Introduction to the analysis of EXAFS data

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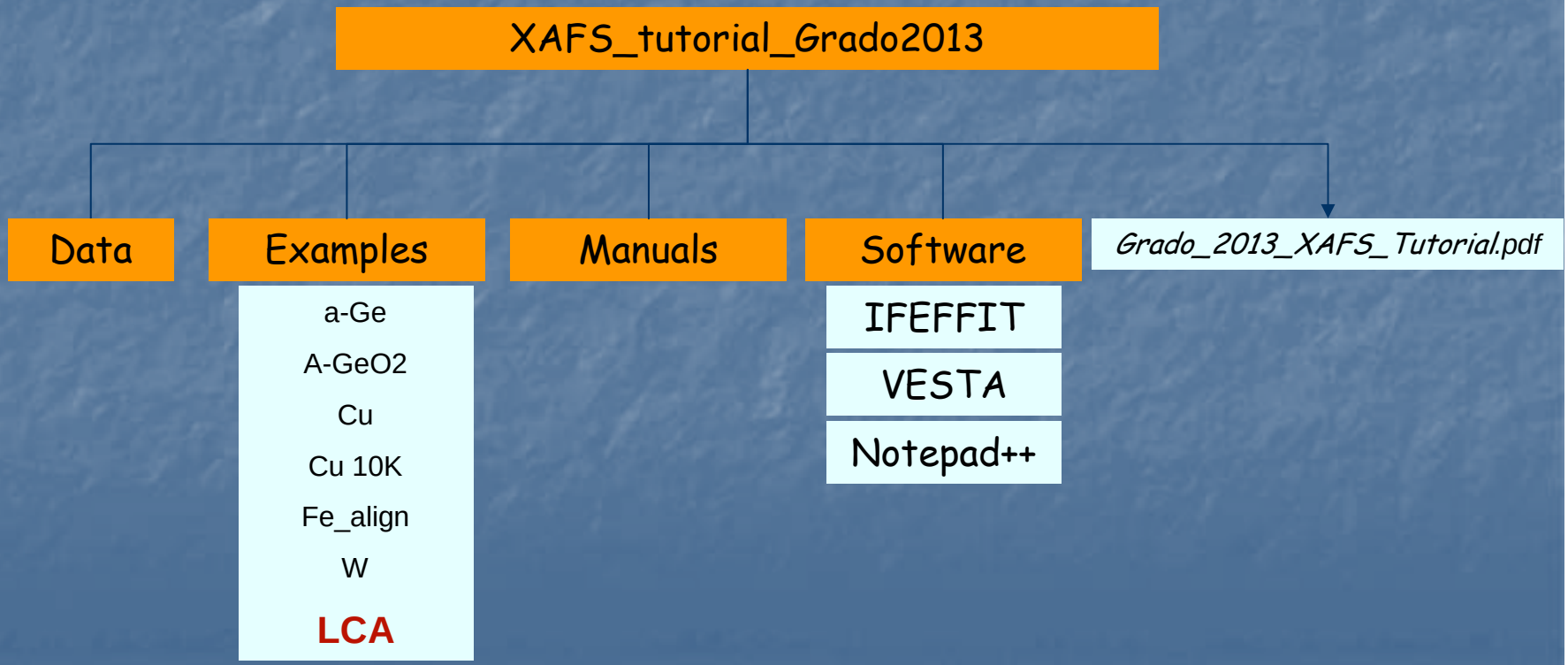
Grado2013_XAFS_TUTORIAL

