00000000	8 0 9 5 3 3 3 3	
Guess parameter enot s_02 sigs1 sigs2 sigw1 sigw2 sigw3 da dc dc ds1z	$\begin{array}{rcrr} = & 0.7\\ = & 0.6\\ = & 0.0\\ = & 0.0\\ = & 0.0\\ = & 0.0\\ = & 0.0\\ = & 0.0\\ = & 0.0\\ = & 0.5\end{array}$	a intie 7332520 8801200 0025320 0051660 0026570 0033690 0055440 0072510 5146890 0061430	+/- 0 +/- 0 +/- 0 +/- 0 +/- 0 +/- 0 +/- 0 +/- 0	uess): .4972210 .0448530 .0004010 .0014340 .0002730 .0011960 .0014310 .0027340 .1757690 .0016870	(0.6808) (0.8821) (0.0025) (0.0052) (0.0034) (0.0034) (0.0055) (0.0071) (0.5032) (0.0060)
Def parameters s1_2z s1_3z a b c d0x d0y d0z d1x d1y d1y	= 0.1 = 0.3 = 3.1 = 3.1 = 12.8 = 0.0 = 0.0 = 0.0 = 0.3	70: P1 1286430 713570 1604510 1604510 3376890 0000000 0000000 0000000 333400 333400		[51]"):	Y
M					×



ws2-bulk-ucb.apj

14

10

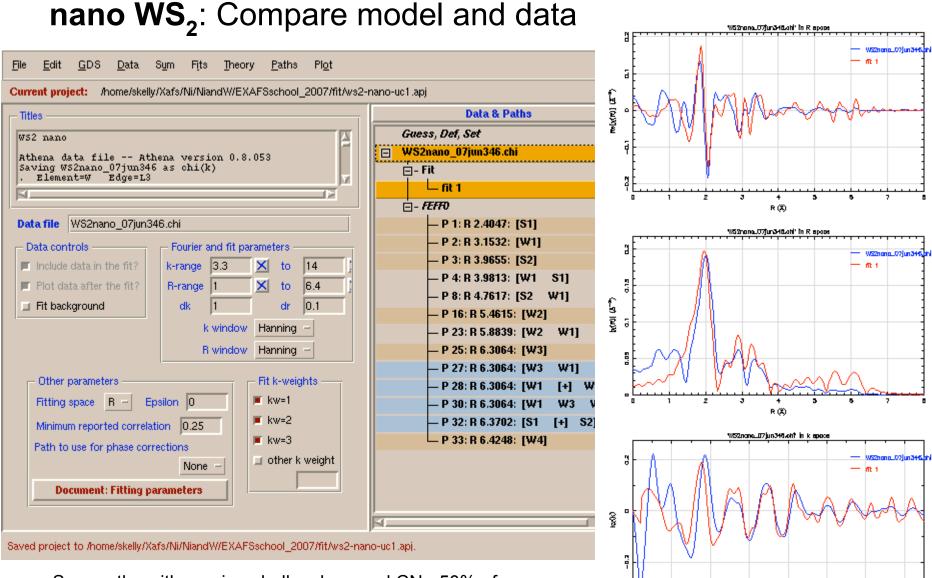
0

z

4

5

∎ k(X<sup>\_-1</sup>) 12



- Sum paths with previous bulk values and CN ~50% of bulk values
- need to add short oxygen signal

ws2-nano-uc1.apj

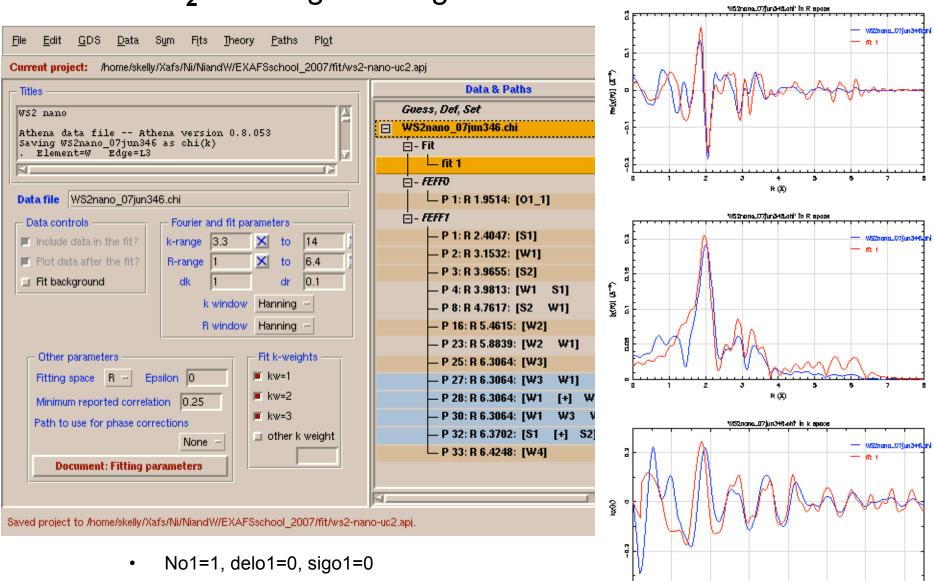
12

14

10

k (X<sup>-1</sup>)

