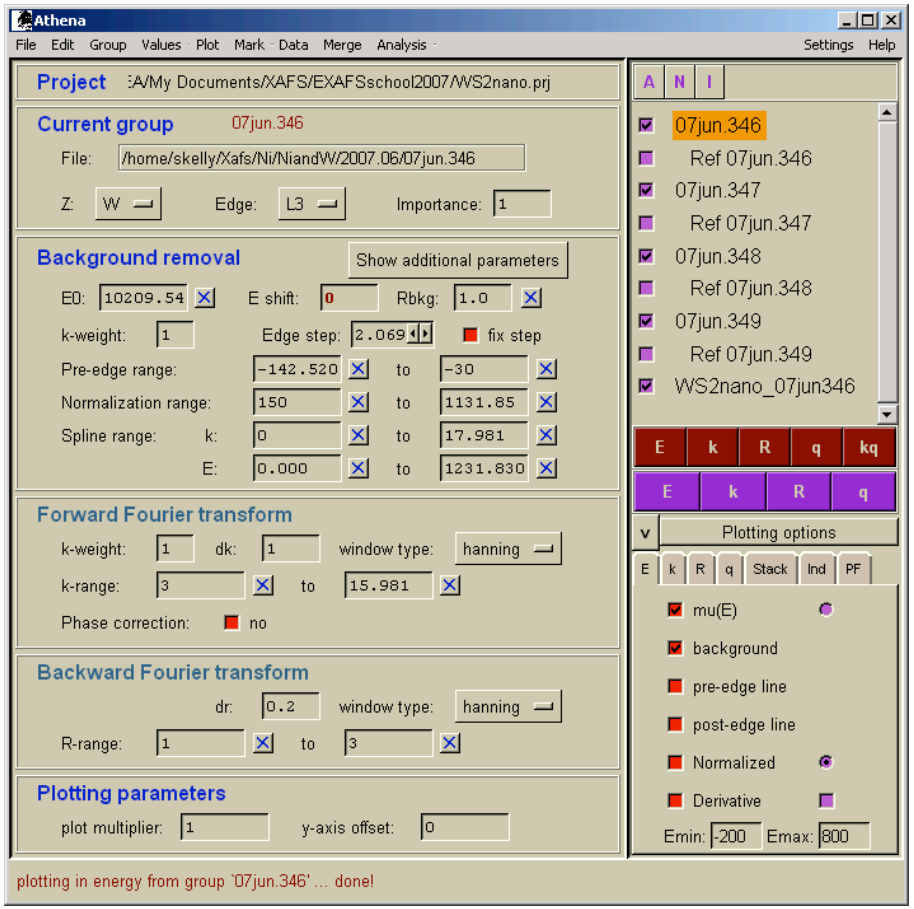
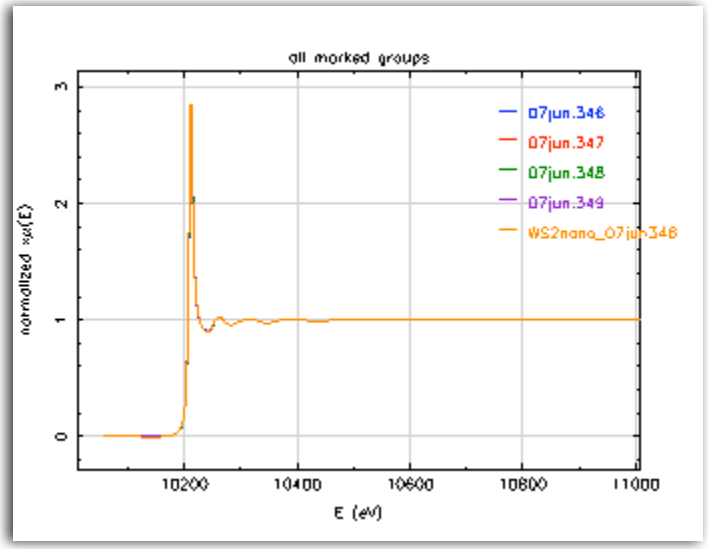
Modeling bulk and nano WS_2

Shelly Kelly

Read data into Athena

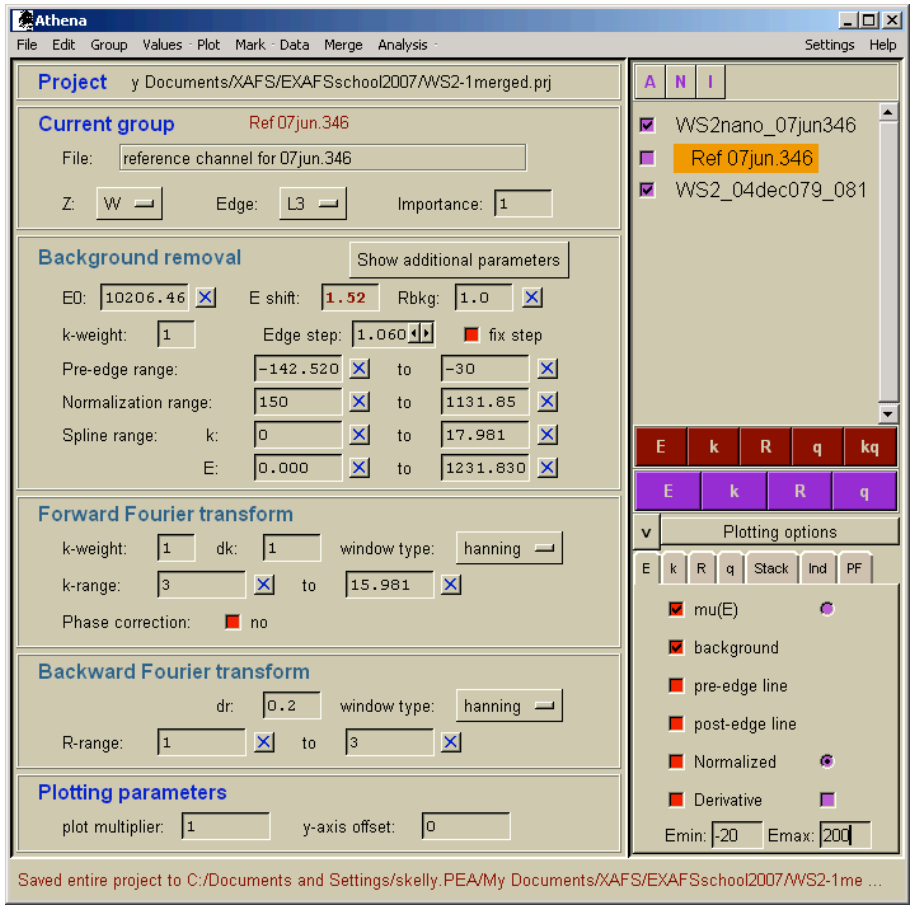


- Read individual files into Athena
  - Align data using the reference spectra
  - Merge data in μ(E)
  - Overplot merged data and aligned spectra

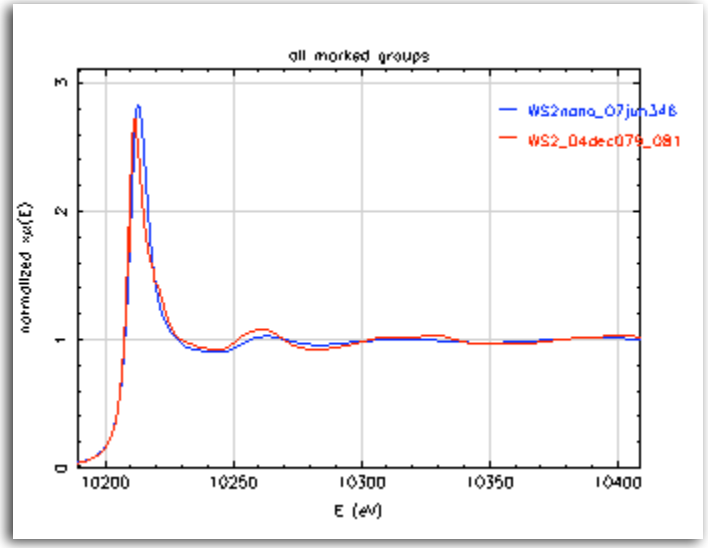


WS2nano.prj

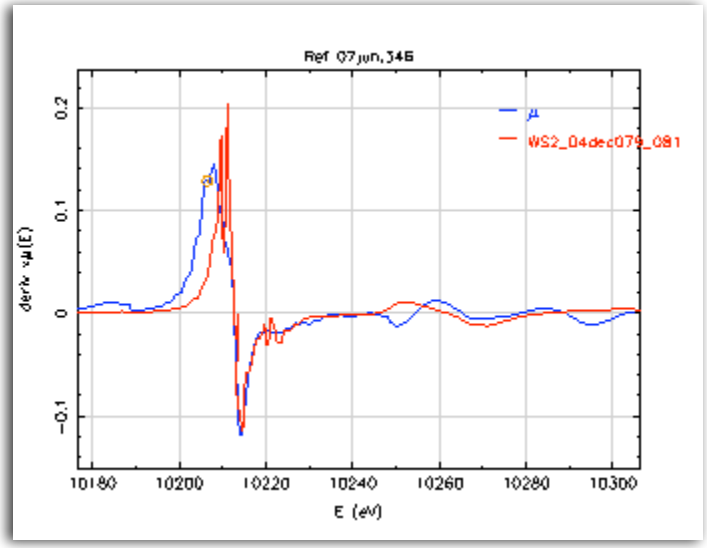
Merged Athena project file



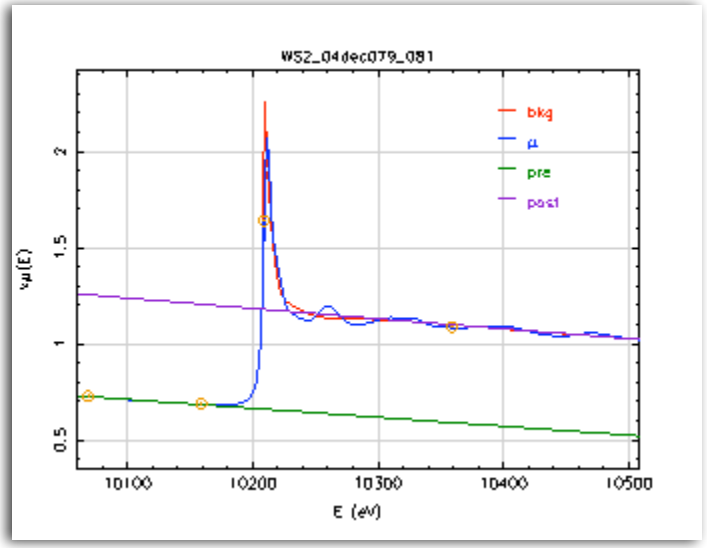
- Keep merged data files together for one project
- Compare χ(k) spectra and Fourier Transform



`WS2-1merged.prj`

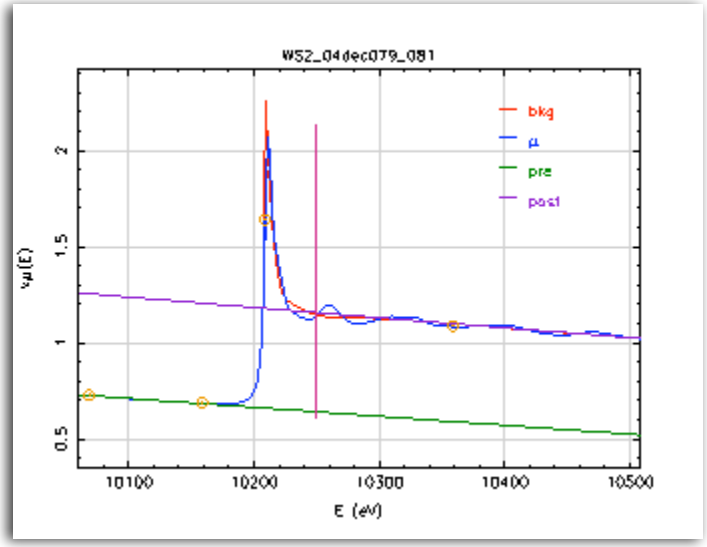


Align spectra to a reference spectrum from the nanoparticles



Check the pre-edge and post-edge ranges in Athena

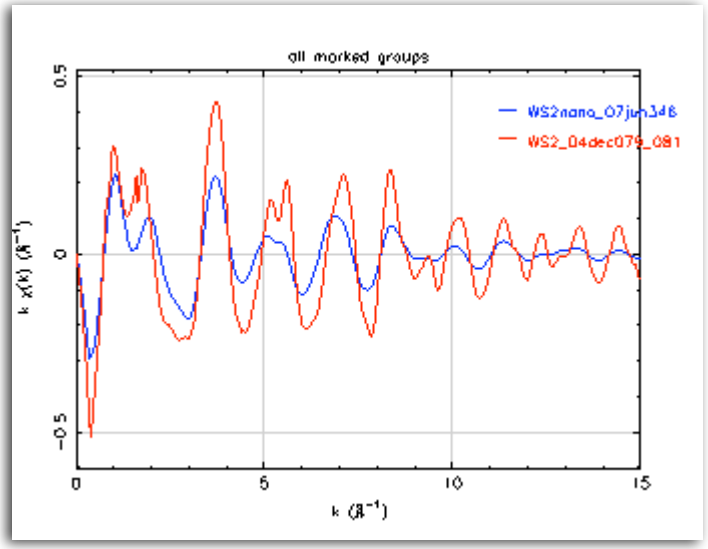
Set pre-edge range: -30 to -50 eV



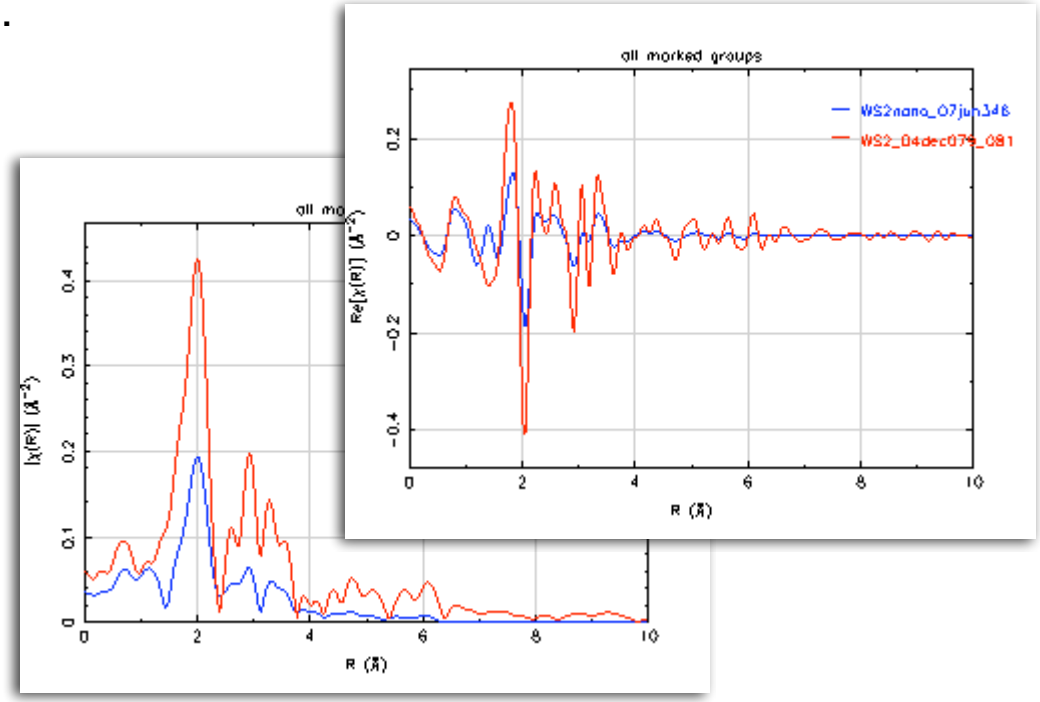
Use IND (indicator) menu to locate k_{min}=3.3 of FT compared to the edge

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
  - except at low R ~ 1.8 Ang.

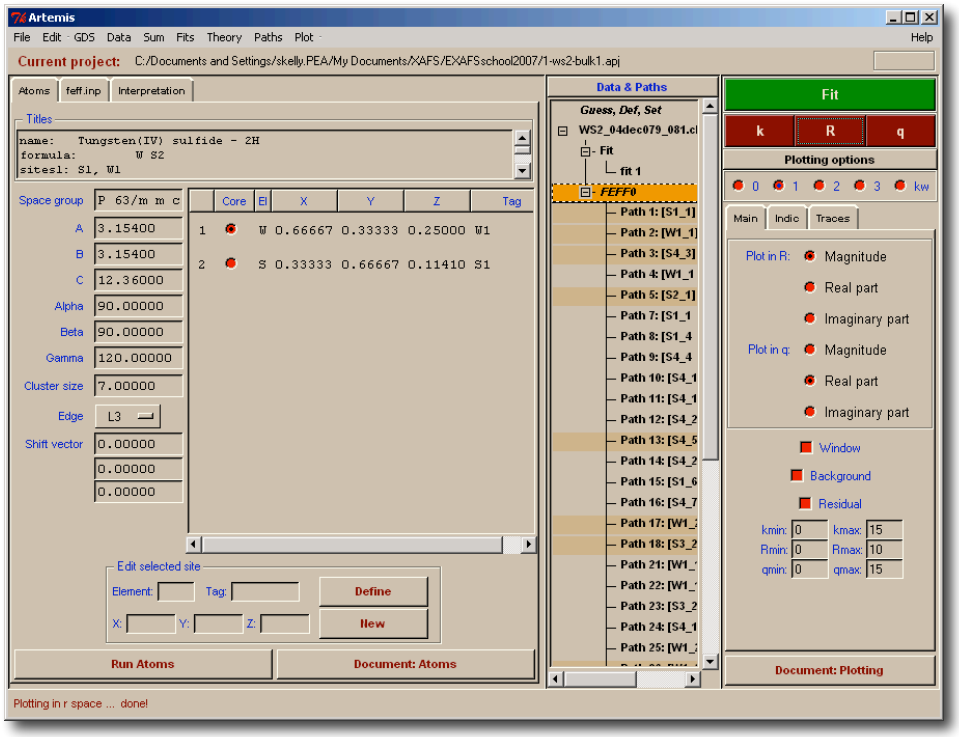


Check that chi(k) spectra oscillate about zero



Compare FT

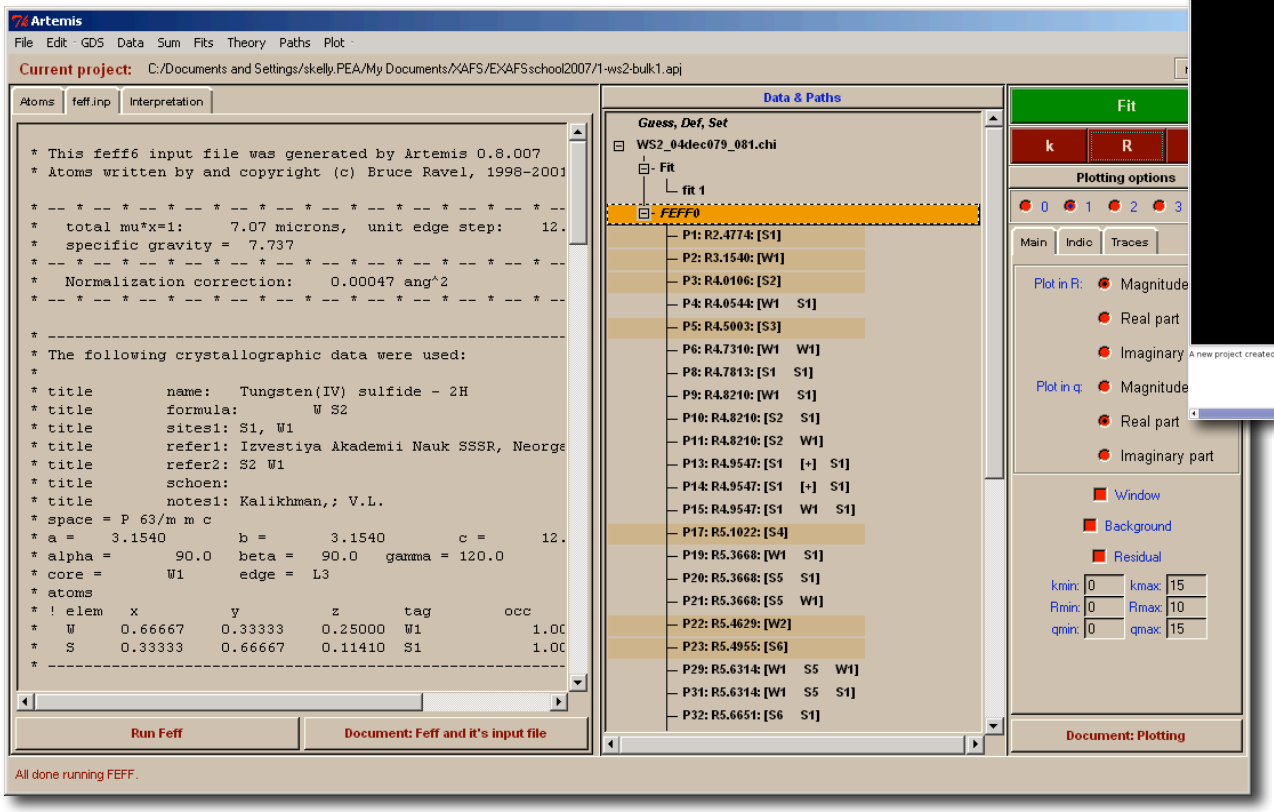
Get WS_2 theory

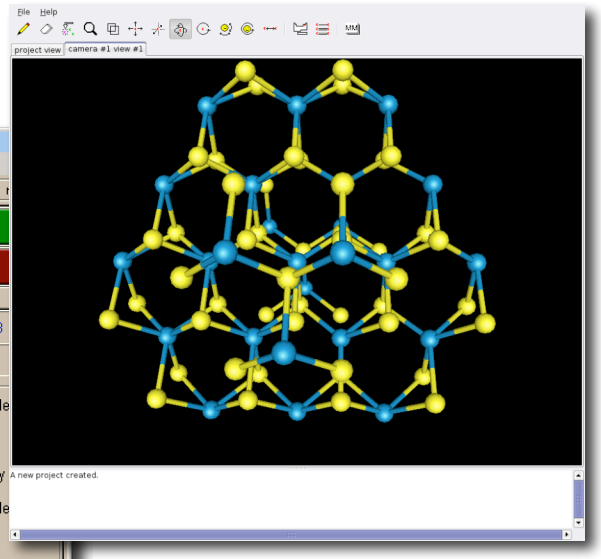


- Fill out Atoms page from icsd_ws2.cif file
- Check edge, Core atom radial button
- Push run atoms button
- Check feff.inp page for reasonable interatomic distances
- Run feff and include all paths in the model