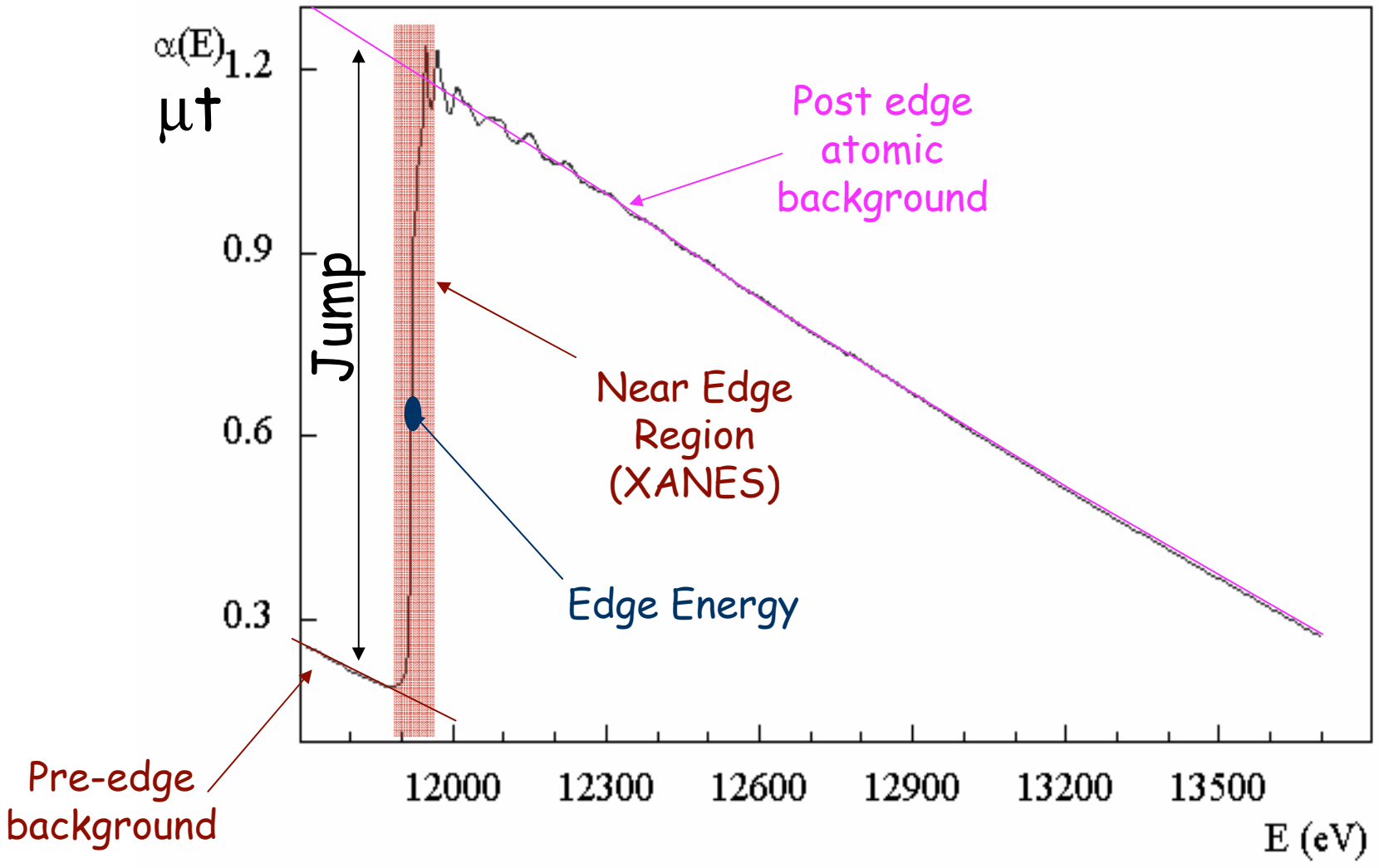
http://dl.dropbox.com/u/20746560/Meneghini_EXAFS-Tutorial-DUINO-2011.zip