7



#### nano WS<sub>2</sub>: Adding W-O signal

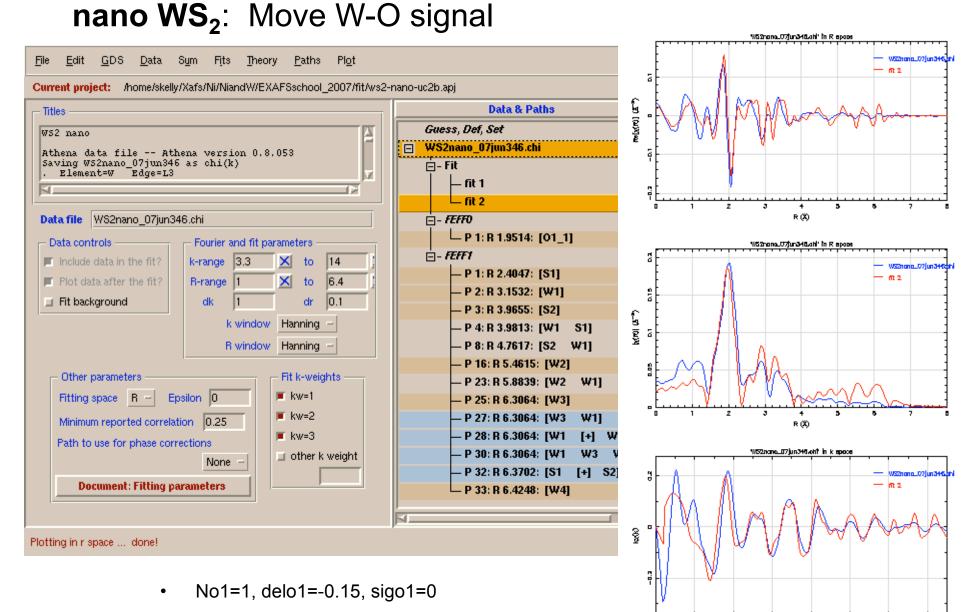
need to shift oxygen signal -0.15 Ang

ws2-nano-uc2.apj

12

10

k (X<sup>-1</sup>)



• need to optimize parameters

ws2-nano-uc2b.apj

12

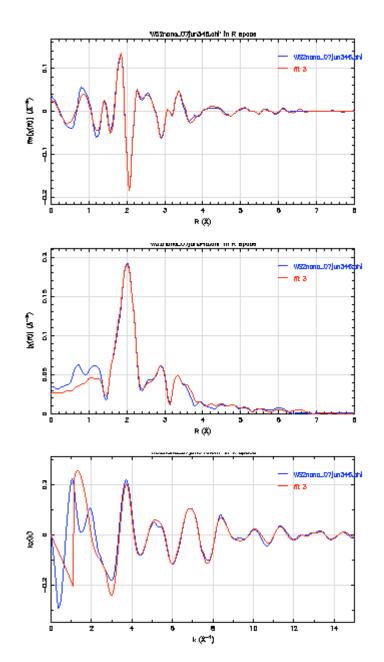
10

k (X<sup>-1</sup>)