Understand the structure of WS_2

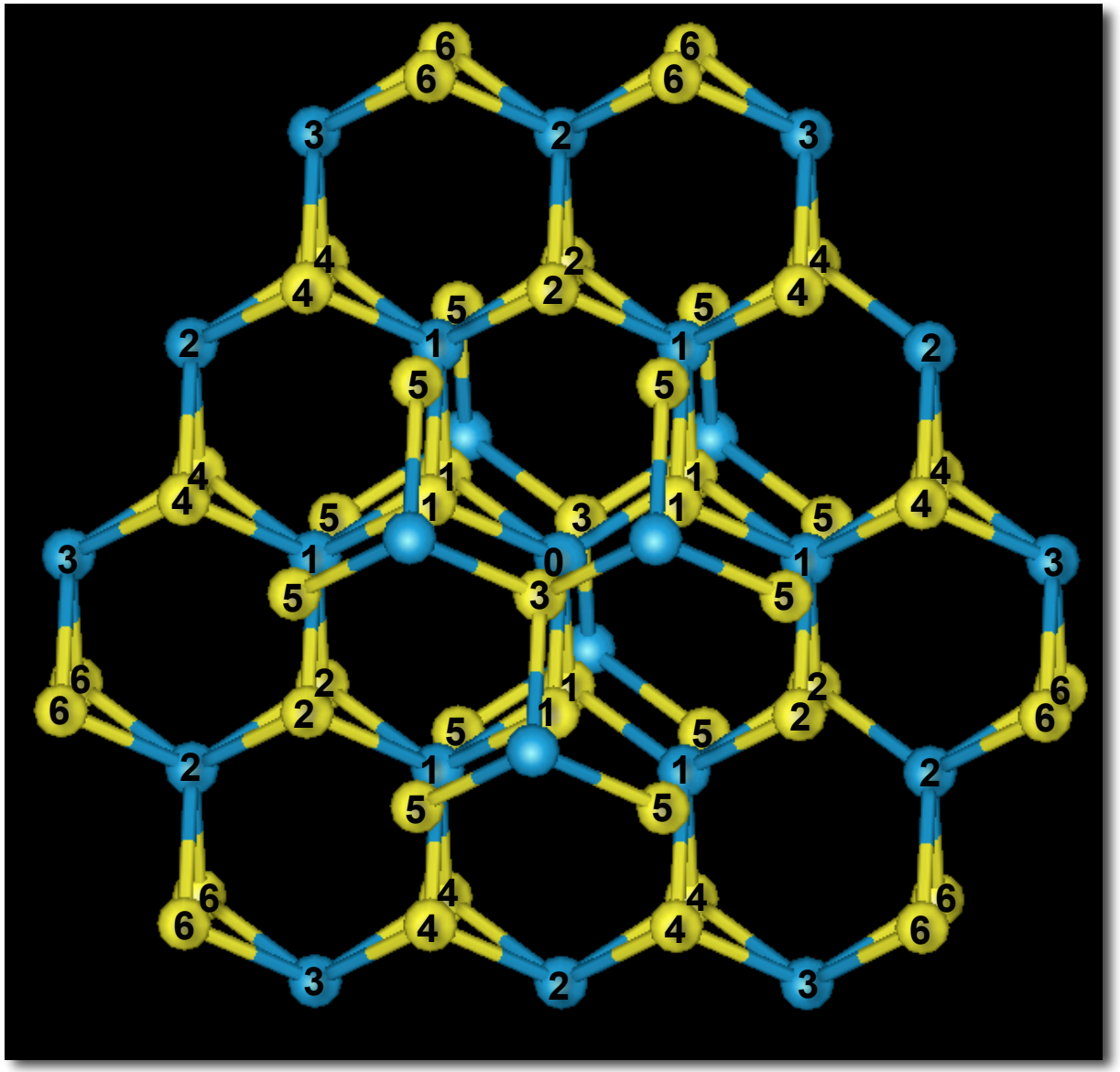
- Make sense of the path names
  - Edit feff.inp tags to decrease the degeneracy of tag names
  - Set preferences to show path number, length and atom type
  - Make ball-n-stick by writing out alc file for ghemical
    http://www.uku.fi/~thassine/projects/ghemical/





Ghemical screen shot

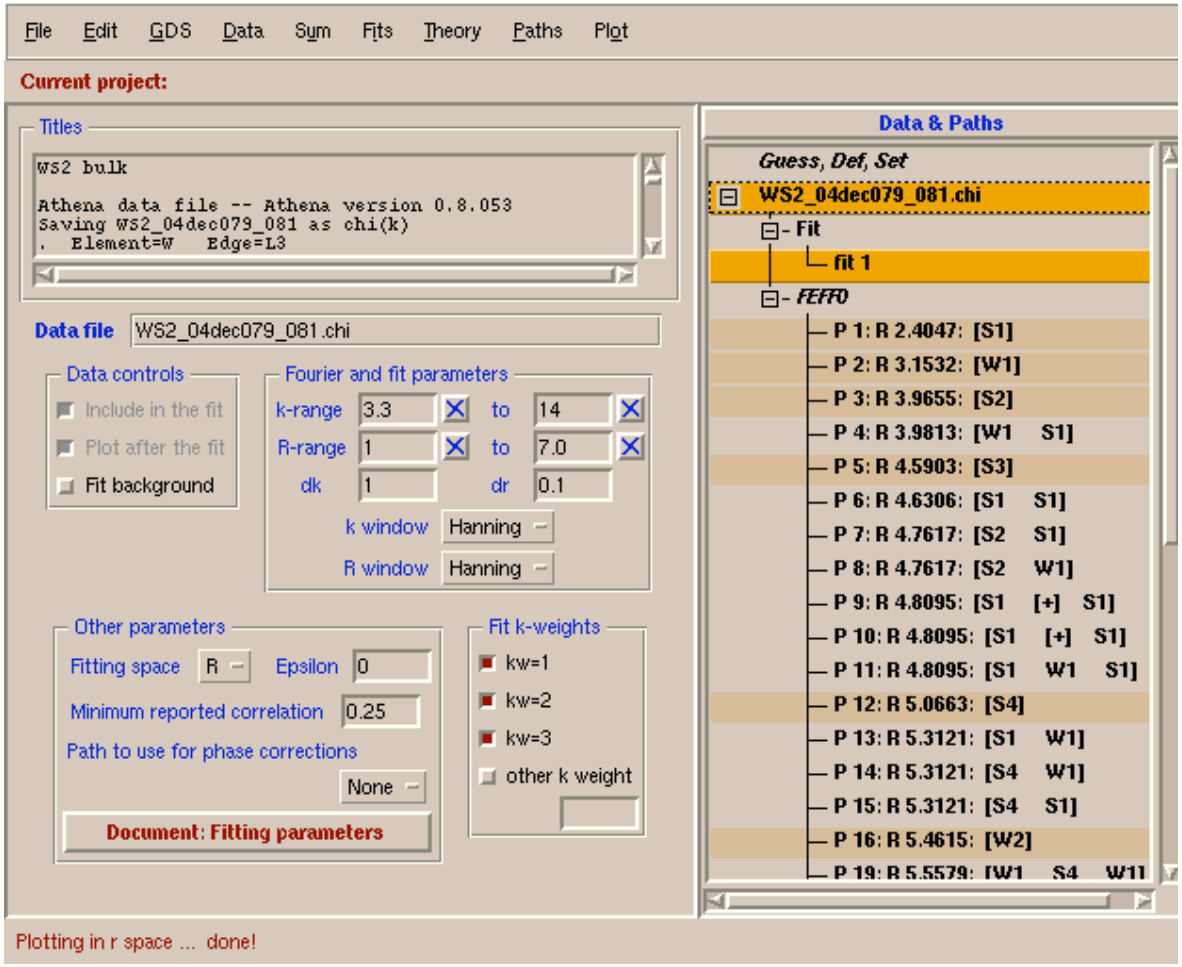
Understand the structure of WS_2

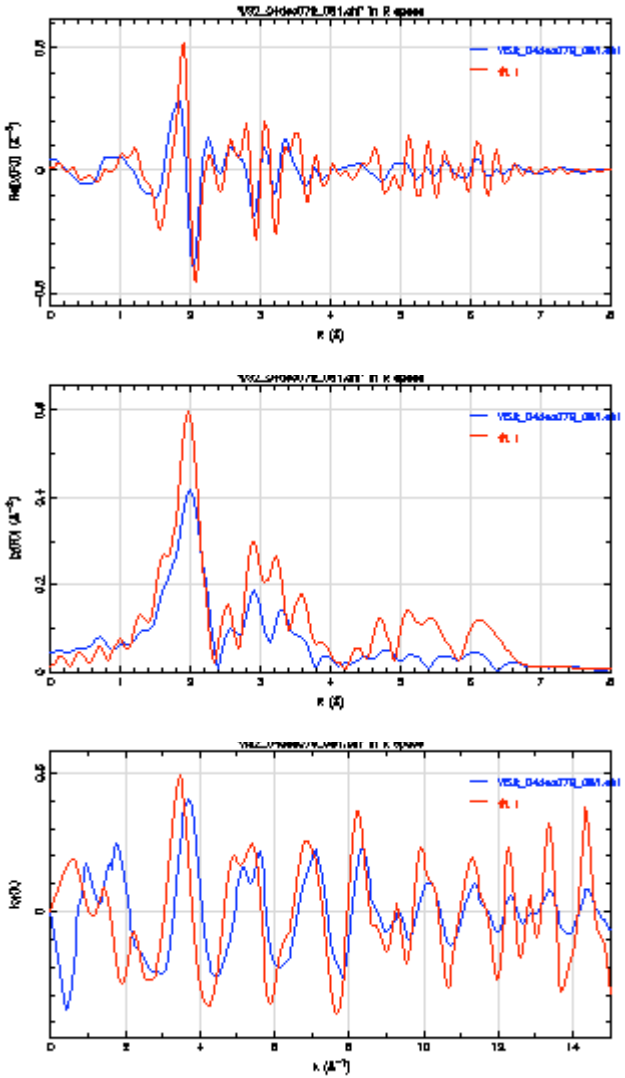


Scattering Paths

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_2 FEFF calculation to WS_2 bulk data





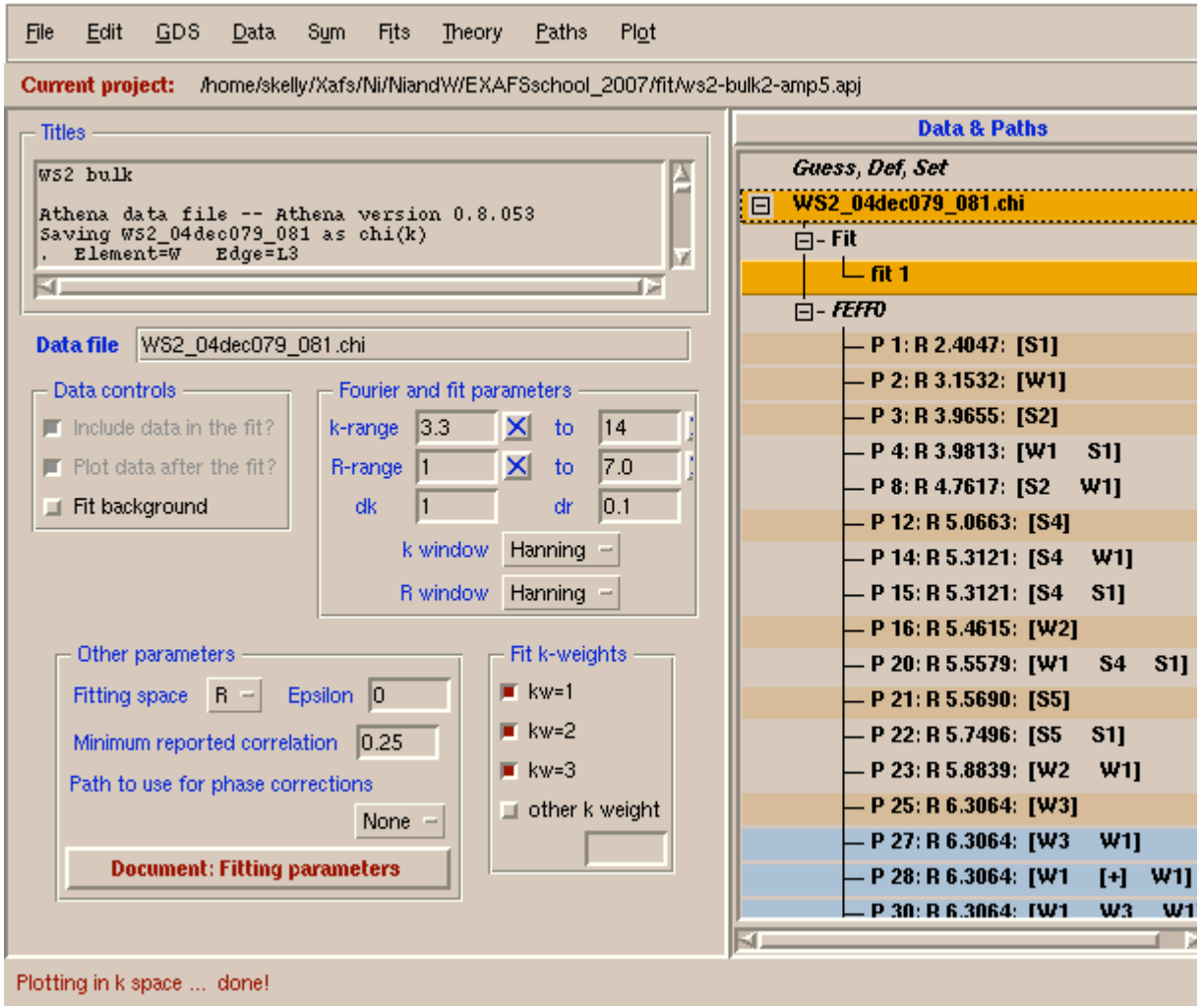
- Set e0=0; S_02=1.0; sigma2=0; delr=0
- chi(k) spectra shows difference in background removal and in e0.
- FT crosses zero at the same places and has the same structure.
- FT amplitude is always larger than that of the data
- Notice that the shape of the spectra from 5 to 7 Å is different in the mag of FT but the data look similar in the real part of the FT –Need to use the real part of the FT

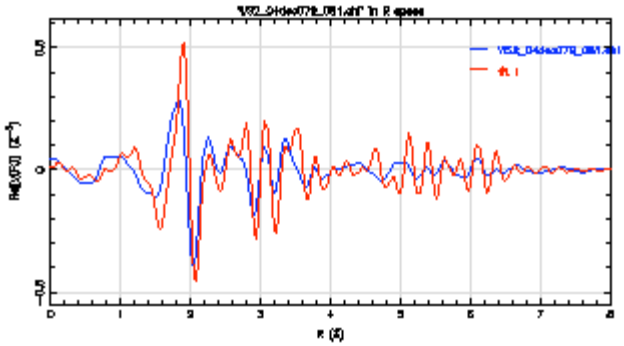
ws2-bulk1.apj

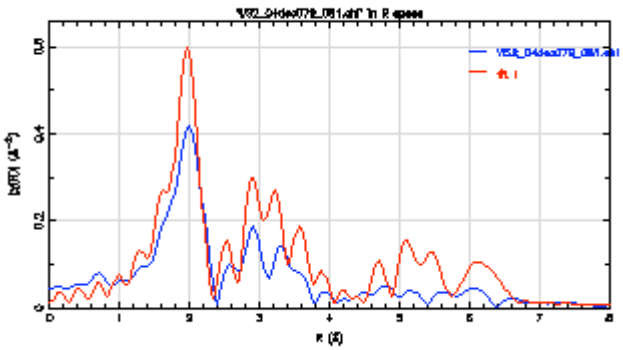
Decisions, Decisions

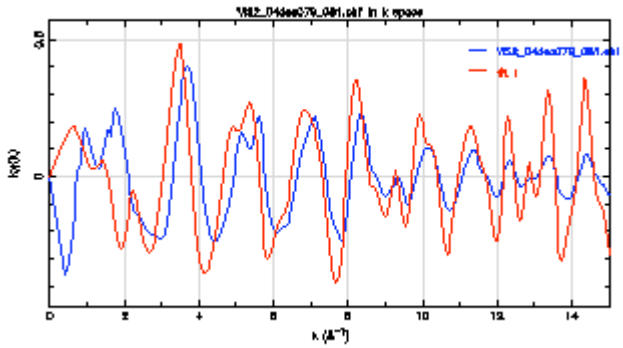
- Keep all the paths
  - go onto the next slide
- Keep only the “big” paths
  - skip to slide 27

Bulk WS_2: How many paths can we eliminate?