PDF slides: https://db.tt/UmF9HOc2

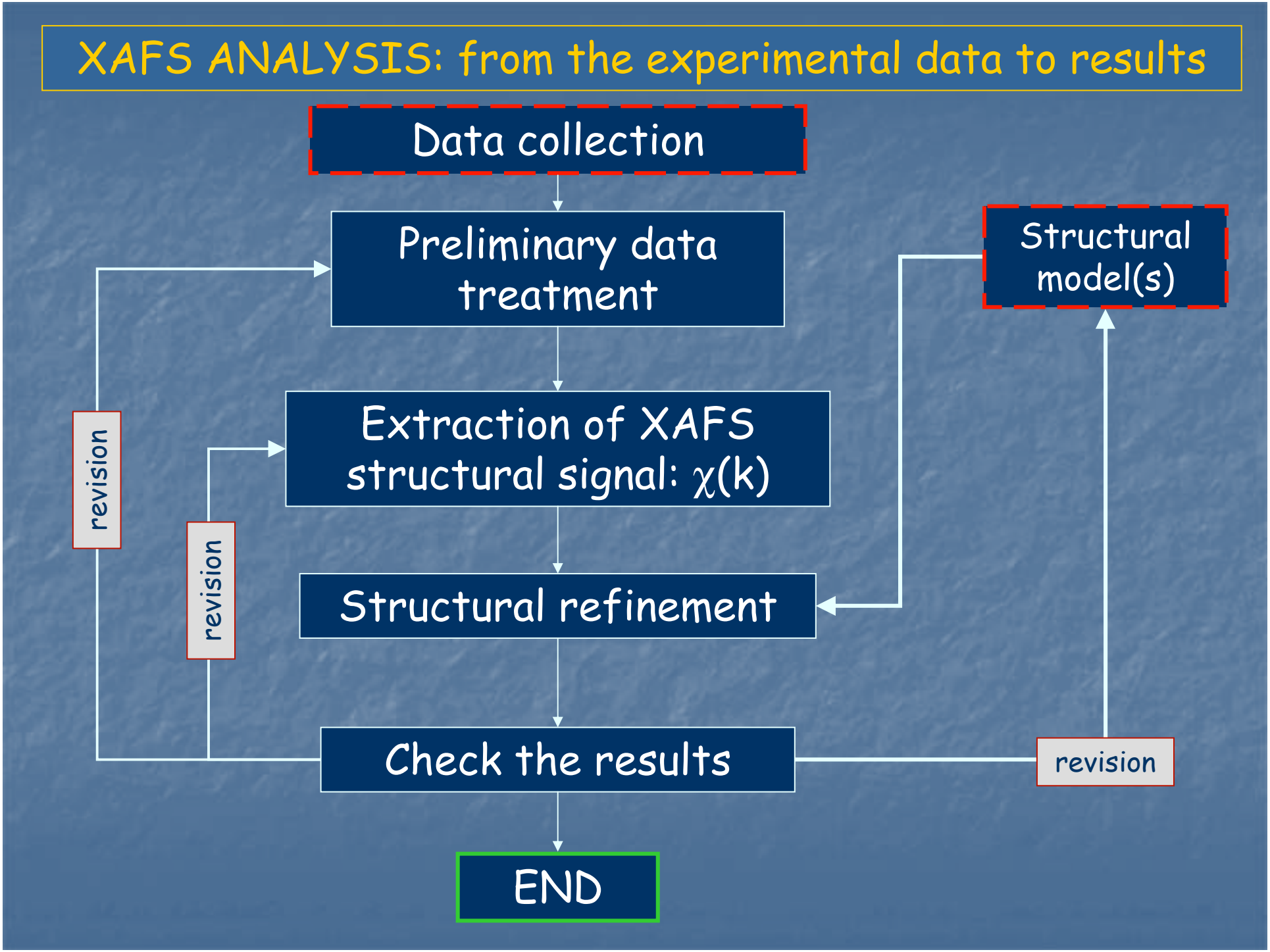
Complete directory

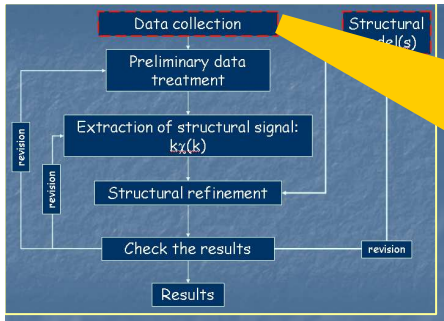


Characteristics of a XAS spectrum



XAFS ANALYSIS: from the experimental data to results





Data collection

Proposal submission + proposal evaluation + beamtime scheduling = 6 to 12 months !

It is difficult to obtain new beamtime for the same proposal in case of failure!!!!

XANES/EXAFS
Fluo/TEY/transmission
....

Choose properly the experimental set-up & sample preparation

Optimize your beamtime!

Check the data quality during the experiment

Quality is better than quantity

Always measure reference data

XAFS rarely gives absolute quantitative details

Choose properly data collection strategy

- Check the proposal submission deadlines,
- discuss your experiment with local contacts,
- check your data during the experiment

ELETTRA: 15-09 + 15-03
ESRF: 01-09 + 01-03

Data collection

Errors in XAFS data analysis are dominated by systematic errors:

- spurious structures
- background subtraction
- wrong models
- inaccurate theory

a Experimental set-up & sample preparation

Transmission: massive concentrated samples

$0.5 \leq \Delta\mu t \leq 1.5$ $\mu t \leq 2.$

inhomogeneities, holes, not parallel surfaces, etc...