#### **nano WS<sub>2</sub>**: optimize parameters

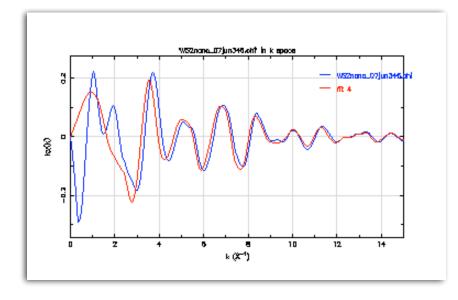
Ifeffit Results	Files Message	es   Echo   Jou	rnal Properties	
Results from th	e last fit	Raw	log file 🚽 🕏	ave Dismiss
Project title Comment Prepared by Contact Started This fit at Environment Figure of merit	: Fit #1 ; ; : 13:23:18 : 13:31:15 : Artemis ( ; : 3	-	07 07 linux, perl 5.0	ŕ
Independent poi Number of varia Chi-square Reduced Chi-squ R-factor Measurement und Measurement und Number of data	nts bles ware sertainty (k) sertainty (R)	= 36.401 = 18.000 = 104858.309 = 5698.397 = 0.015 = 0.000 = 0.000		
Guess parameter enot sigs1 sigs2 sigw2 sigw3 da dc ds1z ns1 nw1 ns2 nw2 nw3 nw4 no1 delo1 sigo1	$\begin{array}{rcrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	560740         +/-           143040         +/-           143040         +/-           155830         +/-           155830         +/-           155830         +/-           155830         +/-           155830         +/-           155830         +/-           110020         +/-           1117510         +/-           1117510         +/-           1117510         +/-           1117510         +/-           1117510         +/-           11117510         +/-           11117510         +/-           11117510         +/-           11117510         +/-           11117510         +/-           11117510         +/-           11117510         +/-           11117510         +/-           1111770         +/-           1111770         +/-           1111770         +/-           1111770         +/-	<pre>ial guess): 0.5681080 0.0005230 0.0079470 0.012770 0.0149970 0.0121140 0.0068210 0.1902890 0.2093210 0.6109970 2.4929180 1.5518340 1.7557080 8.7709550 0.1821170 0.0052930 0.0013850</pre>	$ \begin{pmatrix} 0.6808 \\ 0.0025 \\ (0.0052) \\ (0.0034) \\ (0.0055) \\ (0.0071) \\ (0.5032) \\ (0.0060) \\ (3.0000) \\ (3.0000) \\ (3.0000) \\ (3.0000) \\ (3.0000) \\ (5.0000) \\ (6.0000) \\ (6.0000) \\ (1.0000) \\ (-0.1500) \\ (0.0050) \\ \end{pmatrix} $
Def parameters s1_2z s1_3z	= 0.12 = 0.37	): P 1: R 1.95 271830 728170 749510	14: [01_1]"):	v
M				×

• need to fix background

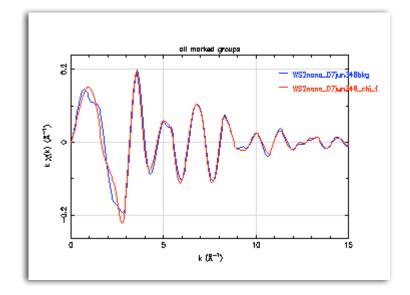


ws2-nano-uc2c.apj

#### **nano WS<sub>2</sub>**: Refining the background



- set all parameters to best fit values, except for e0=0
- write fit chi(k) to disk to be read into Athena

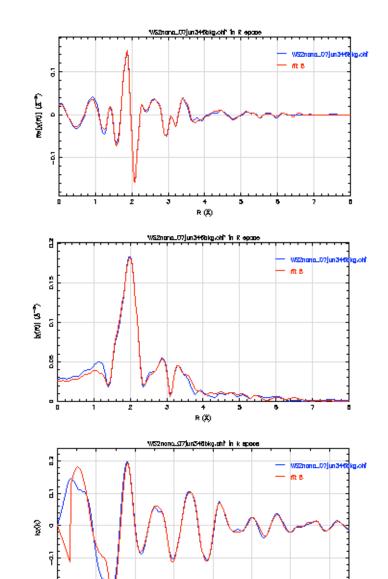


read theory for chi(k) into AthenaMake new background for data

ws2-nano-bkg.prj

#### nano WS<sub>2</sub>: Refining the model

Ifeffit Results	Files Messages	Echo Journal Properti	ies
Results from th	ie last fit	Raw log file -	Save Dismiss
Project title Comment Prepared by Contact Started This fit at Environment Figure of merit	: Fit #1 ; ; ; 13:23:18 on 5 ; 13:41:07 on 5 ; Artemis 0.8.0		5.008008, Tk 81
Independent poi Number of varia Chi-square Reduced Chi-squ R-factor Measurement und Measurement und Number of data	ints = ubles = uare = certainty (k) = certainty (R) =	36.401367188 18.00000000 86981.135954150 4726.884424829 0.013848613 0.000036481 0.000097776 1.00000000	
enot sigs1 sigw1 sigw2 sigw3 da dc ds1z nw1 ns2 nw2 nw3 nw4 no1 delo1 sigo1	rs +/- uncertaint: = 1.690276 = 0.00413: = 0.005547 = 0.007537 = 0.007537 = 0.002722 = 0.488877 = 0.004685 = 0.004685 = 3.471555 = 2.346355 = 5.690997 = 0.450236 = 1.011704 = 4.081947 = 1.045745 = -0.174326 = 0.002086 (using "FEFF0: P	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	(guessed :           (guessed :
s1_2z s1_3z	(USING "FEFFO: P = 0.127185 = 0.37281: - 0.1000	10	N N



k (X<sup>-1</sup>)