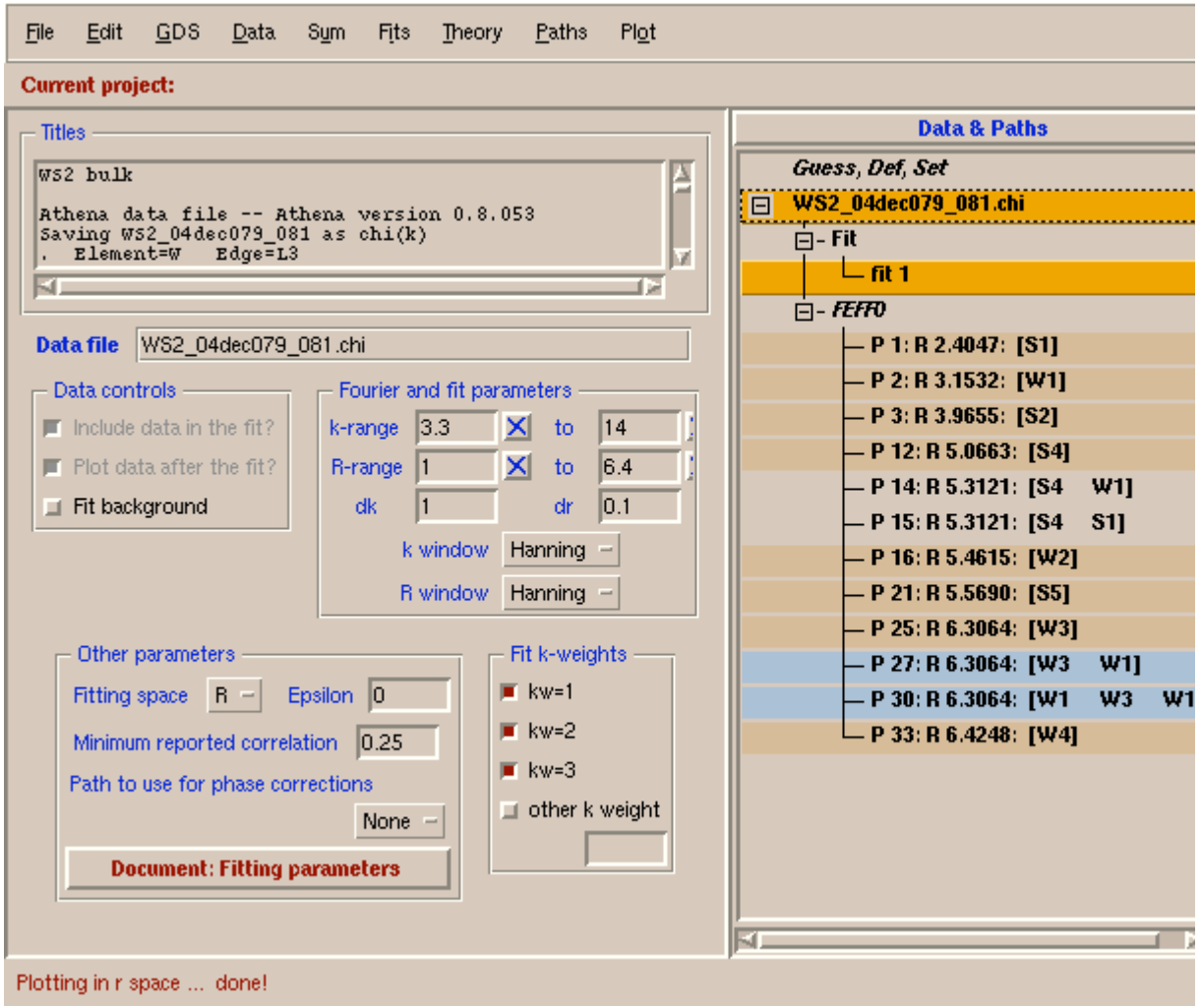


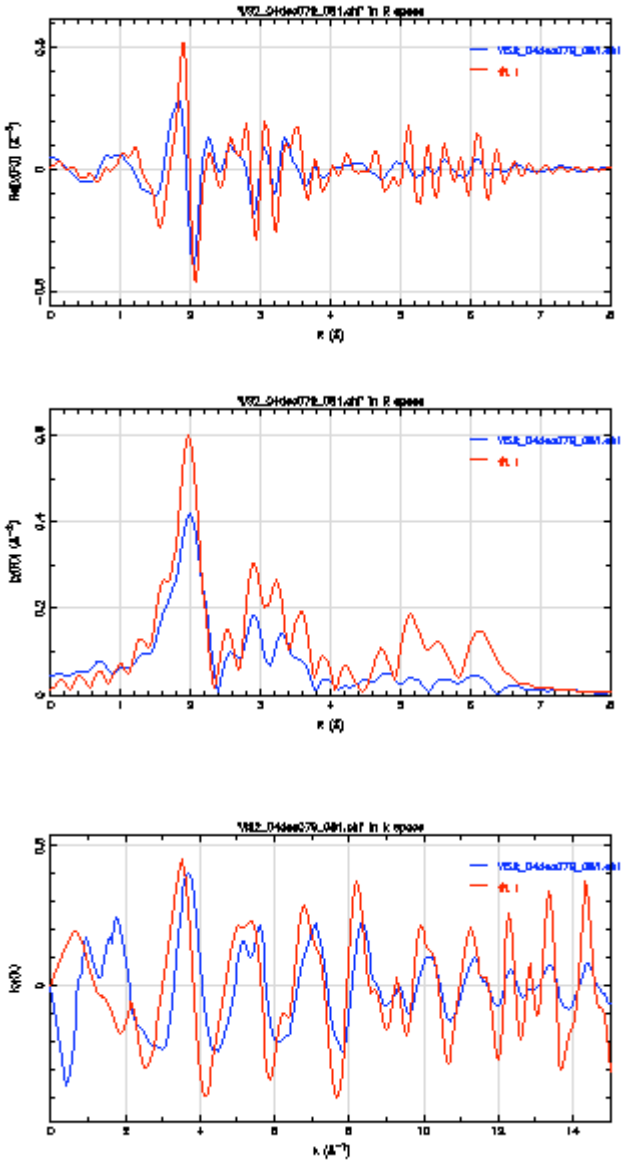


- Use FEFF relative amplitude term to decrease the number of paths.
  - Cutoff at 5%: This keeps all single scattering paths and linear multiple scattering paths.
  - Structure in the data is still present in the model.

`ws2-bulk2-amp5.apj`

Bulk WS_2: How many paths can we eliminate?





- Use FEFF relative amplitude term to decrease the number of paths.
  - Cutoff at 10%: This keeps all single scattering paths and linear multiple scattering paths.
  - Structure in the data is still present in the model.

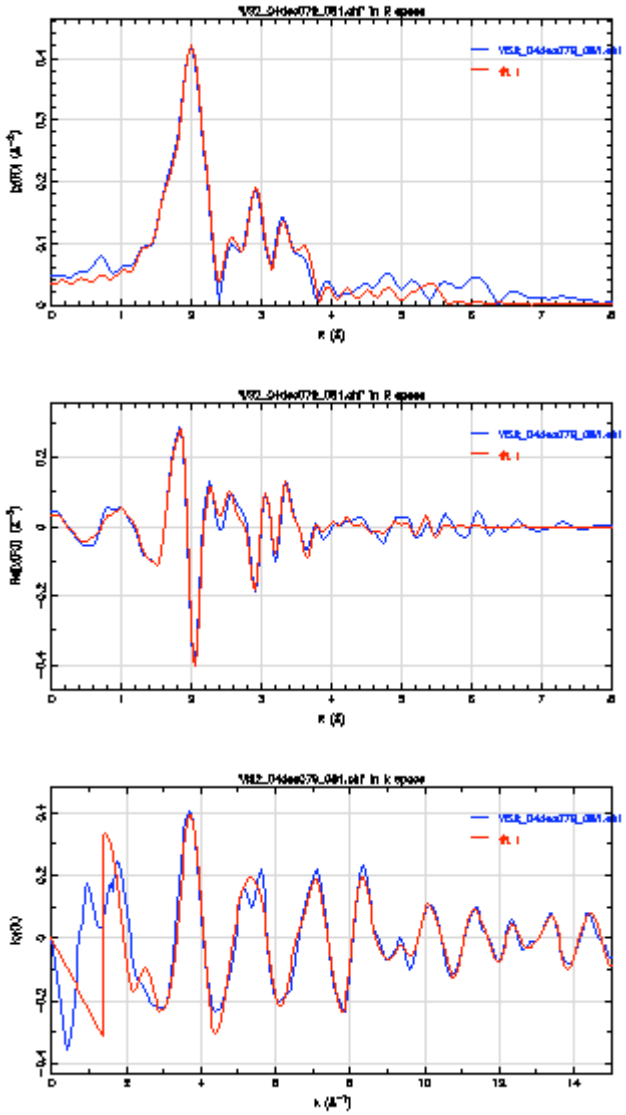
ws2-bulk3-amp10.apj

Bulk WS_2: Model WS_2 with as few variables as possible

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title     :  Fitting WS2_04dec079_081.chi
Comment           :  Fit #1
Prepared by       :
Contact           :
Started           :  12:37:04 on 9 July, 2007
This fit at       :  12:37:49 on 9 July, 2007
Environment       :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit   :  1

------------------------------------------------------------

Independent points           =      36.401367188
Number of variables          =       9.000000000
Chi-square                   =  144139.981035478
Reduced Chi-square           =    5260.320773382
R-factor                     =       0.038557521
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
!!
!! Uncertainties could not be estimated.
!!

Guess parameters +/- uncertainties  (initial guess):
  enot             =      7.3231170   +/-       0.0000000     (7.3212)
  s_02             =      0.8799000   +/-       0.0000000     (0.8797)
  alpha            =      0.0014620   +/-       0.0000000     (0.0015)
  sigs1            =      0.0025010   +/-       0.0000000     (0.0025)
  sigs2            =      0.0053490   +/-       0.0000000     (0.0054)
  sigs4            =      2.2804790   +/-       0.0000000     (2.2805)
  sigw1            =      0.0025770   +/-       0.0000000     (0.0026)
  sigw2            =     -0.0030720   +/-       0.0000000     (-0.0031)
  sigw3            =   -272.3234680   +/-       0.0000000     (-272.323

Correlations between variables:
All other correlations are below 0.25
```



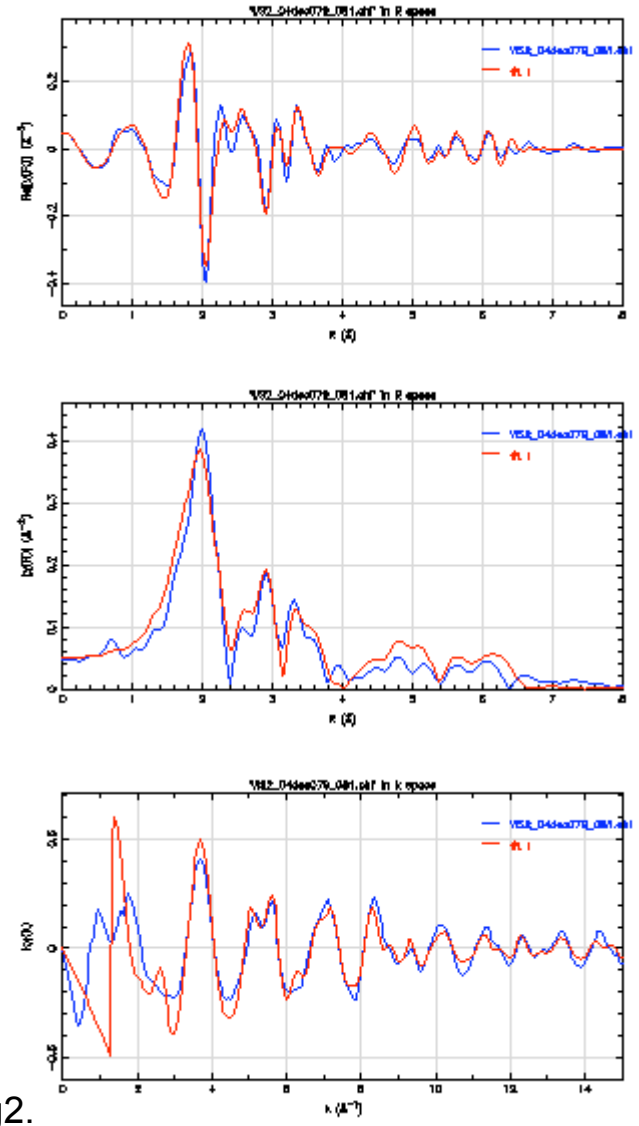
- Model includes e0, alpha*reff, and 6 σ^2 terms.
- Model fails at large R because restriction on ΔR is too strong

Bulk WS_2: Model WS_2 relaxing constraint on delr

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title     :  Fitting WS2_04dec079_081.chi
Comment           :  Fit #1
Prepared by       :
Contact           :
Started           :  12:41:29 on 9 July, 2007
This fit at       :  12:41:50 on 9 July, 2007
Environment       :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit   :  1

-------------------------------------------------------------

Independent points           =      36.401367188
Number of variables          =      12.000000000
Chi-square                   =     427344.123
Reduced Chi-square           =   17513.122093724
R-factor                     =       0.121995343
Measurement uncertainty (k)  =       0.000161388
Measurement uncertainty (R)  =       0.000432548
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
   enot             =     6.3243200   +/-       1.2941090     (6.3327)
   s_02             =     1.3493790   +/-       0.1006830     (1.3494)
   dels1            =    -0.0038970   +/-       0.0125000     (-0.0038)
   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)
   dels5            =     0.0296260   +/-       0.0371610     (0.0297)
   delw1            =     0.0107270   +/-       0.0106580     (0.0107)
   delw2            =    -0.0318760   +/-       0.0454950     (-0.0320)
   delw3            =     0.0499580   +/-       0.0280620     (0.0503)
   delw4            =    -0.2720220   +/-       0.0573720     (-0.2718)

Set parameters:
   sigs1            =  0.008380
   sigs2            =  0.009596
   sigs4            =  0.005101
   sigw1            =  0.005474
   sigw2            =  0.005408
   sigw3            =  0.0050282


Correlations between variables:
```



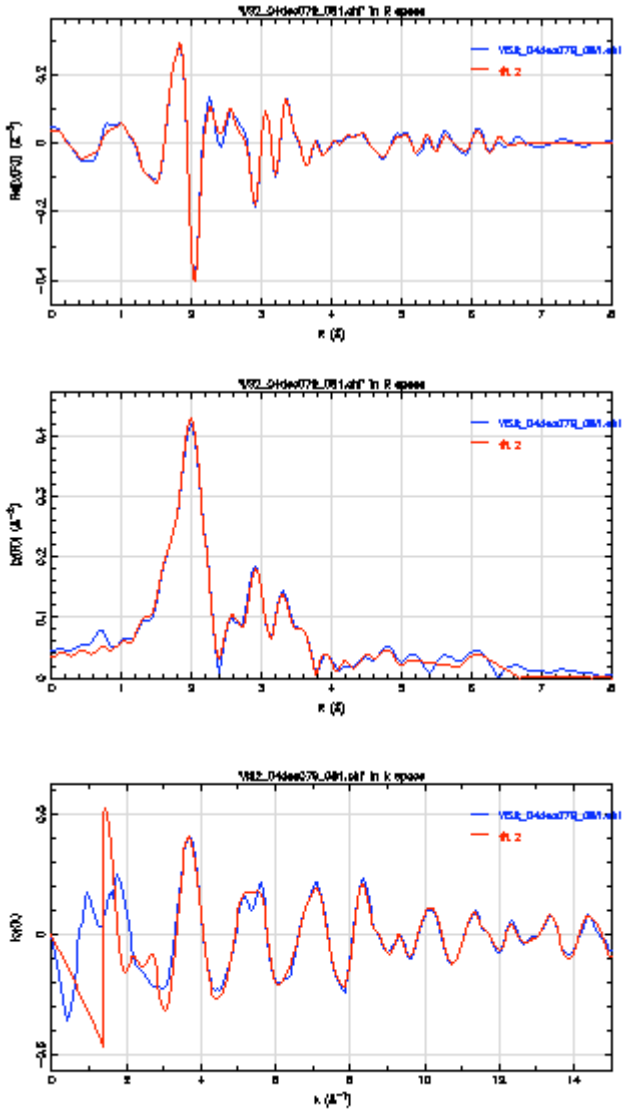
- Model includes e0,10 ΔR terms, set 6 σ^2 terms to ~0.005 Ang2.
- Model works fairly well, now that ΔR are close, vary all params

Bulk WS_2: Model WS_2 relaxing constraint on delr

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

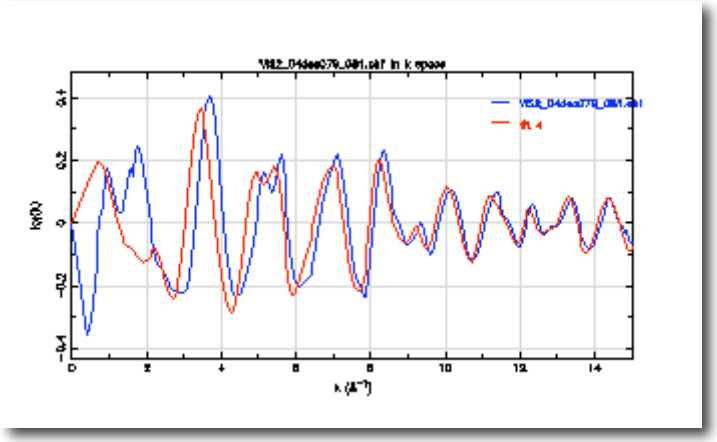
Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2_04dec079_081.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  12:45:38 on 9 July, 2007
This fit at      :  12:47:02 on 9 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit  :  2

------------------------------------------------------------

Independent points           =      36.401367188
Number of variables          =      18.000000000
Chi-square                   =   43315.563177051
Reduced Chi-square           =    2353.931788638
R-factor                     =       0.011819824
Measurement uncertainty (k)  =       0.000161388
Measurement uncertainty (R)  =       0.000432548
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =     7.1436230   +/-       0.4943730     (0.0000)
  s_02             =     0.8927770   +/-       0.0449740     (0.8836)
  sigs1            =     0.0025740   +/-       0.0004100     (0.0025)
  sigs2            =     0.0039670   +/-       0.0012470     (0.0048)
  sigs4            =     0.0246940   +/-       0.0063430     (0.0183)
  sigw1            =     0.0026340   +/-       0.0002810     (0.0026)
  sigw2            =     0.0028640   +/-       0.0009650     (0.0034)
  sigw3            =     0.0050980   +/-       0.0014160     (0.0062)
  dels1            =    -0.0029720   +/-       0.0033710     (-0.0057)
  dels2            =    -0.0126710   +/-       0.0120090     (-0.0087)
  dels4            =    -0.8637700   +/-       0.0413950     (-0.3256)
  dels4w1          =    -0.1700870   +/-       0.0838860     (-0.2590)
  dels4s1          =    -0.2497940   +/-       0.1254600     (-0.2973)
  dels5            =     0.0606240   +/-       0.1020410     (0.0502)
  delw1            =     0.0083950   +/-       0.0030080     (0.0063)
  delw2            =     0.0132480   +/-       0.0116360     (0.0112)
  delw3            =     0.0405430   +/-       0.0146790     (0.0457)
  delw4            =    -0.5438930   +/-       0.0292780     (-0.2395)