Fluorescence: thin concentrated

thick diluted samples

Self absorption, detector linearity, Bragg reflections

TEY: thick concentrated

Surface sensitivity, sample charge, Bragg reflections

IXS Standards and Criteria Subcommittee Reports

b Collection strategy

- step scan / quick EXAFS
- Fixed Energy or K steps
- single scan/repeated scans
- temperature points
- . . .

c Data quality

S/N ratio

glitches

discontinuities

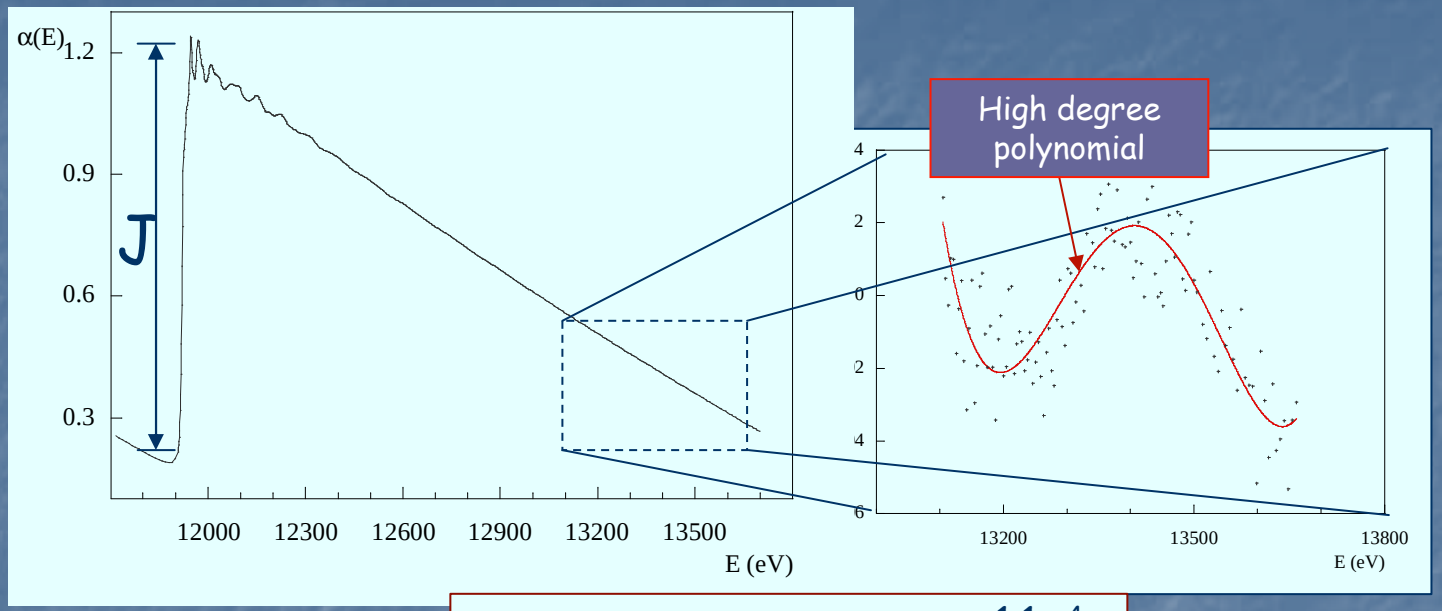
d Measure reference samples

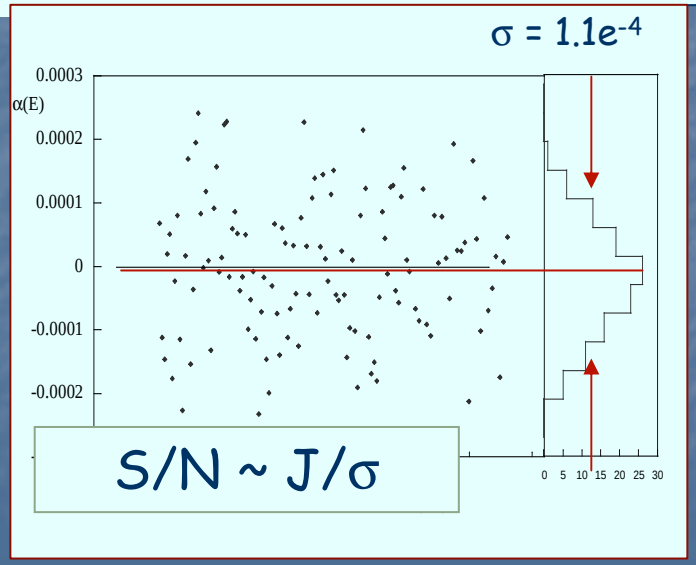
1-energy calibration

2-data analysis procedures calibration

The power of XAFS technique consists in highlighting the smallest structural differences