10

12

5

ŝ

z

4

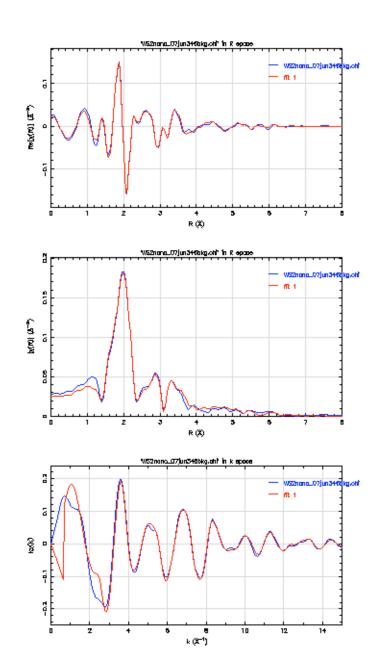
ws2-nano-uc3b.apj

14

#### **nano WS<sub>2</sub>** : Refining the model

Ifeffit Results File	es   Messages   E	cho   Journal	Properties	
Results from the la	ast fit	Raw log file	- Save	Dismiss
Project title : Comment :	Fitting WS2nar Fit #1	.o_07jun346bkg.	chi	A
Prepared by : Contact : Started :	13:44:38 on 9			
This fit at : Environment :	13:45:17 on 9		ner1 5,00800	8 TE 81
Figure of merit :	1	o using intur,	perr 5.00000	o, in o.
Independent points Number of variable	s =	10.816406250 5.00000000	)	
Chi-square Reduced Chi-square		6538.889730369 1124.214755523	3	
R-factor Measurement uncert	ainty (k) =	0.235362466	Ĺ	
Measurement uncert Number of data set	:s =	0.000097776 1.000000000		
Guess parameters +	-/- uncertaintie	s (initial gu	less):	
sigw2 sigw3	= 0.0044960 = 0.0075700	i +/- 0,	.0035760 (O	.0045) .0076)
nw2 nw3	= 0.8248320 = 1.2075320	i +/- 0,	6821310 (1	.8240) .2083)
nw4 Def parameters (us	= 2.2013950			.1990)
s1_2z s1_3z	= 0.1272350 = 0.3727650		01_1] );	
a b	= 3.1561530 = 3.1561530	l i i i i i i i i i i i i i i i i i i i		
c d0x	= 12.8201570 = 0.0000000	l i i i i i i i i i i i i i i i i i i i		
d0y d0z	= 0.0000000 = 0.0000000			
d1x d1y	= 0.3333400 = 0.3333400	l i i i i i i i i i i i i i i i i i i i		
d1z d3x	= 0.5000000 = 0.3333400	l i i i i i i i i i i i i i i i i i i i		
d3y d3z	= 0.3333400 = 0.1227650	l i i i i i i i i i i i i i i i i i i i		
d4x 44	= 0.3333400 - 0.9999400			Y
M				X

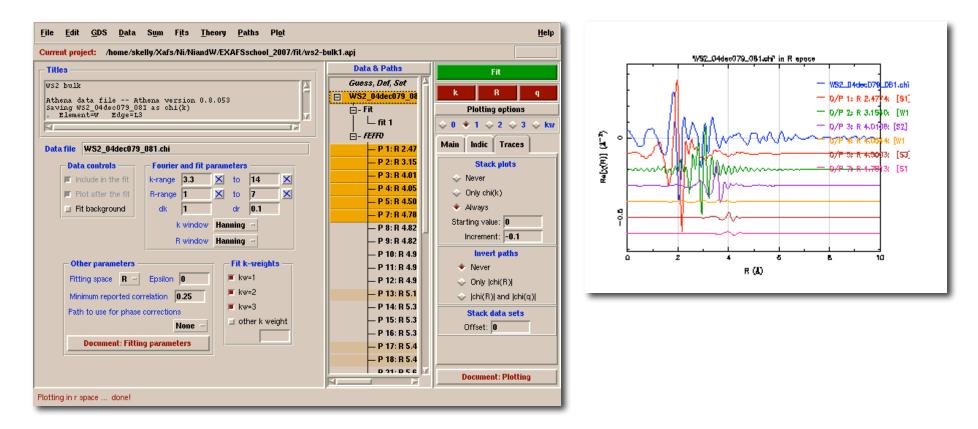
- determine Nw2, Nw3, and Nw4
- Model fit region from 5 to 6.4 Ang