Correlations between variables:
       s_02 and sigs1       -->  0.8126
       enot and dels1       -->  0.7281
```

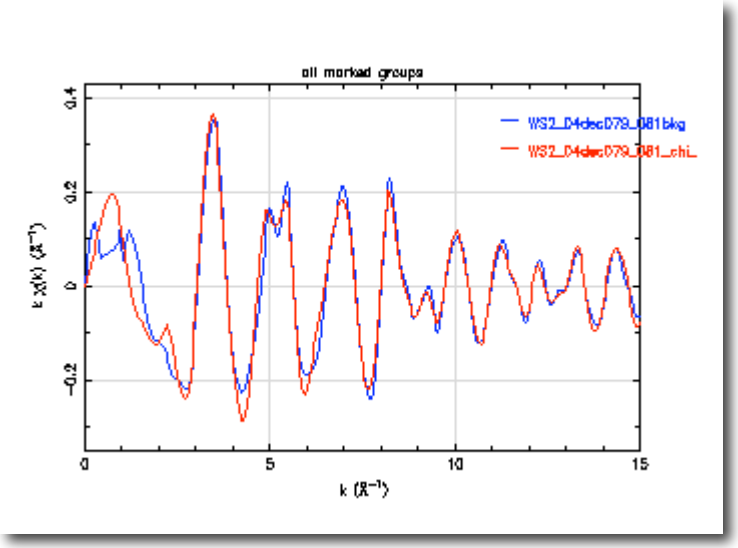


- Model includes e0,10 ΔR terms, 6 σ^2 terms.
- Model works fairly well.

Bulk WS_2: 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

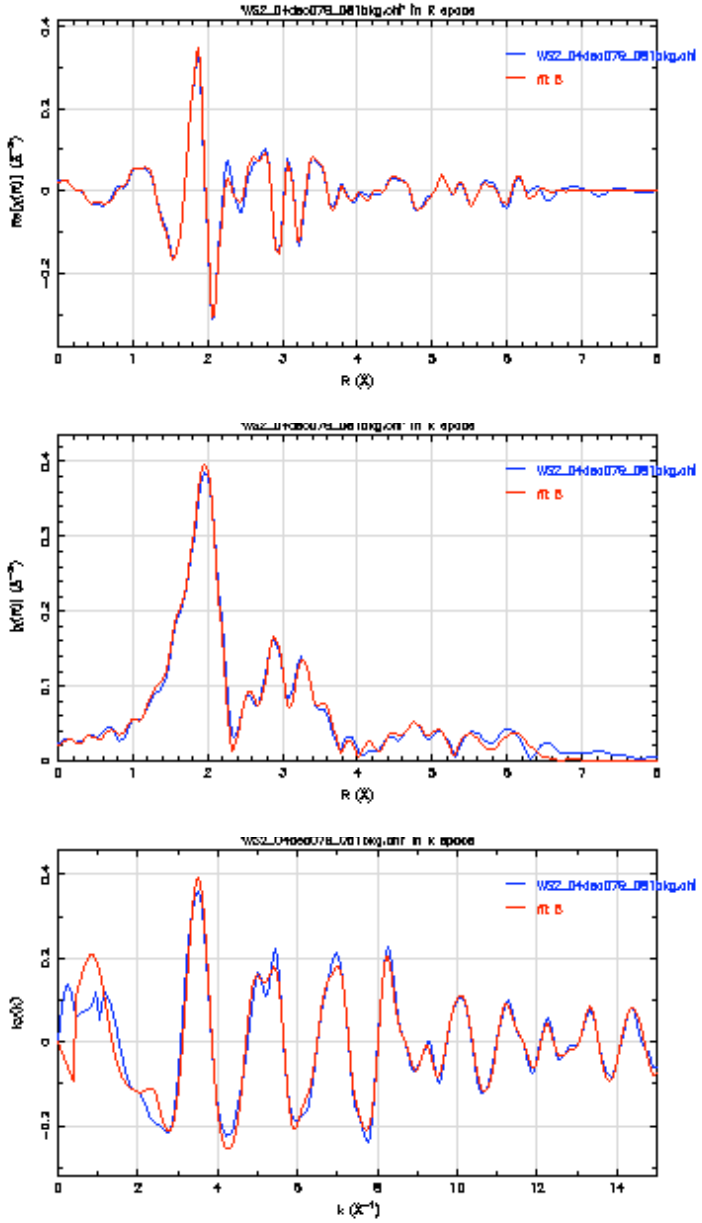
`ws2-bkg.prj`

Bulk WS_2: Making a theory for pretty background removal

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2_04dec079_081.chi
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

============================================================

Independent points           =      36.401367188
Number of variables          =      18.000000000
Chi-square                   =   47831.822404141
Reduced Chi-square           =    2599.362423279
R-factor                     =       0.014139526
Measurement uncertainty (k)  =       0.000161333
Measurement uncertainty (R)  =       0.000432403
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =     0.7593290   +/-       0.5887570     (0.0000)
  s_02             =     0.8759420   +/-       0.0490590     (guessed
  sigs1            =     0.0024960   +/-       0.0004350     (guessed
  sigs2            =     0.0046840   +/-       0.0014430     (guessed
  sigs4            =     0.0199540   +/-       0.0106960     (guessed
  sigw1            =     0.0026180   +/-       0.0002960     (guessed
  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   +/-       0.0921570     (guessed
  dels4w1          =    -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


Correlations between variables:
        s_02 and sigs1       -->  0.8144
```



- Beautiful background
- too Many ΔR values highly unsatisfactory.....

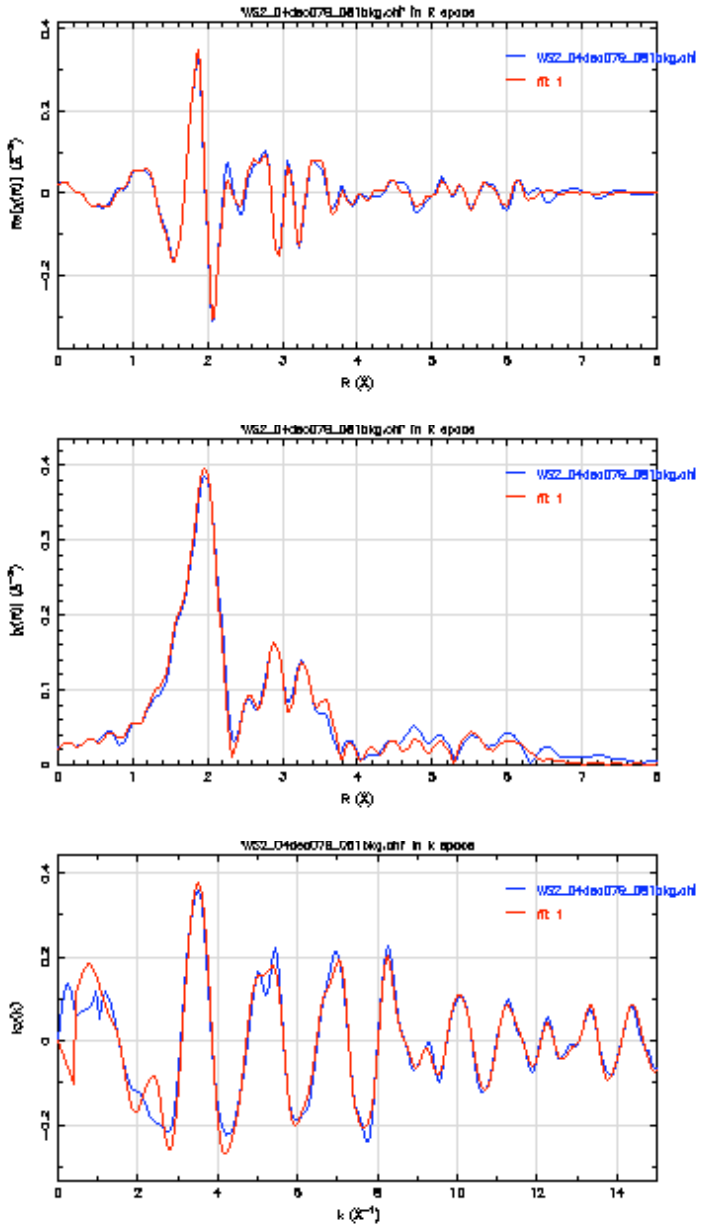
ws2-vars2d.apj

Bulk WS_2: Reformulate ΔR list in terms of unit cell parameters

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2_04dec079_081bkg.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  13:06:29 on 9 July, 2007
This fit at      :  13:08:07 on 9 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit  :  1

------------------------------------------------------------

Independent points           =      36.401367188
Number of variables          =      12.000000000
Chi-square                   =   59713.930562177
Reduced Chi-square           =    2447.155116487
R-factor                     =       0.017650277
Measurement uncertainty (k)  =       0.000161333
Measurement uncertainty (R)  =       0.000432403
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =      0.7683830   +/-       0.5653740     (0.6649)
  s_02             =      0.8816770   +/-       0.0486940     (0.8834)
  sigs1            =      0.0025410   +/-       0.0004250     (0.0026)
  sigs2            =      0.0051770   +/-       0.0014840     (0.0052)
  sigs4            =      0.1438630   +/-       4.4316550     (0.0050)
  sigs5            =      0.0322980   +/-       0.0473520     (0.0050)
  sigw1            =      0.0026660   +/-       0.0002890     (0.0027)
  sigw2            =      0.0033220   +/-       0.0012440     (0.0034)
  sigw3            =      0.0052420   +/-       0.0013970     (0.0055)
  da               =      0.0072600   +/-       0.0028860     (0.0070)
  dc               =      0.4114840   +/-       0.1255630     (0.4994)
  ds1z             =      0.0051340   +/-       0.0012720     (0.0060)

Def parameters (using "FEFF0: P 1: R 2.4047:  [S1]"):
  s1_2z            =      0.1276340
  s1_3z            =      0.3723660
  s1_4z            =      0.8723660
  a                =      3.1604600
  b                =      3.1604600
  c                =     12.7344840
  d0x              =      0.0000000
  d0y              =      0.0000000
  d0z              =      0.0000000
```



MS paths do not contribute because of large sigma values

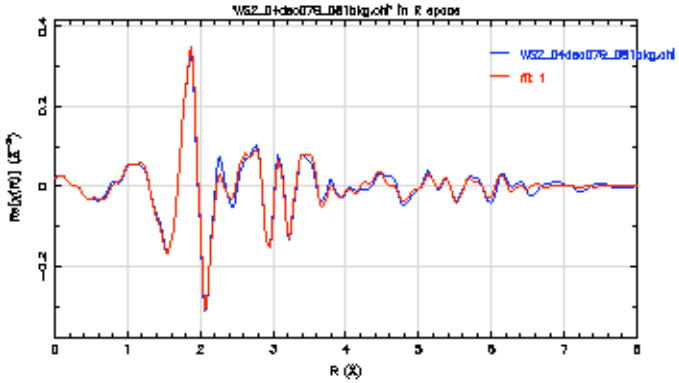
ws2-bulk-uc2.apj

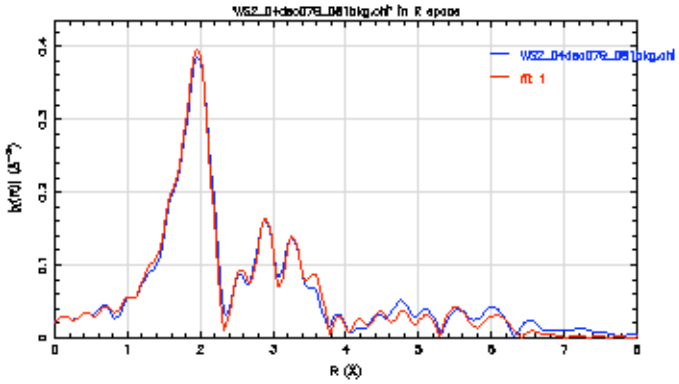
Bulk WS_2: Reformulate ΔR list in terms of unit cell parameters

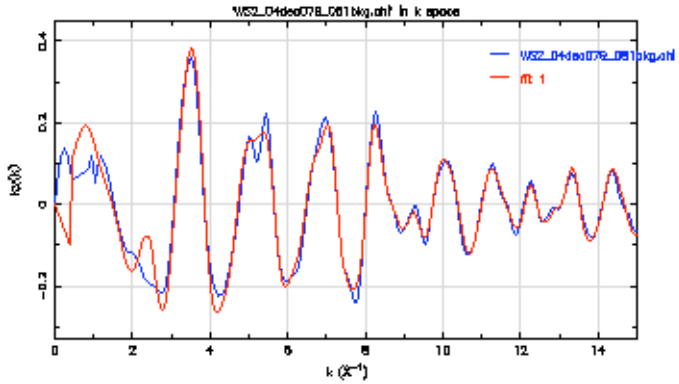
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2_04dec079_081bkg.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  13:14:12 on 9 July, 2007
This fit at      :  13:15:01 on 9 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit  :  1

------------------------------------------------------------

Independent points           =      36.401367188
Number of variables          =      10.000000000
Chi-square                   =   60719.764164219
Reduced Chi-square           =    2299.871962425
R-factor                     =       0.017944873
Measurement uncertainty (k)  =       0.000161333
Measurement uncertainty (R)  =       0.000432403
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =      0.7332520   +/-       0.4972210     (0.6808)
  s_02             =      0.8801200   +/-       0.0448530     (0.8821)
  sigs1            =      0.0025320   +/-       0.0004010     (0.0025)
  sigs2            =      0.0051660   +/-       0.0014340     (0.0052)
  sigw1            =      0.0026570   +/-       0.0002730     (0.0027)
  sigw2            =      0.0033690   +/-       0.0011960     (0.0034)
  sigw3            =      0.0055440   +/-       0.0014310     (0.0055)
  da               =      0.0072510   +/-       0.0027340     (0.0071)
  dc               =      0.5146890   +/-       0.1757690     (0.5032)
  ds1z             =      0.0061430   +/-       0.0016870     (0.0060)

Def parameters (using "FEFF0: P 1: R 2.4047:  [S1]"):
  s1_2z            =      0.1286430
  s1_3z            =      0.3713570
  a                =      3.1604510
  b                =      3.1604510
  c                =     12.8376890
  d0x              =      0.0000000
  d0y              =      0.0000000
  d0z              =      0.0000000
  d1x              =      0.3333400
  d1y              =      0.3333400
  d1z              =      0.5000000
```