Evaluate S/N ratio

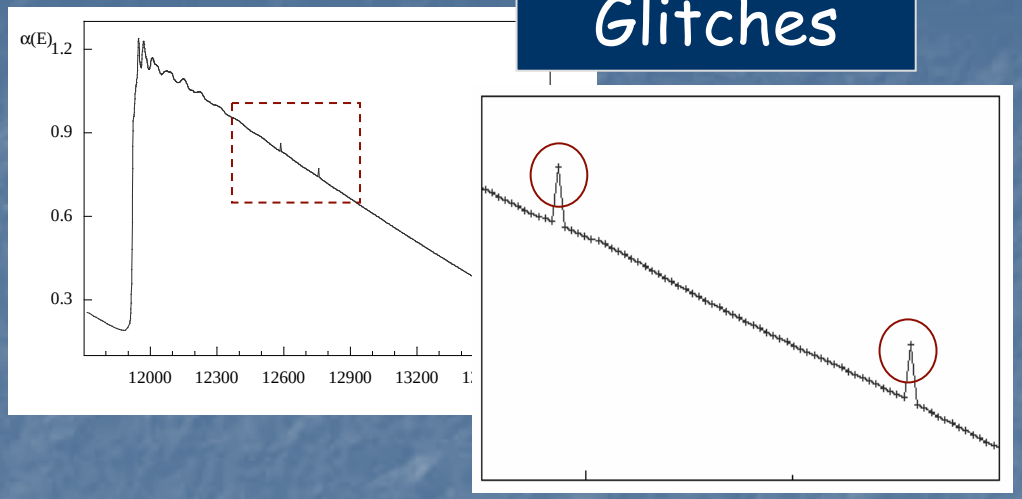




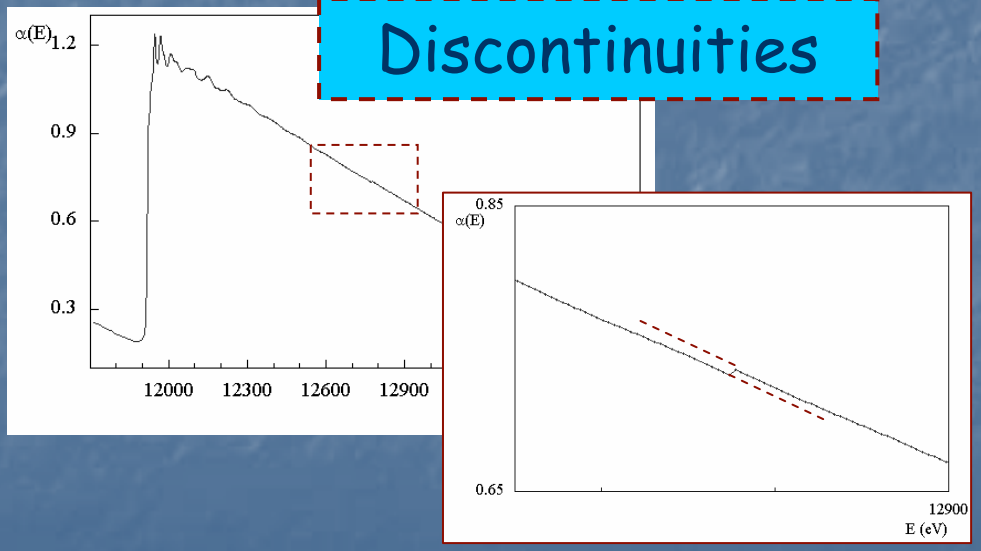
Check regularly during the experiment

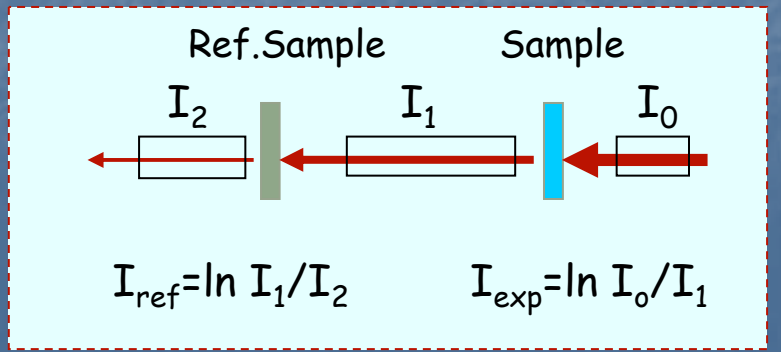
Check systematically during the experiment