ws2-nano-uc4.apj

Done and Starting over using just the BiG paths

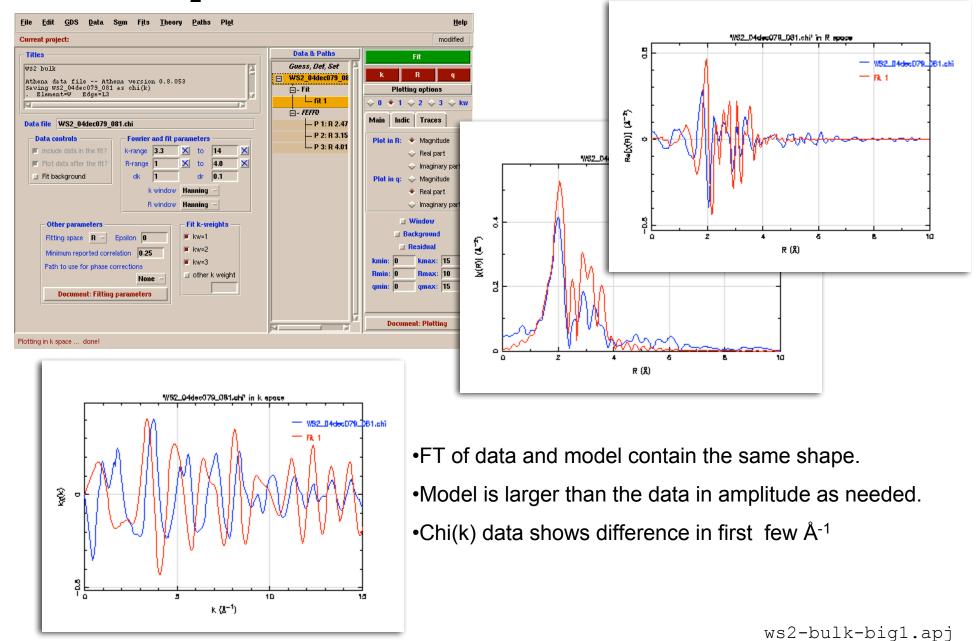
# **Bulk WS<sub>2</sub>**: Look for big paths and a region in R where paths do not overlap

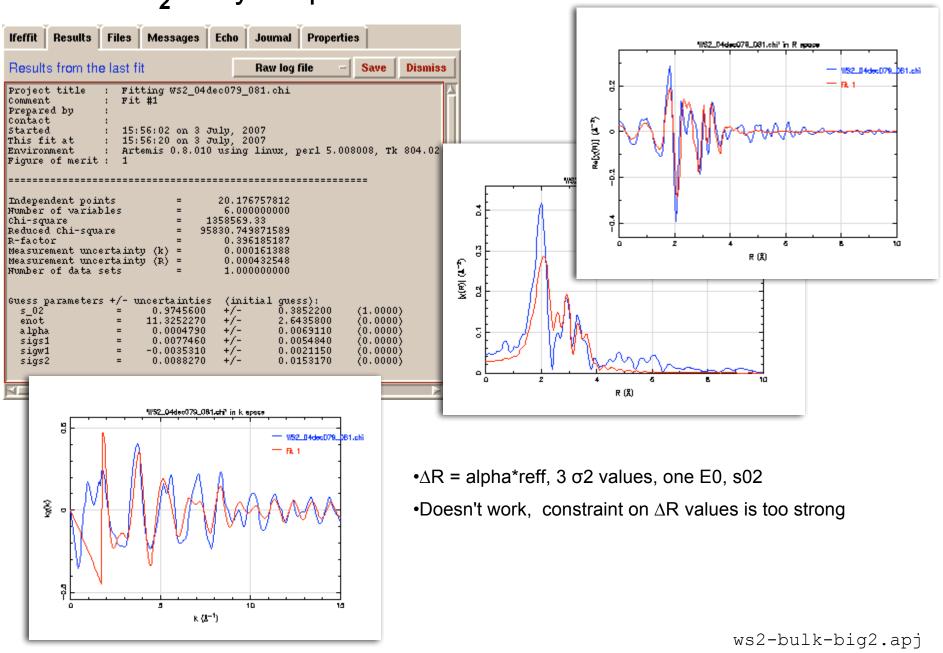


First three paths (red, green, and purple) are much bigger and well separated from other paths

ws2-bulk1.apj

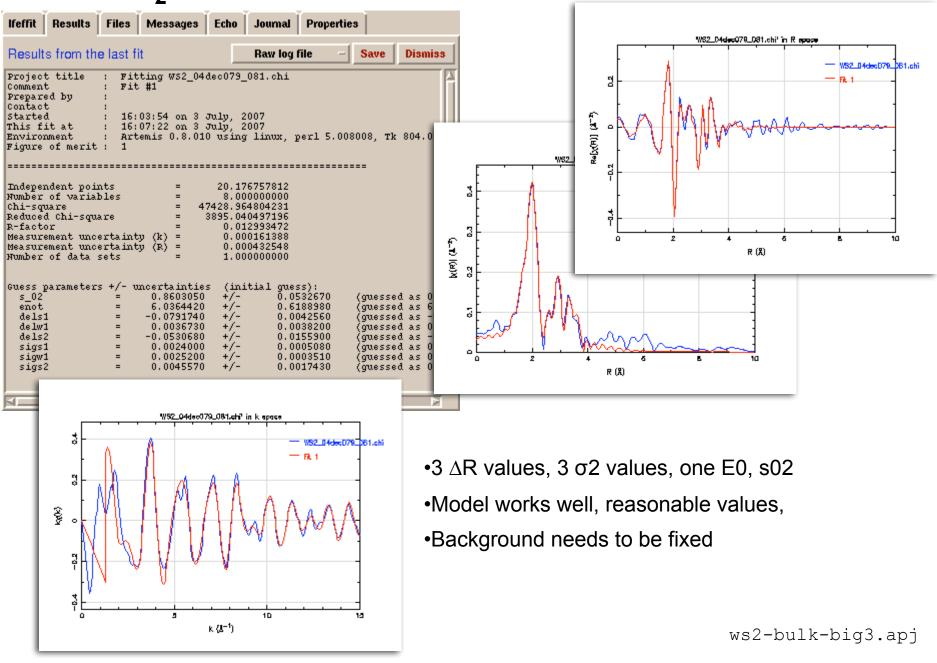
#### Bulk WS<sub>2</sub>: Sum up first three paths and compare to data