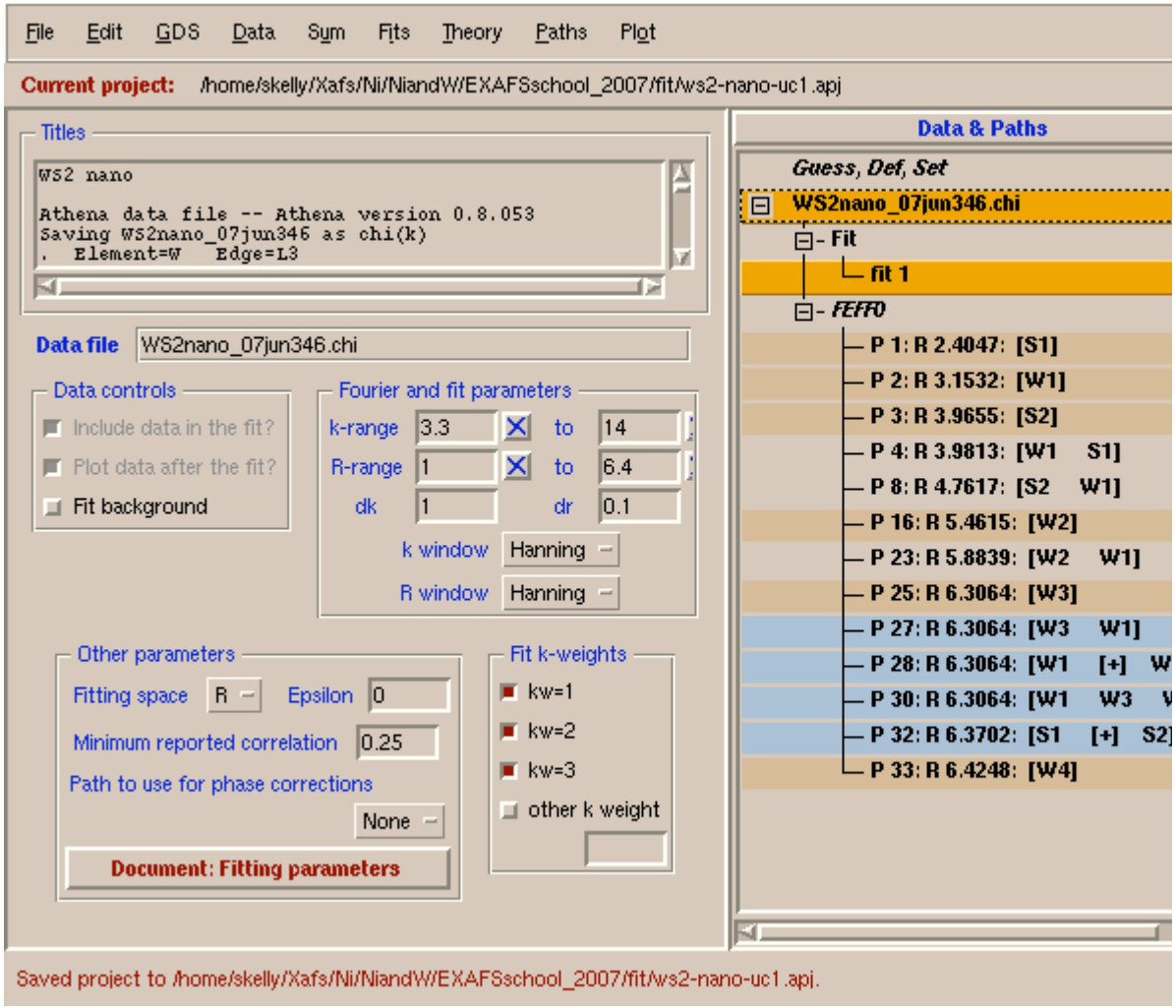


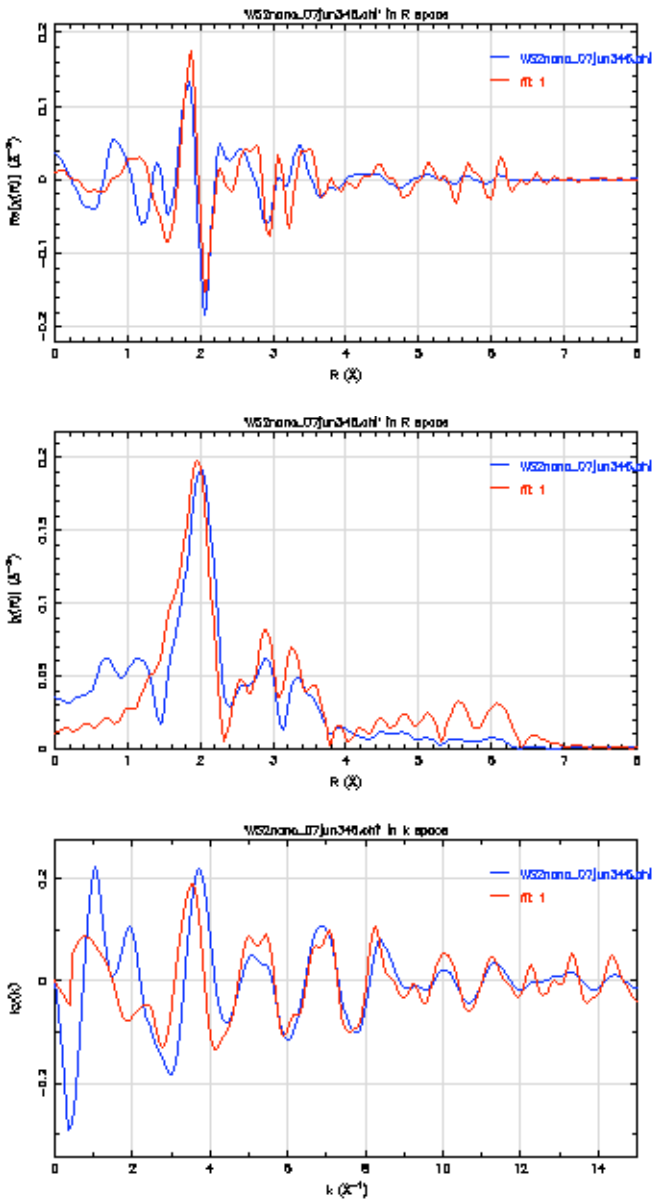




ws2-bulk-ucb.apj

nano WS_2: Compare model and data

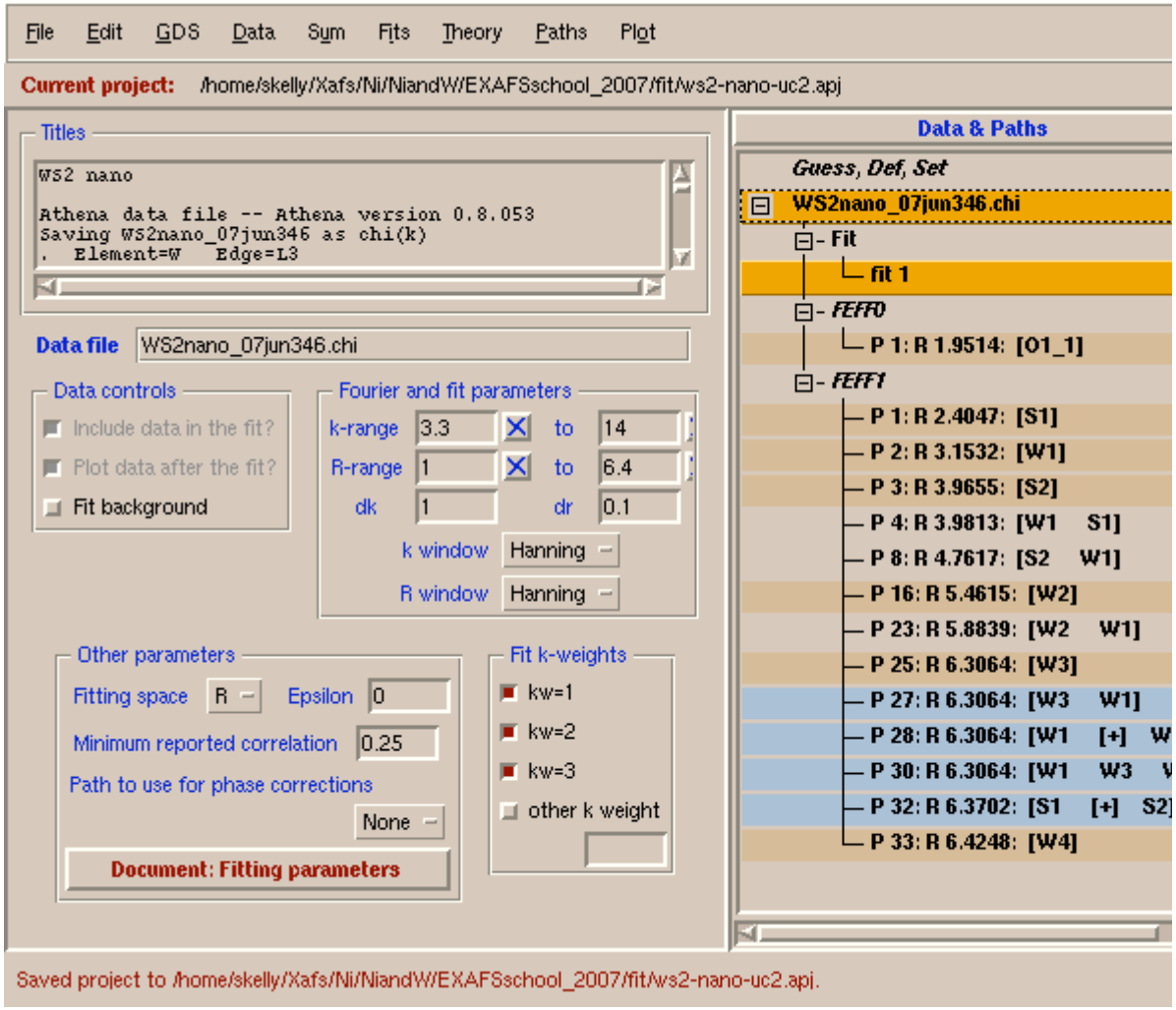


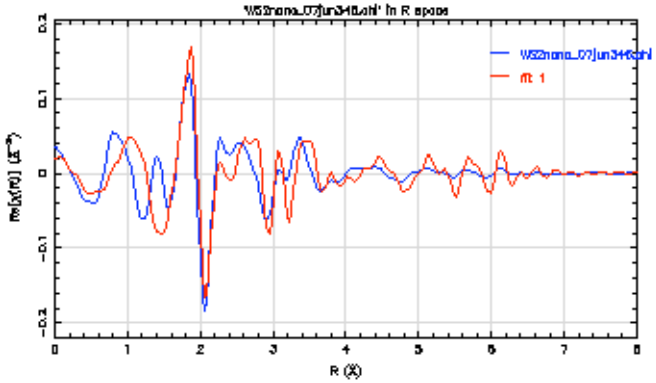


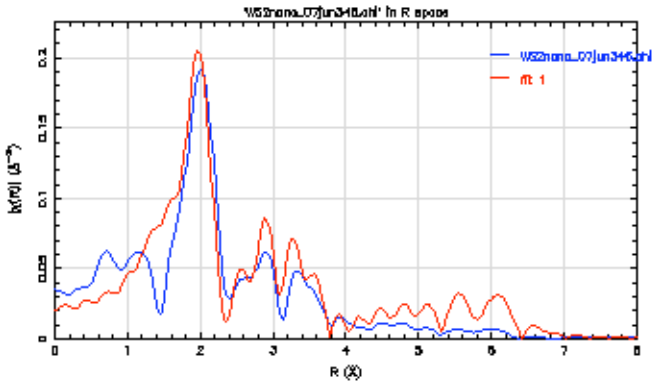
- Sum paths with previous bulk values and CN ~50% of bulk values
- need to add short oxygen signal

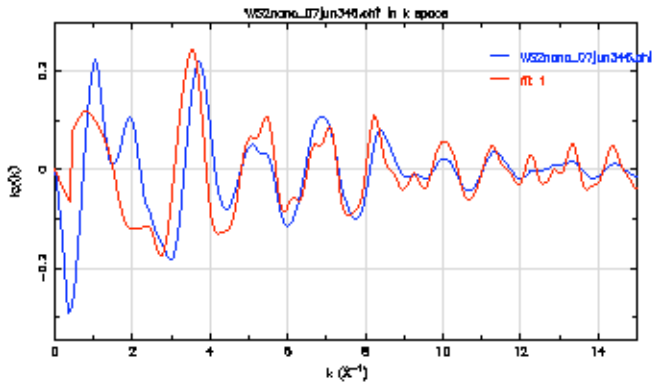
ws2-nano-uc1.apj

nano WS_2: Adding W-O signal





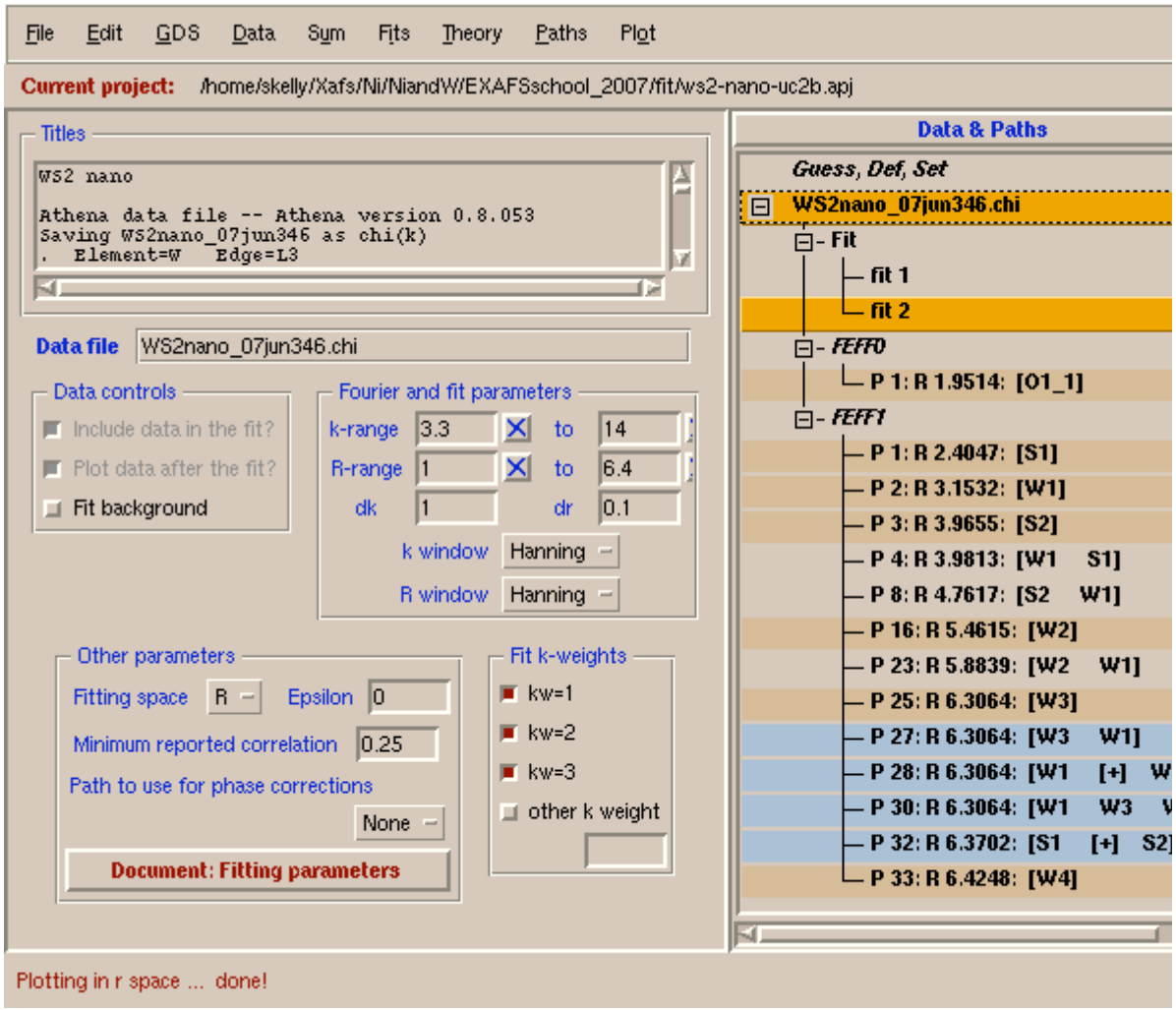


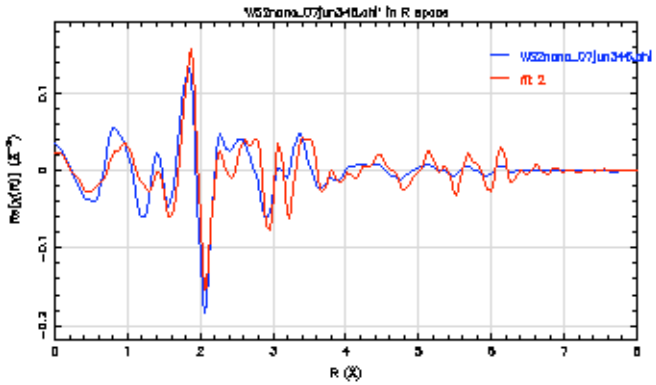


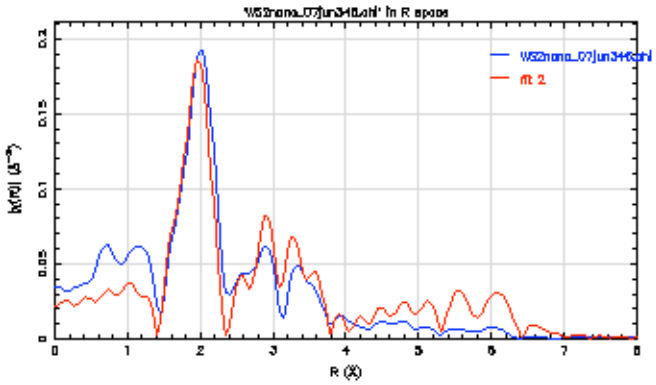
- No1=1, delo1=0, sigo1=0
- need to shift oxygen signal -0.15 Ang

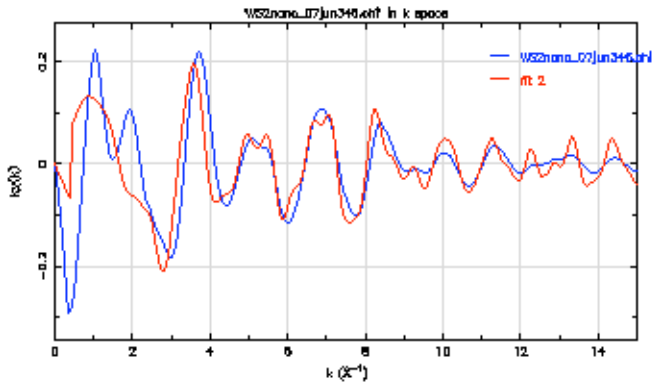
ws2-nano-uc2.apj

nano WS_2: Move W-O signal









- No1=1, delo1=-0.15, sigo1=0
- need to optimize parameters

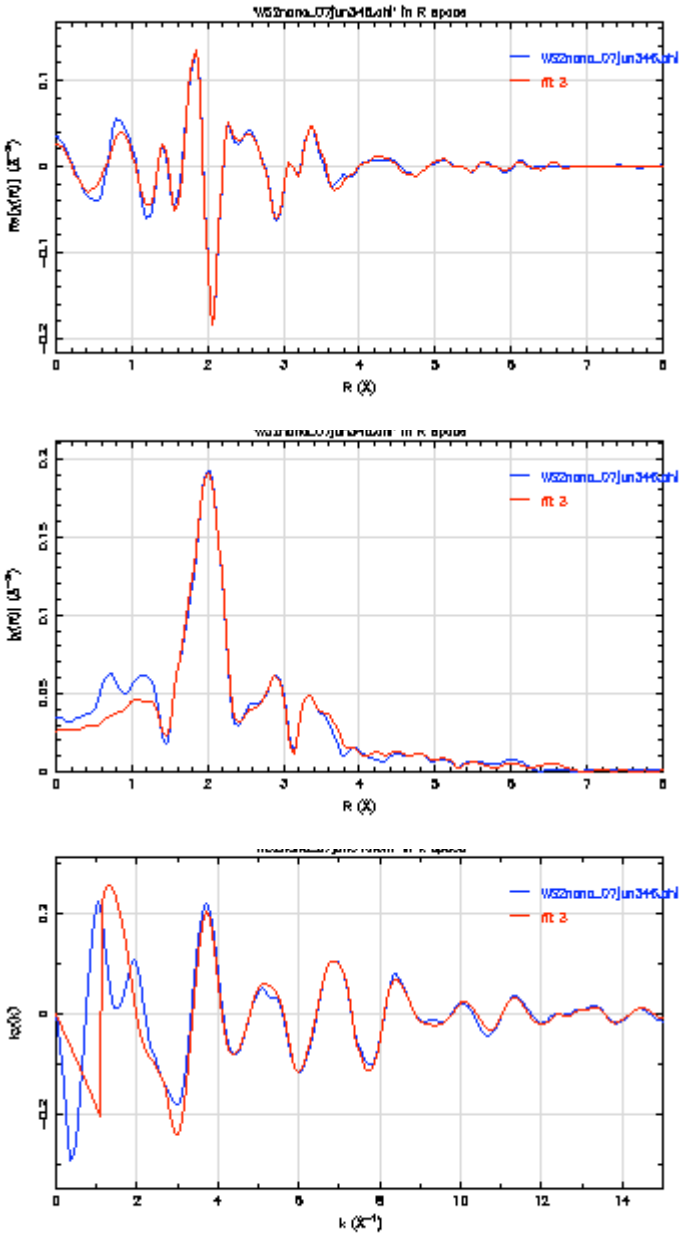
ws2-nano-uc2b.apj

nano WS_2: optimize parameters

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

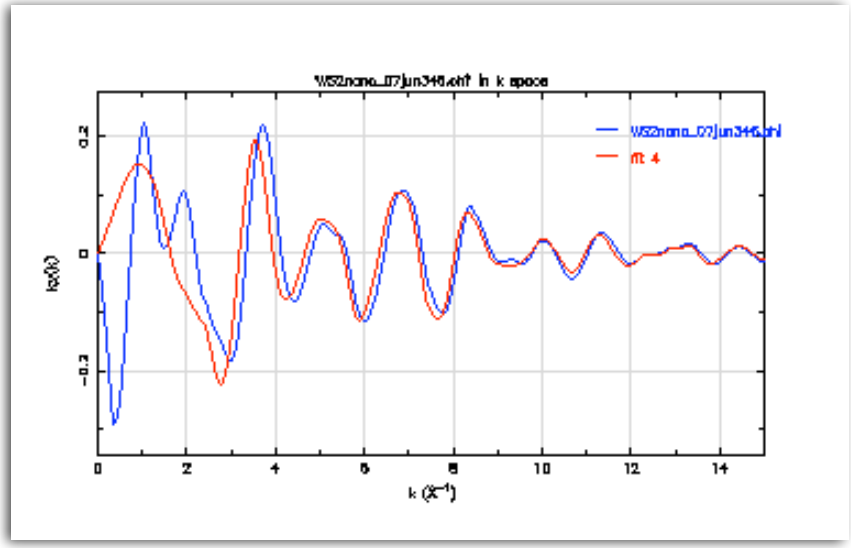
```
Project title     :  Fitting Ws2nano_07jun346.chi
Comment           :  Fit #1
Prepared by       :
Contact           :
Started           :  13:23:18 on 9 July, 2007
This fit at       :  13:31:15 on 9 July, 2007
Environment       :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit   :  3

------------------------------------------------------------

Independent points               =      36.401367188
Number of variables              =      18.000000000
Chi-square                       =  104858.309963899
Reduced Chi-square               =    5698.397781831
R-factor                         =       0.015294443
Measurement uncertainty (k)      =       0.000037342
Measurement uncertainty (R)      =       0.000100084
Number of data sets              =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =     4.8660740   +/-       0.5681080     (0.6808)
  sigs1            =     0.0043040   +/-       0.0005230     (0.0025)
  sigs2            =     0.0185730   +/-       0.0079470     (0.0052)
  sigw1            =     0.0055830   +/-       0.0012770     (0.0027)
  sigw2            =    -0.0010020   +/-       0.0149970     (0.0034)
  sigw3            =     0.0083360   +/-       0.0121140     (0.0055)
  da               =     0.0017510   +/-       0.0068210     (0.0071)
  dc               =     0.4750370   +/-       0.1902890     (0.5032)
  ds1z             =     0.0046830   +/-       0.0018780     (0.0060)
  ns1              =     3.5949700   +/-       0.2093210     (3.0000)
  nw1              =     2.3805920   +/-       0.6109970     (3.0000)
  ns2              =     5.3561670   +/-       2.4929180     (3.0000)
  nw2              =     0.3719320   +/-       1.5518340     (3.0000)
  nw3              =    -1.0876670   +/-       1.7557080     (6.0000)
  nw4              =     5.4086450   +/-       8.7709550     (6.0000)
  no1              =     1.2131890   +/-       0.1821170     (1.0000)
  delo1            =    -0.1711470   +/-       0.0052930     (-0.1500)
  sigo1            =     0.0028900   +/-       0.0013850     (0.0050)

Def parameters (using "FEFF0: P 1: R 1.9514:  [01_1]"):
  s1_2z            =     0.1271830
  s1_3z            =     0.3728170
```

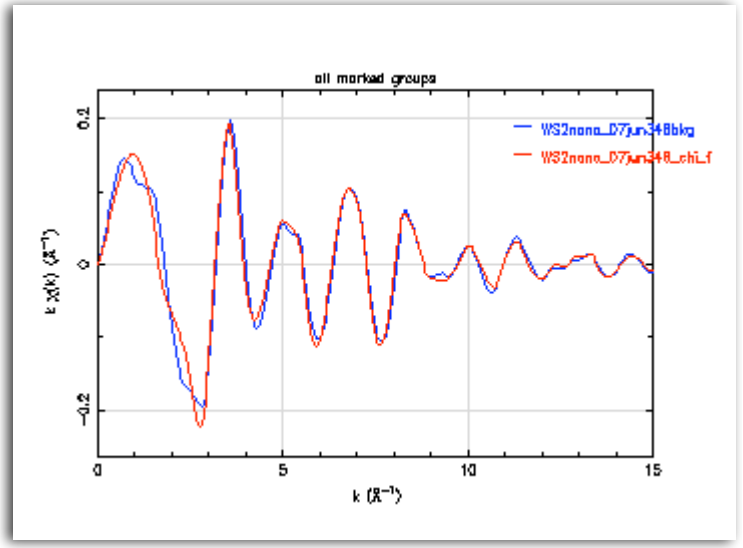


- need to fix background

ws2-nano-uc2c.apj

nano WS_2: 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 Athena
- Make new background for data