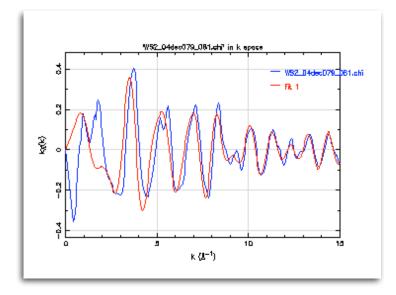


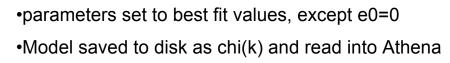
#### **Bulk WS**<sub>2</sub>: Try simple model

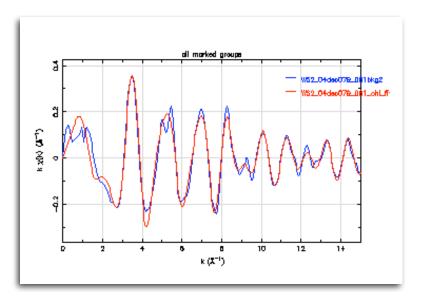
#### **Bulk WS**<sub>2</sub>: relax constraints on $\Delta R$



#### **Bulk WS<sub>2</sub>**: re-work background



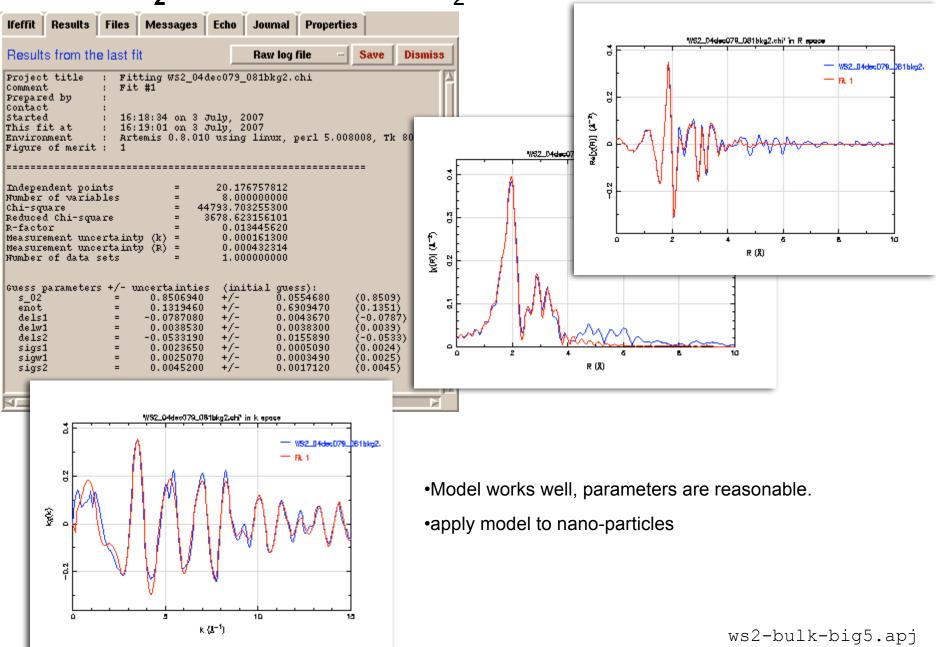




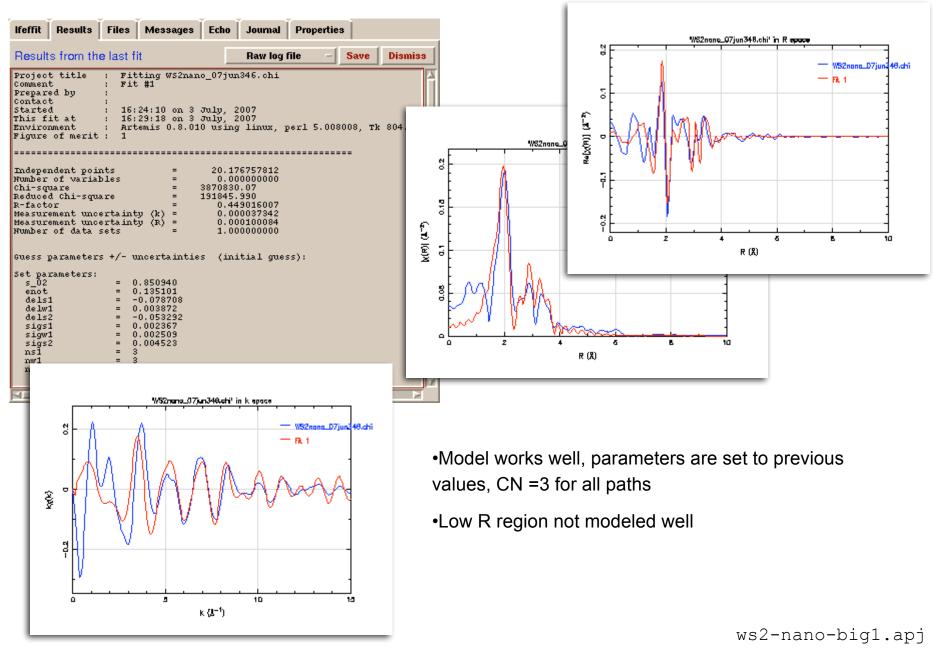
- •Model read into Athena
- •New background made for data

ws2-bulk-big4.apj
ws2-bkg2.prj

#### Bulk WS<sub>2</sub>: Model of Bulk WS<sub>2</sub> data



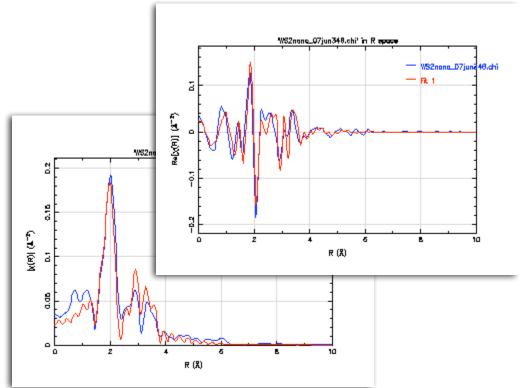
#### Apply bulk model to Nano data



#### nano WS<sub>2</sub>: Add oxygen path to model

48.chi

lfeffit	Results	Files	Messages	Echo	Journal	Propert	tie
Result	s from th	e last fit	Raw log f	ile –	Save	Dismiss	
Commen Prepar Contac starte This f. Envirou Figure ====== Number Chi-sq Reduce Refact Measur Number Guess 1	ed by t d of merit of merit of varial uare d chi-squi or ement unco- of data : parameter: rameters: 1 1 2 1	: Fit : : : 16:: : 16:: : Art: : 1 : : Art: : : : : 1 : : : : : : : : : : : : : :	37:14 on 3 3 37:31 on 3 3 smis 0.8.01 = = = = 12: = 0 (k) =	July, 2 July, 2 0 using 20.17 0.00 2501122 3960.60 0.36 0.00 1.00	007 007 1 linux, 00000000 09 0000000 4716463 00037342 00100084 0010008	-	
delo: sigo:		= -( = 0	). 15 WS	i2nana_0	7)un348.chi'	in k space	ź
	kg(k) -0.2 0.2				к (2 <sup>-1</sup> )	10	- WS2none_D7 - Fk 1



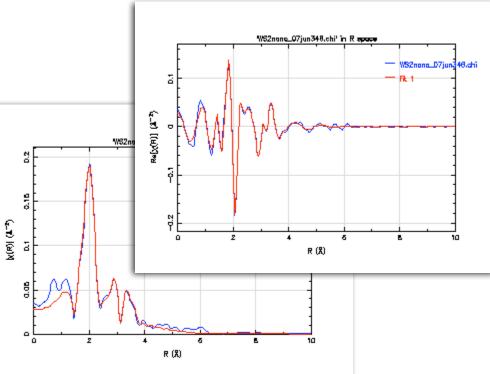
•Model works well, parameters are set to previous values, CN =3 for all paths,