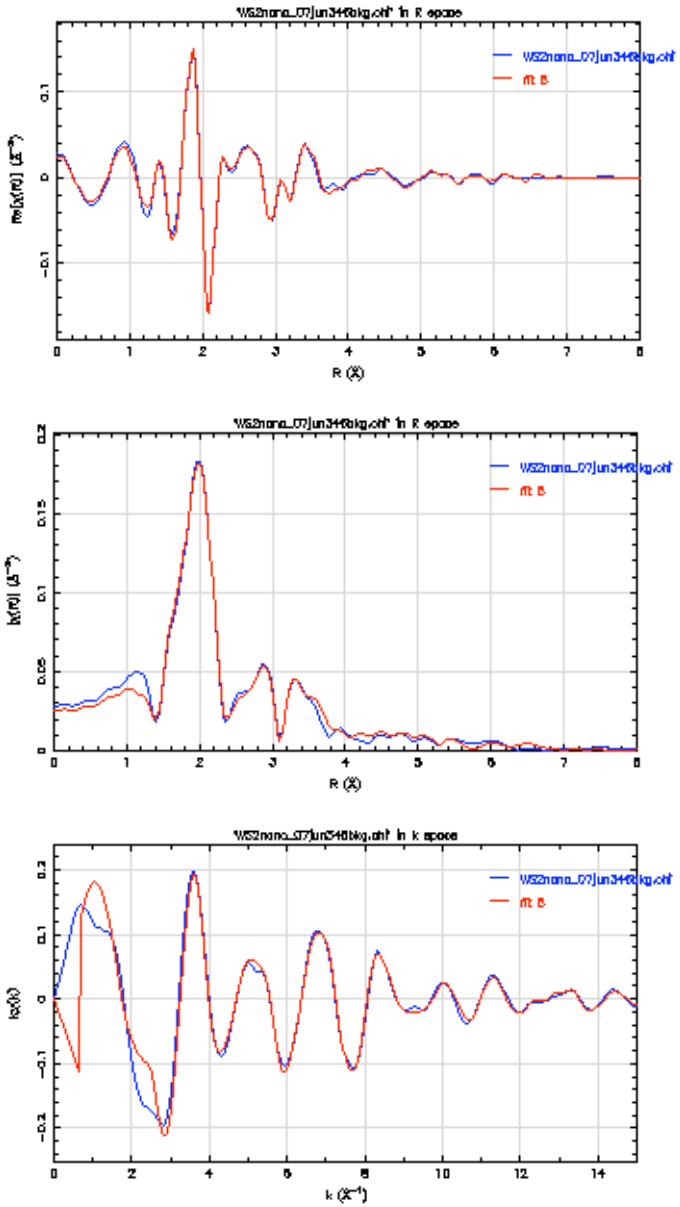
ws2-nano-bkg.prj

nano WS_2 : Refining the model

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2nano_07jun346.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  13:23:18 on 9 July, 2007
This fit at      :  13:41:07 on 9 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit  :  5

------------------------------------------------------------

Independent points           =      36.401367188
Number of variables          =      18.000000000
Chi-square                   =   86981.135954150
Reduced Chi-square           =    4726.884424829
R-factor                     =       0.013848613
Measurement uncertainty (k)  =       0.000036481
Measurement uncertainty (R)  =       0.000097776
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =     1.6902760   +/-       0.5448750     (0.0000)
  sigs1            =     0.0041310   +/-       0.0004820     (guessed
  sigs2            =     0.0192240   +/-       0.0072930     (guessed
  sigw1            =     0.0055470   +/-       0.0011680     (guessed
  sigw2            =     0.0018550   +/-       0.0132430     (guessed
  sigw3            =     0.0075330   +/-       0.0099620     (guessed
  da               =     0.0027220   +/-       0.0062390     (guessed
  dc               =     0.4888730   +/-       0.1932460     (guessed
  ds1z             =     0.0046890   +/-       0.0019010     (guessed
  ns1              =     3.4715650   +/-       0.1917730     (guessed
  nw1              =     2.3463510   +/-       0.5571650     (guessed
  ns2              =     5.6909970   +/-       2.4440560     (guessed
  nw2              =     0.4502380   +/-       1.6031410     (guessed
  nw3              =     1.0117040   +/-       1.5065430     (guessed
  nw4              =     4.0819410   +/-       6.5422230     (guessed
  no1              =     1.0457450   +/-       0.1495530     (guessed
  delo1            =    -0.1743200   +/-       0.0050360     (guessed
  sigo1            =     0.0020800   +/-       0.0012140     (guessed

Def parameters (using "FEFF0: P 1: R 1.9514:  [01_1]"):
  s1_2z            =     0.1271890
  s1_3z            =     0.3728110
```



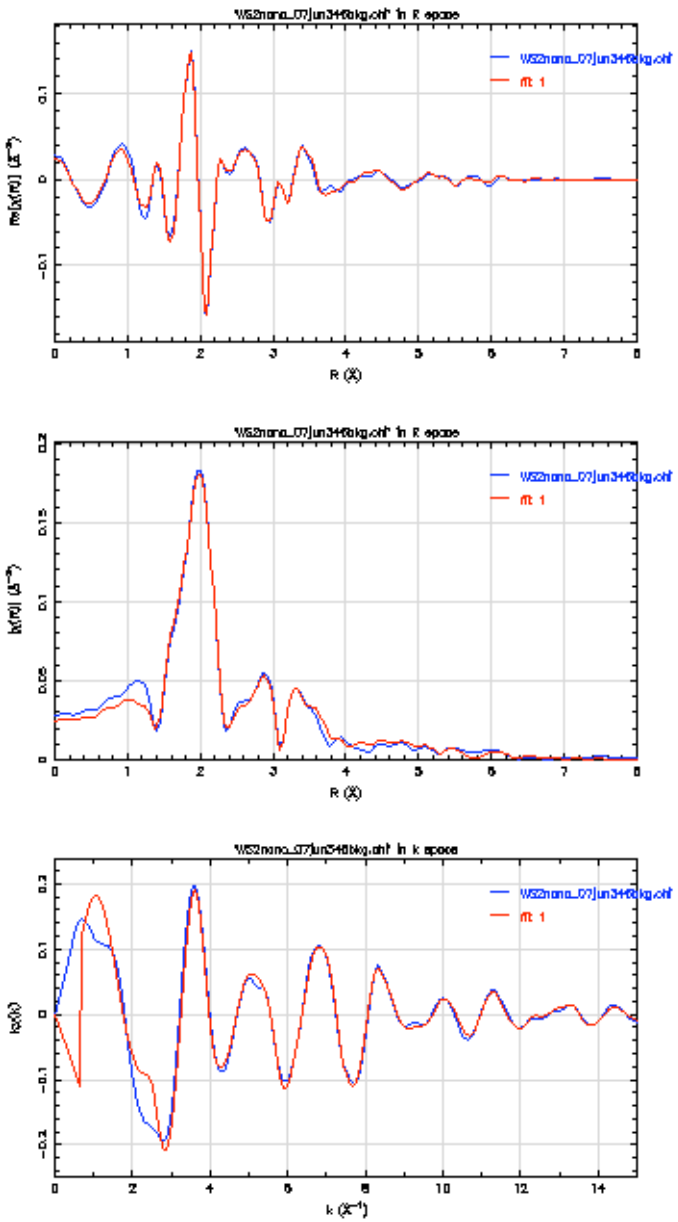
ws2-nano-uc3b.apj

nano WS_2 : Refining the model

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2nano_07jun346bkg.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  13:44:38 on 9 July, 2007
This fit at      :  13:45:17 on 9 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 8
Figure of merit  :  1

------------------------------------------------------------

Independent points           =      10.816406250
Number of variables          =       5.000000000
Chi-square                   =    6538.889730369
Reduced Chi-square           =    1124.214755523
R-factor                     =       0.235362466
Measurement uncertainty (k)  =       0.000036481
Measurement uncertainty (R)  =       0.000097776
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
   sigw2             =      0.0044960   +/-       0.0079210     (0.0045)
   sigw3             =      0.0075700   +/-       0.0035760     (0.0076)
   nw2               =      0.8248320   +/-       1.5519620     (0.8240)
   nw3               =      1.2075320   +/-       0.6821310     (1.2083)
   nw4               =      2.2013950   +/-       1.9160020     (2.1990)

Def parameters (using "FEFF0: P 1: R 1.9514:  [01_1]"):
   s1_2z             =      0.1272350
   s1_3z             =      0.3727650
   a                 =      3.1561530
   b                 =      3.1561530
   c                 =     12.8201570
   d0x               =      0.0000000
   d0y               =      0.0000000
   d0z               =      0.0000000
   d1x               =      0.3333400
   d1y               =      0.3333400
   d1z               =      0.5000000
   d3x               =      0.3333400
   d3y               =      0.3333400
   d3z               =      0.1227650
   d4x               =      0.3333400
   d4y               =      0.3333400
```

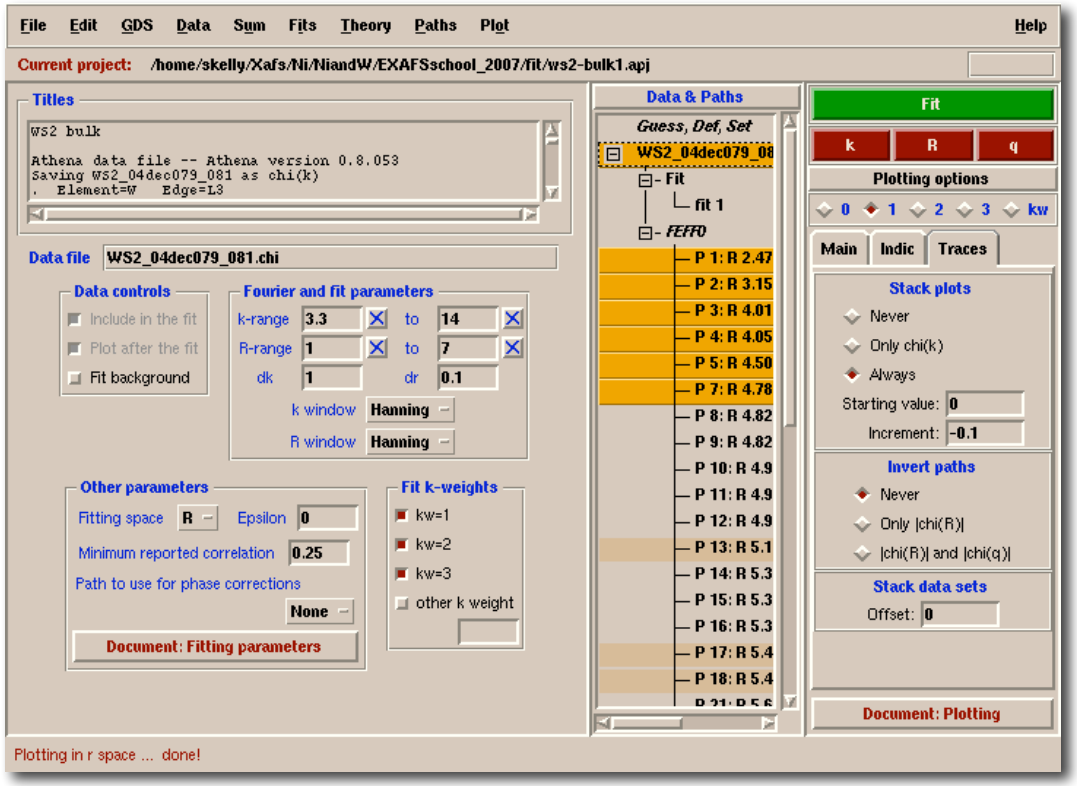


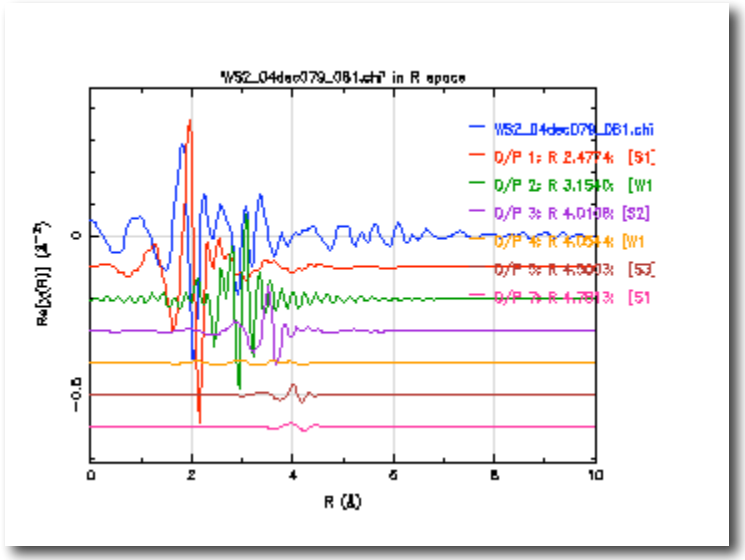
- determine Nw2, Nw3, and Nw4
- Model fit region from 5 to 6.4 Ang

ws2-nano-uc4.apj

Done
and
Starting over using just the
BiG paths

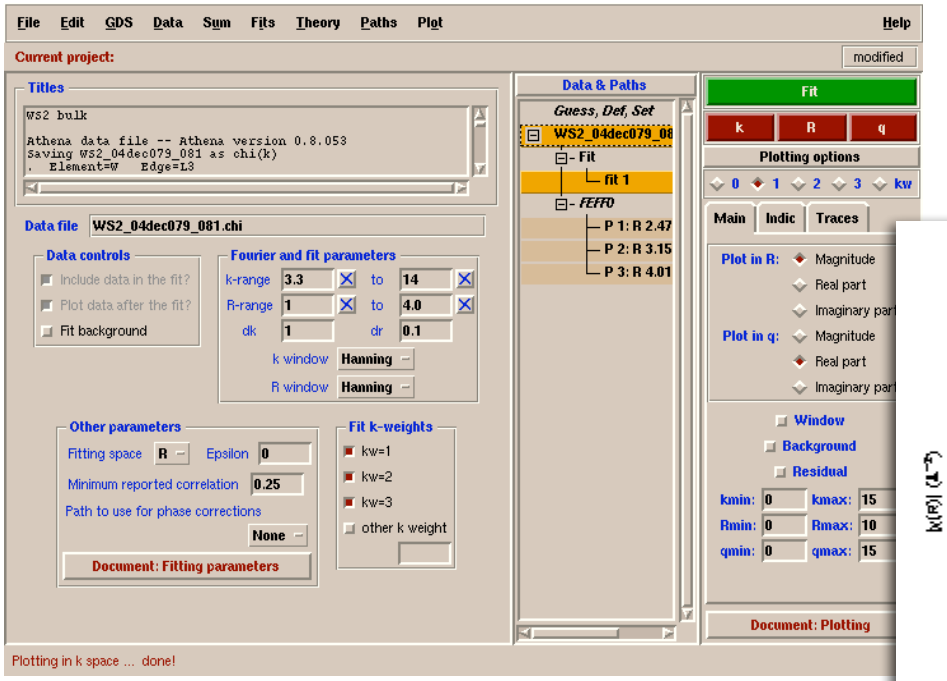
Bulk WS_2 : Look for big paths and a region in R where paths do not overlap

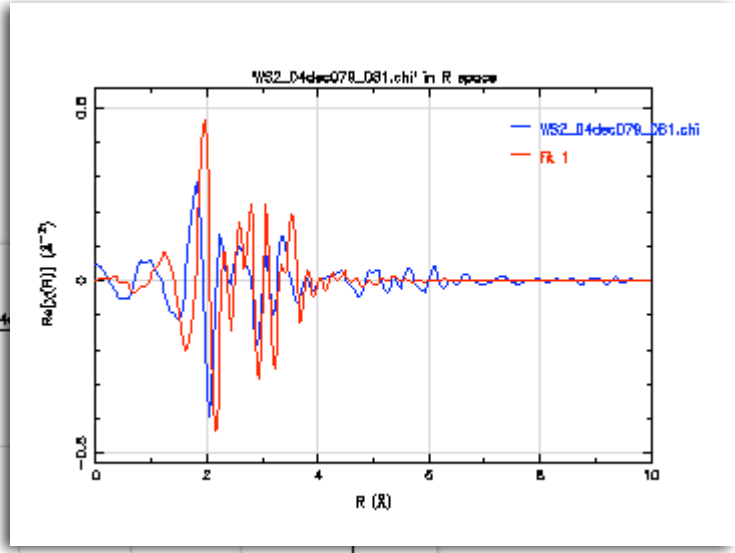


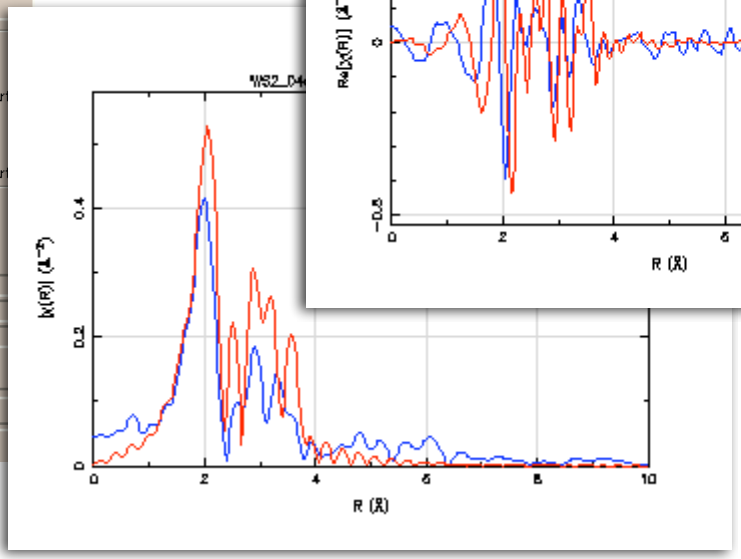


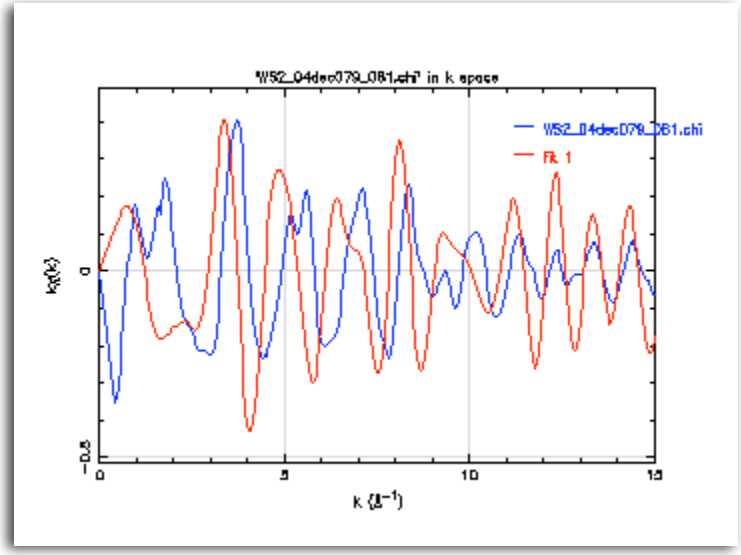
First three paths (red, green, and purple)
are much bigger and well separated from other paths

Bulk WS_2 : Sum up first three paths and compare to data









- FT of data and model contain the same shape.
- Model is larger than the data in amplitude as needed.
- Chi(k) data shows difference in first few $Å^{-1}$