•W-O path, CN=1, delr=-0.15, ss=0

•fixes low k-region

ws2-nano-big2.apj

Ifeffit Results	[ Files ]		Í Eaba Í I		Duranautica
iremit Results	rnes	messages	ECNO	ournau	Properties
Results from the	e last fi	t Raw log	file –	Save	Dismiss
Project title Comment Prepared by Contact Started This fit at Environment Figure of merit	: Fit : : 16: : 16: : Art : 1	"- 45:23 on 3 45:55 on 3 emis 0.8.01	July, 200 July, 200 0 using 1	7 7 inux, <u>r</u>	er1 5.0
Independent poin Number of varial Chi-square Reduced Chi-squ R-factor Measurement unco Number of data	bles are ertaint ertaint	= 1 = y (k) =	20.1767 13.0000 3170.5103 1588.8695 0.0128 0.0000 0.0001 1.0000	00000 05937 81342 87617 37342 00084	
Guess parameter: enot dels1 dels2 sigs1 sigw1 sigs2 ns1 nw1 ns2 no1 delo1 sigo1	s +/- u = = = = = = = = = = = =	ncertaintie 3.6987390 -0.0751680 0.0015200 0.0043560 0.0056940 0.0111720 3.7264150 2.5220570 3.6515630 1.3927860 -0.1721410 0.0035320	·//·/· + + //··· + + + + + + //····	0.85 0.00 0.02 0.00 0.00 0.00 0.30 1.97 0.30 0.30	(5): (55040) (57200) (67500) (67500) (07460) (18180) (75160) (66410) (07700) (53900) (77220) (77220) (774140) (21000)



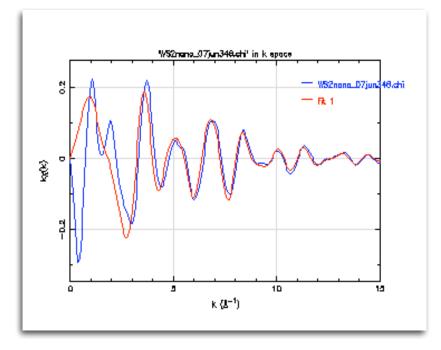
•Model works well, parameters are reasonable

•clean up background

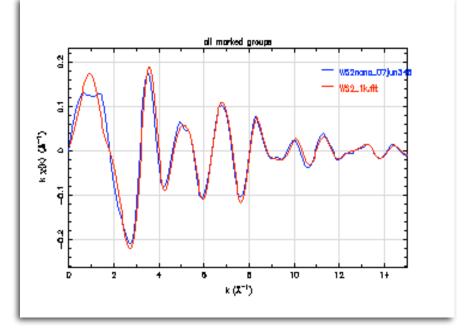
#### nano WS<sub>2</sub> :optimize fit parameters

ws2-nano-big3.apj

#### nano WS<sub>2</sub>:re-work background



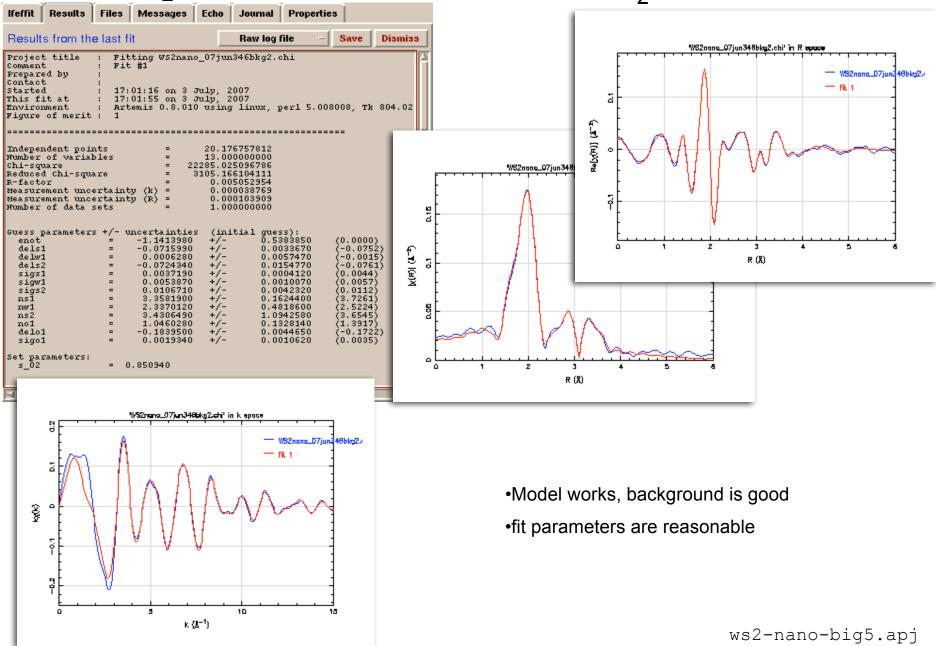
parameters set to best fit values, except e0=0
Model saved to disk as chi(k) and read into Athena



Model read into AthenaNew background made for data

ws2-nano-big4.apj
ws2-nanobkg2.prj

#### nano WS<sub>2</sub>: Modelling Nano-particles of WS<sub>2</sub>



## The End