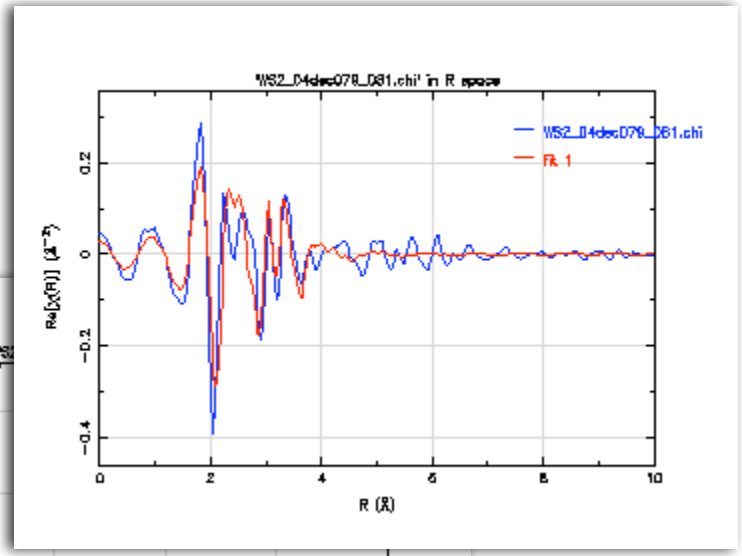
ws2-bulk-big1.apj

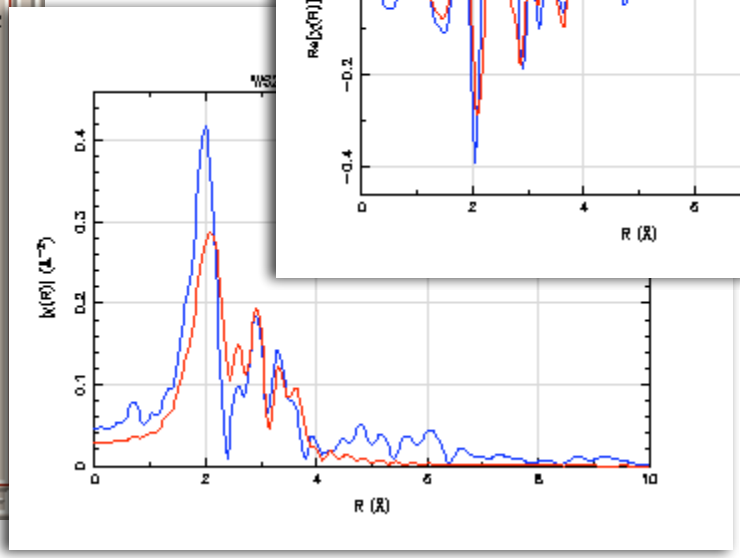
Bulk WS_2 : Try simple model

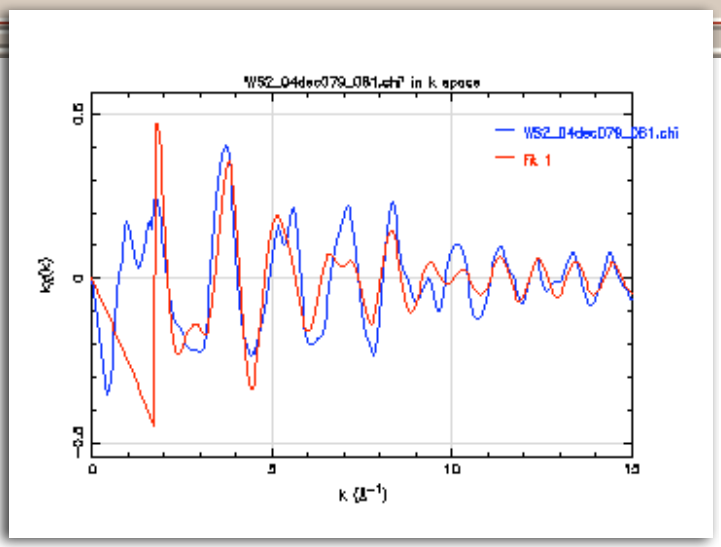
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2_04dec079_081.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  15:56:02 on 3 July, 2007
This fit at      :  15:56:20 on 3 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 804.02
Figure of merit  :  1

-------------------------------------------------------------

Independent points           =      20.176757812
Number of variables          =       6.000000000
Chi-square                   =    1358569.33
Reduced Chi-square           =   95830.749871589
R-factor                     =       0.396185187
Measurement uncertainty (k)  =       0.000161388
Measurement uncertainty (R)  =       0.000432548
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  s_02             =     0.9745600   +/-      0.3852200     (1.0000)
  enot             =    11.3252270   +/-      2.6435800     (0.0000)
  alpha            =     0.0004790   +/-      0.0069110     (0.0000)
  sigs1            =     0.0077460   +/-      0.0054840     (0.0000)
  sigw1            =    -0.0035310   +/-      0.0021150     (0.0000)
  sigs2            =     0.0088270   +/-      0.0153170     (0.0000)
```







- ΔR = alpha*reff, 3 σ2 values, one E0, s02
- Doesn't work, constraint on ΔR values is too strong

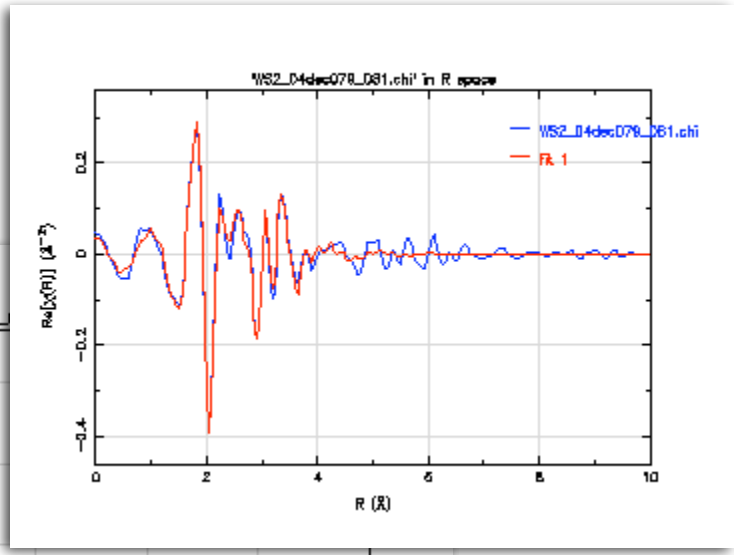
ws2-bulk-big2.apj

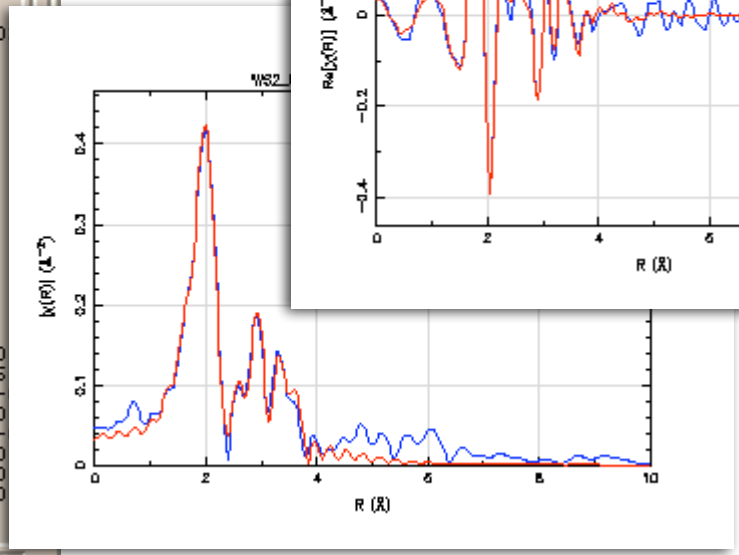
Bulk WS_2 : relax constraints on ΔR

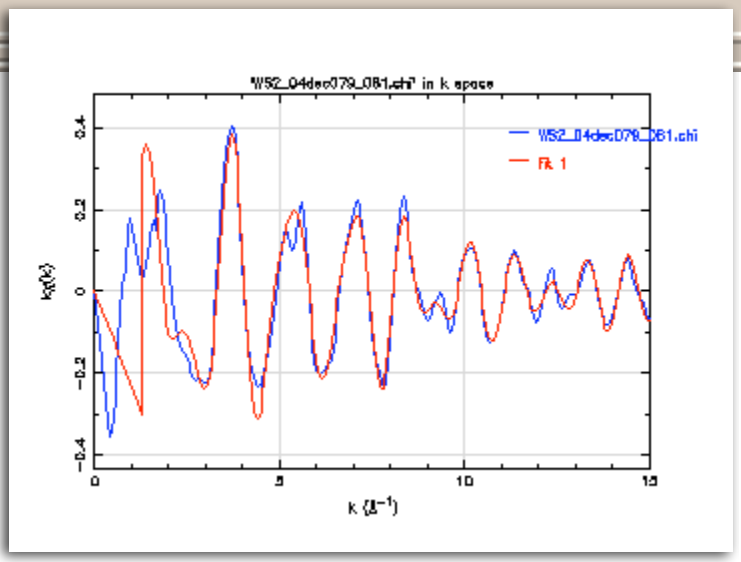
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title     :  Fitting WS2_04dec079_081.chi
Comment           :  Fit #1
Prepared by       :
Contact           :
Started           :  16:03:54 on 3 July, 2007
This fit at       :  16:07:22 on 3 July, 2007
Environment       :  Artemis 0.8.010 using linux, perl 5.008008, Tk 804.0
Figure of merit   :  1

-------------------------------------------------------------

Independent points           =      20.176757812
Number of variables          =       8.000000000
Chi-square                   =   47428.964804231
Reduced Chi-square           =    3895.040497196
R-factor                     =       0.012993472
Measurement uncertainty (k)  =       0.000161388
Measurement uncertainty (R)  =       0.000432548
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  s_02             =     0.8603050   +/-       0.0532670     (guessed as 0
  enot             =     6.0364420   +/-       0.6188980     (guessed as 6
  dels1            =    -0.0791740   +/-       0.0042560     (guessed as -
  delw1            =     0.0036730   +/-       0.0038200     (guessed as 0
  dels2            =    -0.0530680   +/-       0.0155900     (guessed as -
  sigs1            =     0.0024000   +/-       0.0005080     (guessed as 0
  sigw1            =     0.0025200   +/-       0.0003510     (guessed as 0
  sigs2            =     0.0045570   +/-       0.0017430     (guessed as 0
```



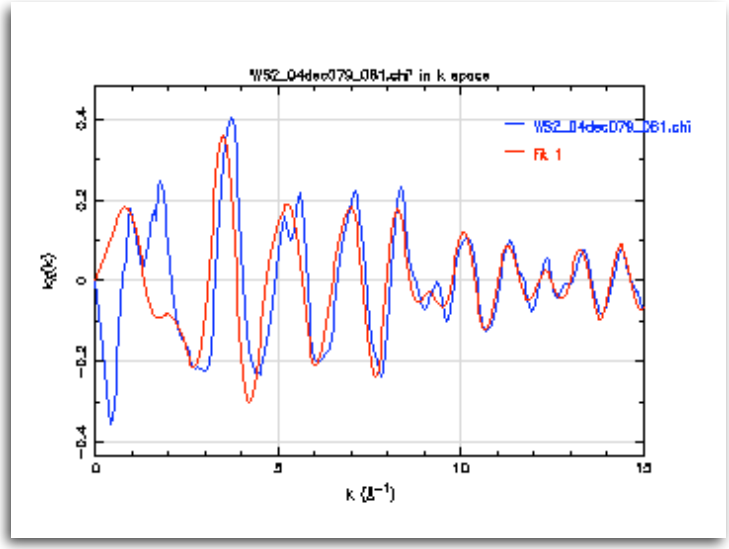


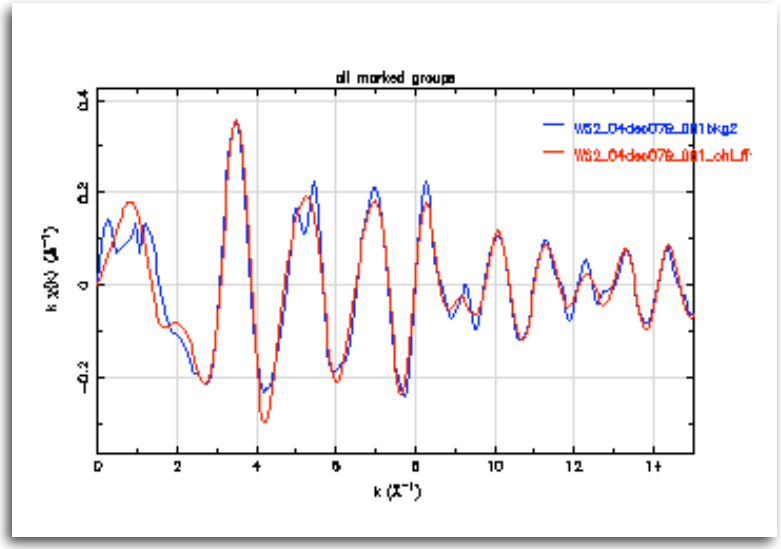


- 3 ΔR values, 3 σ2 values, one E0, s02
- Model works well, reasonable values,
- Background needs to be fixed

ws2-bulk-big3.apj

Bulk WS_2 : 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 Athena
- New background made for data

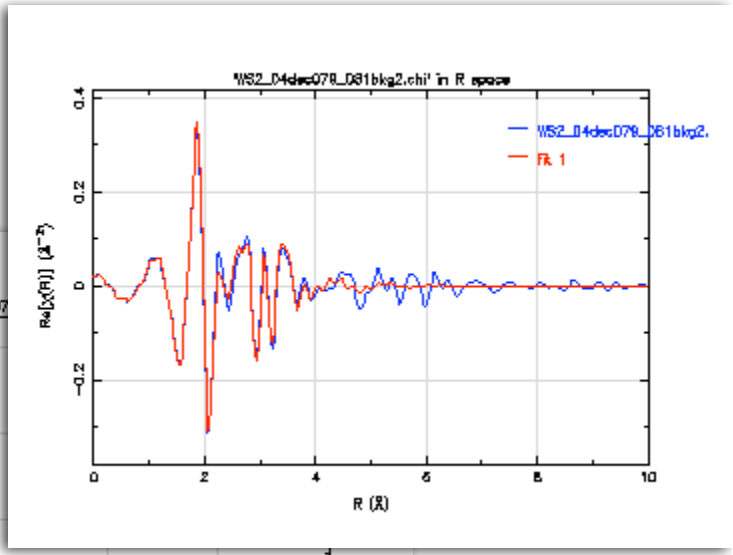
ws2-bulk-big4.apj
ws2-bkg2.prj

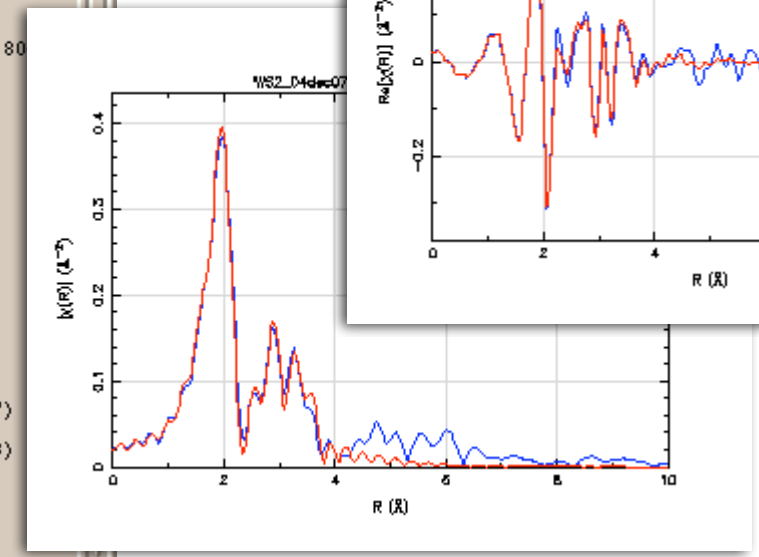
Bulk WS_2 : Model of Bulk WS_2 data

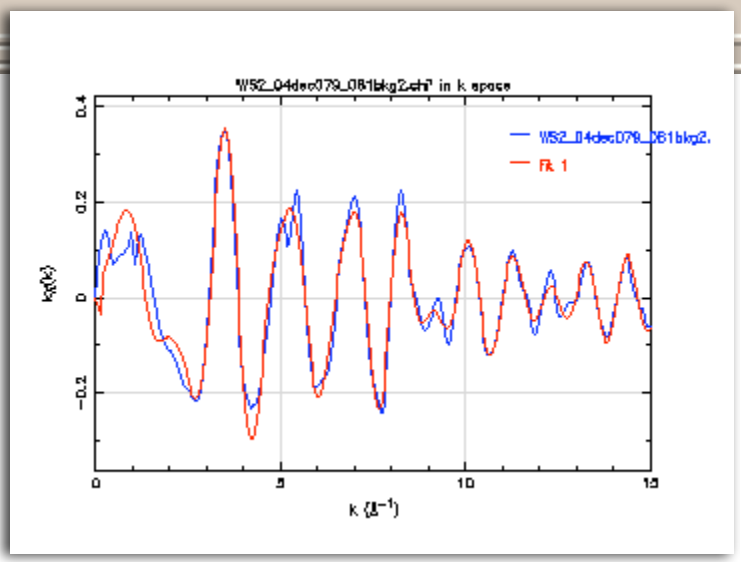
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title     :  Fitting WS2_04dec079_081bkg2.chi
Comment           :  Fit #1
Prepared by       :
Contact           :
Started           :  16:18:34 on 3 July, 2007
This fit at       :  16:19:01 on 3 July, 2007
Environment       :  Artemis 0.8.010 using linux, perl 5.008008, Tk 80
Figure of merit   :  1

-------------------------------------------------------------

Independent points           =      20.176757812
Number of variables          =       8.000000000
Chi-square                   =   44793.703255300
Reduced Chi-square           =    3678.623156101
R-factor                     =       0.013445620
Measurement uncertainty (k)  =       0.000161300
Measurement uncertainty (R)  =       0.000432314
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  s_02             =      0.8506940   +/-       0.0554680     (0.8509)
  enot             =      0.1319460   +/-       0.6909470     (0.1351)
  dels1            =     -0.0787080   +/-       0.0043670     (-0.0787)
  delw1            =      0.0038530   +/-       0.0038300     (0.0039)
  dels2            =     -0.0533190   +/-       0.0155890     (-0.0533)
  sigs1            =      0.0023650   +/-       0.0005090     (0.0024)
  sigw1            =      0.0025070   +/-       0.0003490     (0.0025)
  sigs2            =      0.0045200   +/-       0.0017120     (0.0045)
```



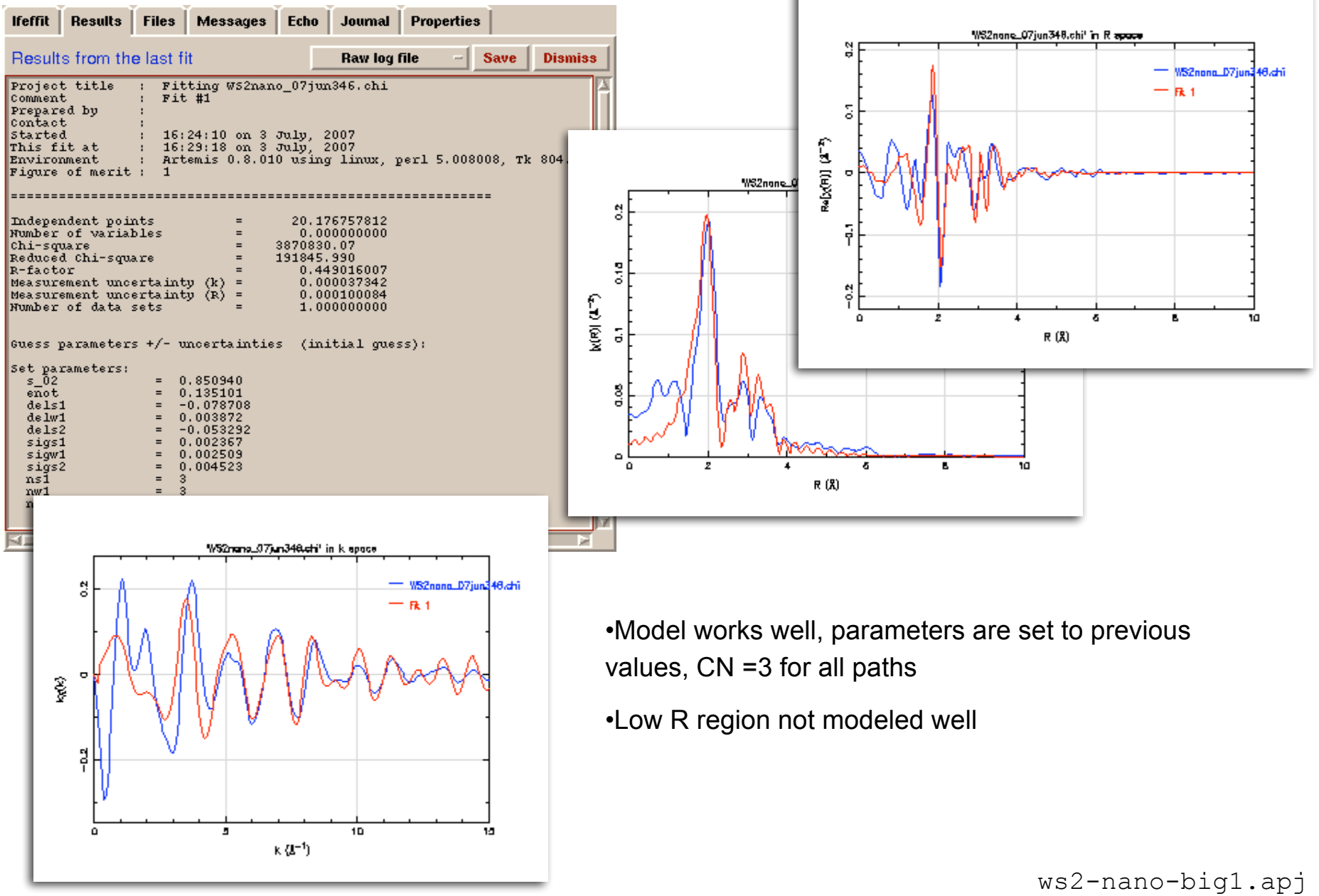




- Model works well, parameters are reasonable.
- apply model to nano-particles

ws2-bulk-big5.apj

Apply bulk model to Nano data



- Model works well, parameters are set to previous values, CN =3 for all paths
- Low R region not modeled well

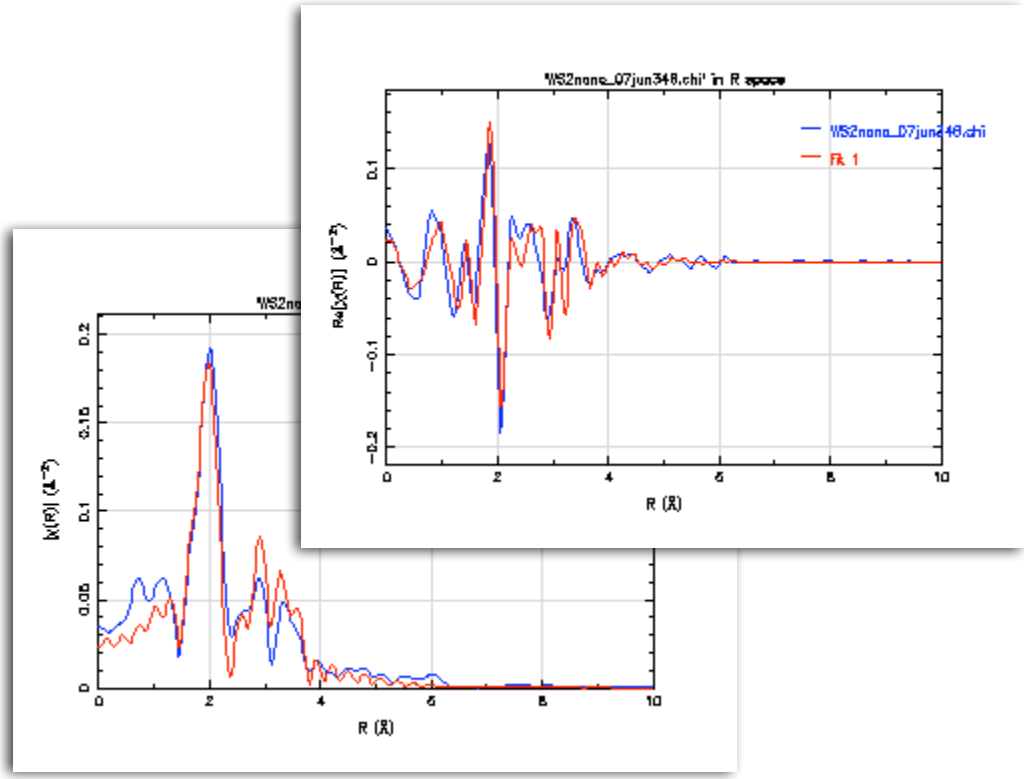
ws2-nano-big1.apj

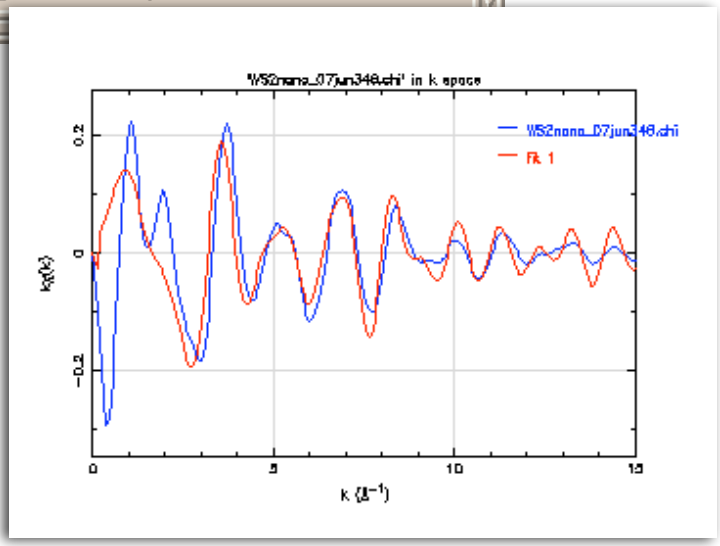
nano WS_2 : Add oxygen path to model

Ifeffit | Results | Files | Messages | Echo | Journal | Propertie

Results from the last fit | Raw log file | Save | Dismiss

```
Project title     :  Fitting WS2nano_07jun346.chi
Comment           :  Fit #1
Prepared by       :
Contact           :
Started           :  16:37:14 on 3 July, 2007
This fit at       :  16:37:31 on 3 July, 2007
Environment       :  Artemis 0.8.010 using linux, perl 5
Figure of merit   :  1

=====================================================

Independent points           =      20.176757812
Number of variables          =       0.000000000
Chi-square                   =    2501123.09
Reduced Chi-square           =  123960.604085908
R-factor                     =       0.364716463
Measurement uncertainty (k)  =       0.000037342
Measurement uncertainty (R)  =       0.000100084
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):

Set parameters:
   s_02             =  0.850940
   enot             =  0.135101
   dels1            =  -0.078708
   delw1            =  0.003872
   dels2            =  -0.053292
   sigs1            =  0.002367
   sigw1            =  0.002509
   sigs2            =  0.004523
   ns1              =  3
   nw1              =  3
   ns2              =  3
   no1              =  1
   delo1            =  -0.15
   sigo1            =  0
```





- 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

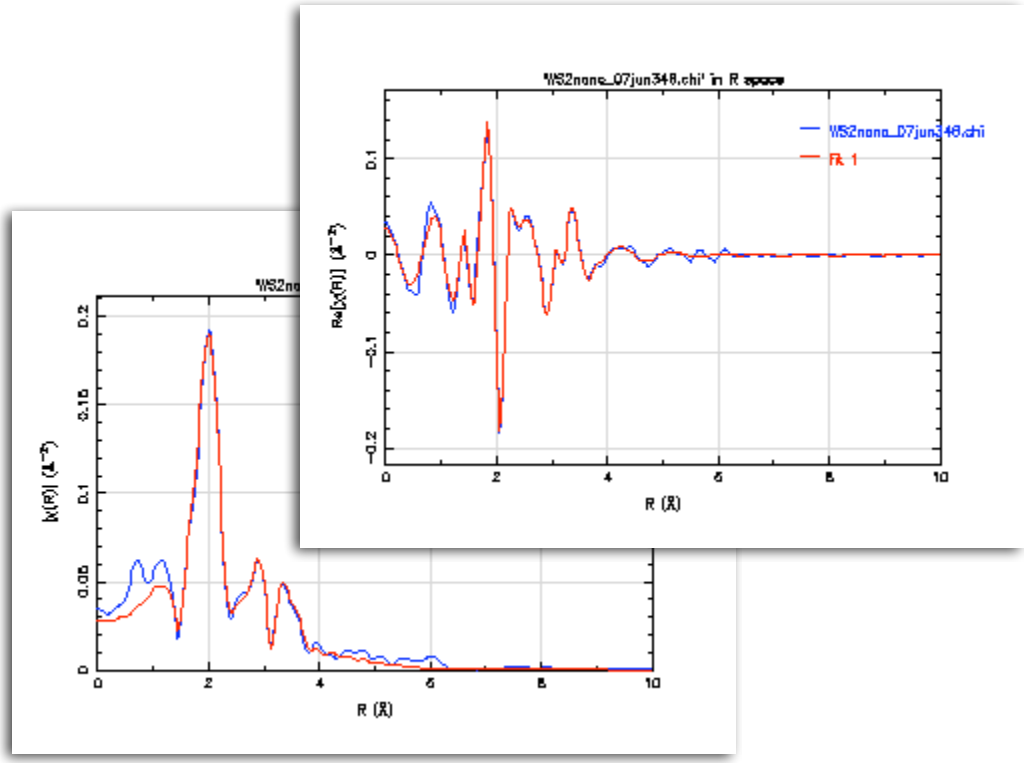
ws2-nano-big2.apj

nano WS_2 :optimize fit parameters

Ifeffit | Results | Files | Messages | Echo | Journal | Properties

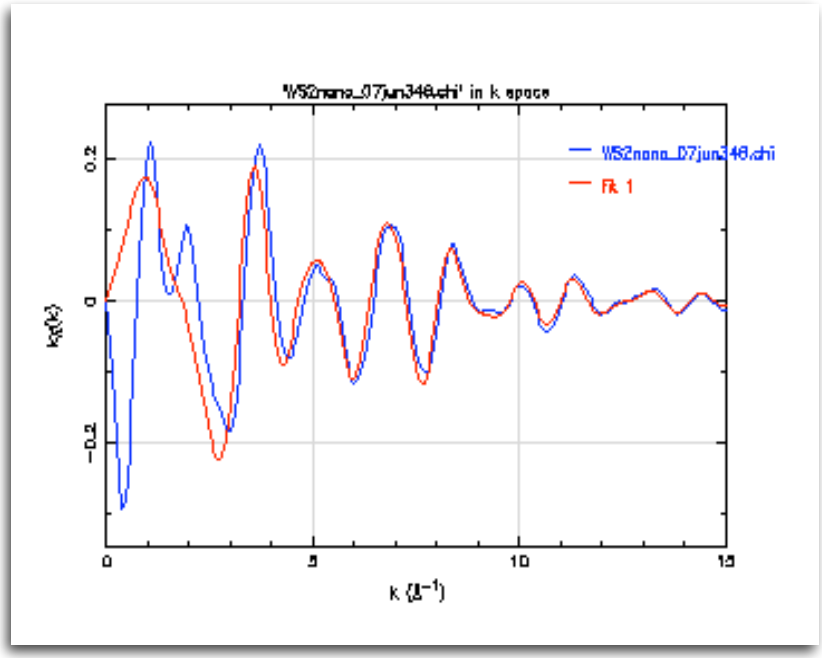
Results from the last fit — Raw log file — Save — Dismiss

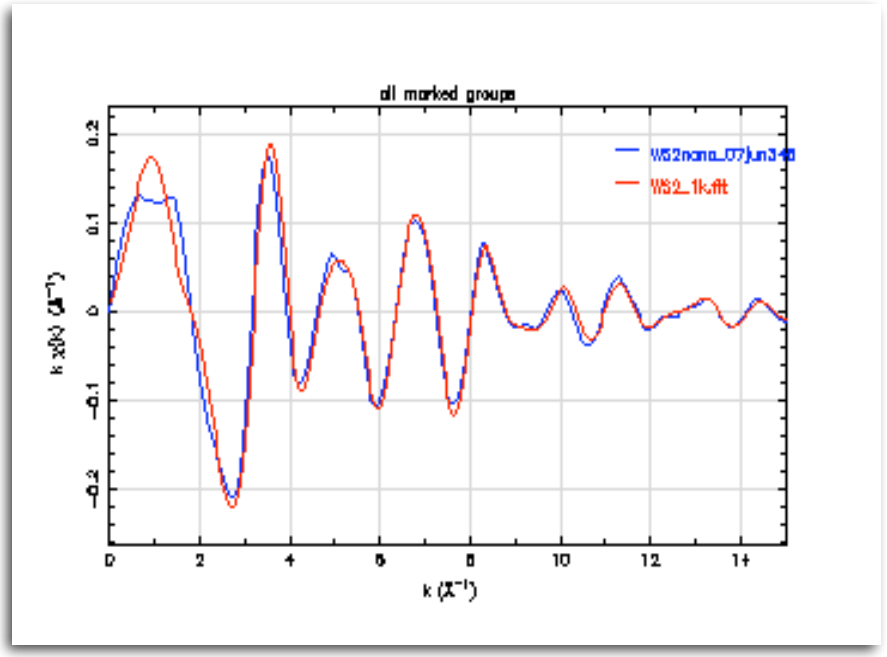
```
Project title    :  Fitting WS2nano_07jun346.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  16:45:23 on 3 July, 2007
This fit at      :  16:45:55 on 3 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.0
Figure of merit  :  1

------------------------------------------------------------

Independent points           =      20.176757812
Number of variables          =      13.000000000
Chi-square                   =   83170.510305937
Reduced Chi-square           =   11588.869581342
R-factor                     =       0.012887617
Measurement uncertainty (k)  =       0.000037342
Measurement uncertainty (R)  =       0.000100084
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =     3.6987390   +/-       0.8555040
  dels1            =    -0.0751680   +/-       0.0057200
  delw1            =    -0.0015200   +/-       0.0102440
  dels2            =    -0.0761520   +/-       0.0267500
  sigs1            =     0.0043560   +/-       0.0007460
  sigw1            =     0.0056940   +/-       0.0018180
  sigs2            =     0.0111720   +/-       0.0075160
  ns1              =     3.7264150   +/-       0.3066410
  nw1              =     2.5220570   +/-       0.9107700
  ns2              =     3.6515630   +/-       1.9753900
  no1              =     1.3927860   +/-       0.3077220
  delo1            =    -0.1721410   +/-       0.0074140
  sigo1            =     0.0035320   +/-       0.0021000
```



- Model works well, parameters are reasonable
- clean up background

nano WS_2 :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 Athena
- New background made for data

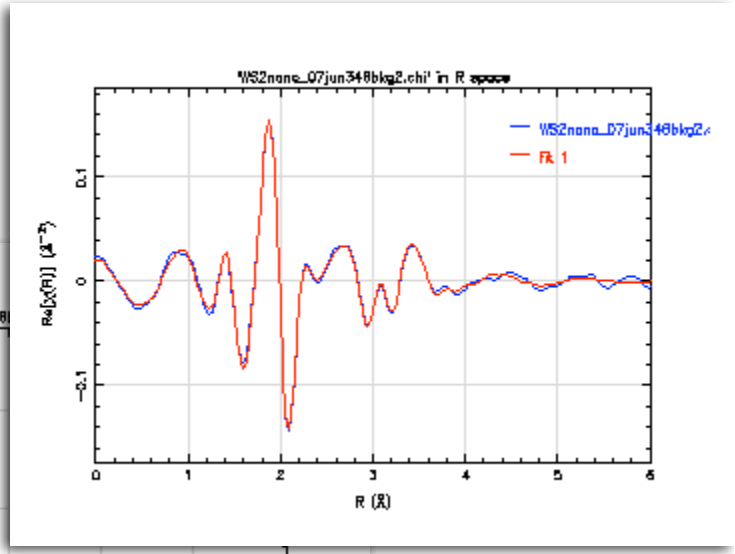
ws2-nano-big4.apj
ws2-nanobkg2.prj

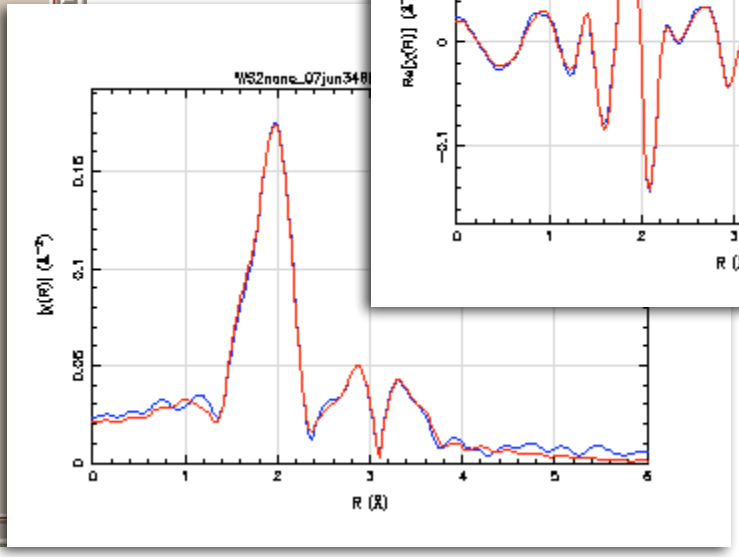
nano WS_2 :Modelling Nano-particles of WS_2

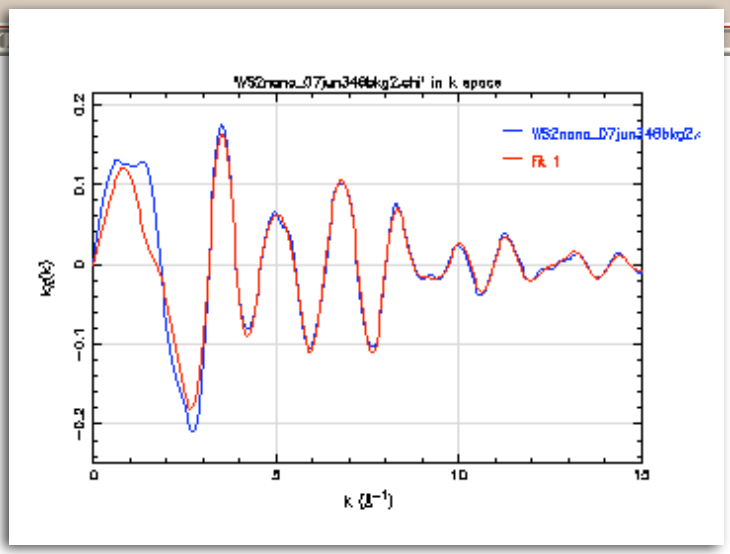
Ifeffit | Results | Files | Messages | Echo | Journal | Properties

Results from the last fit — Raw log file — Save — Dismiss

```
Project title    :  Fitting WS2nano_07jun346bkg2.chi
Comment          :  Fit #1
Prepared by      :
Contact          :
Started          :  17:01:16 on 3 July, 2007
This fit at      :  17:01:55 on 3 July, 2007
Environment      :  Artemis 0.8.010 using linux, perl 5.008008, Tk 804.02
Figure of merit  :  1

-------------------------------------------------------------

Independent points           =      20.176757812
Number of variables          =      13.000000000
Chi-square                   =   22285.025096786
Reduced Chi-square           =    3105.166104111
R-factor                     =       0.005052954
Measurement uncertainty (k)  =       0.000038769
Measurement uncertainty (R)  =       0.000103909
Number of data sets          =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
   enot             =     -1.1413980   +/-       0.5383850     (0.0000)
   dels1            =     -0.0715990   +/-       0.0033670     (-0.0752)
   delw1            =      0.0006280   +/-       0.0057470     (-0.0015)
   dels2            =     -0.0724340   +/-       0.0154770     (-0.0761)
   sigs1            =      0.0037190   +/-       0.0004120     (0.0044)
   sigw1            =      0.0053870   +/-       0.0010070     (0.0057)
   sigs2            =      0.0106710   +/-       0.0042320     (0.0112)
   ns1              =      3.3581900   +/-       0.1624400     (3.7261)
   nw1              =      2.3370120   +/-       0.4818600     (2.5224)
   ns2              =      3.4306490   +/-       1.0942580     (3.6545)
   no1              =      1.0460280   +/-       0.1328140     (1.3917)
   delo1            =     -0.1839500   +/-       0.0044650     (-0.1722)
   sigo1            =      0.0019340   +/-       0.0010620     (0.0035)

Set parameters:
   s_02             =   0.850940
```







- Model works, background is good
- fit parameters are reasonable

ws2-nano-big5.apj

The End