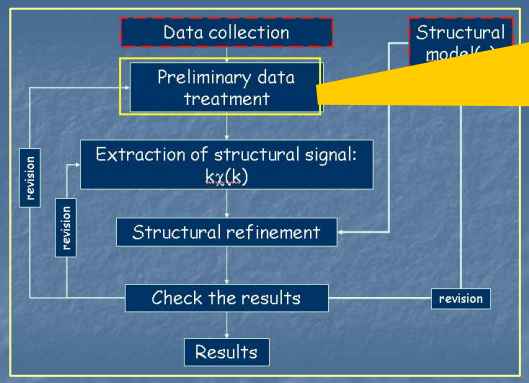
Glitches



Discontinuities



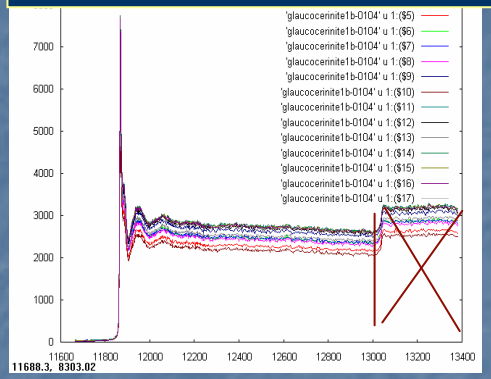


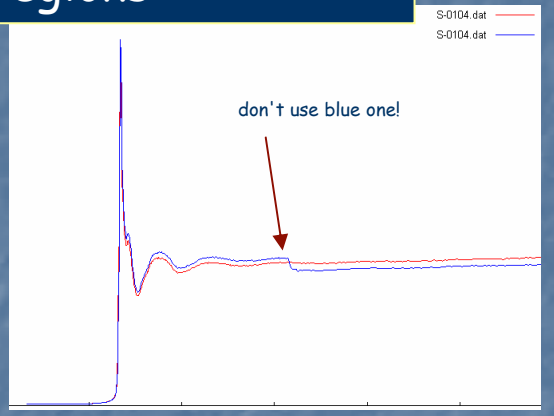


Preliminary data treatment

a

Select properly the best spectra and useful data regions





Absorption signal

Transmission $\alpha(E) = \log_e \frac{I_o}{I_t}$

Fluorescence & TEY $\alpha(E) = \frac{I_f}{I_o}$

μx<<1

b

Preliminary data treatment

- Self absorption corrections
-deglitching
-data interpolation
- data alignement

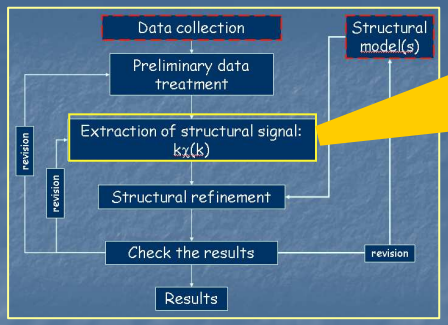
Check carefully the data quality during the experiment

Experimental set-up generally provide macros for automatic data collection over several days: supervise your macros!

c

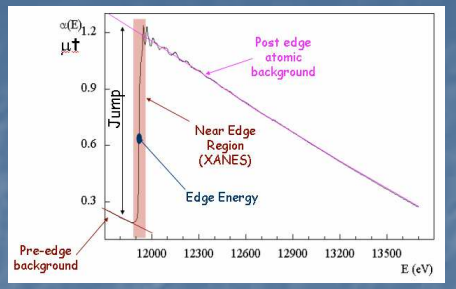
Sum together the best spectra

Weighting by S/N



Extract χ(k) structural signal

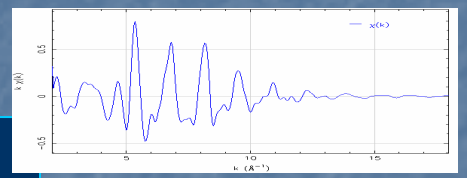
$\alpha(E)$



pre-edge subtraction

revise preliminary tratments

α_o calculation



structural signal χ(k)

Fourier Transform

Fourier Filtering

Structural refinement

Absorption signal

Transmission $\alpha(E) = \log_e \frac{I_o}{I_t}$

Fluorescence & TEY $\alpha(E) = \frac{I_f}{I_o}$

$\alpha = \alpha_o + \alpha_{pre}$

$\alpha_o = (\mu_O + \mu)t$

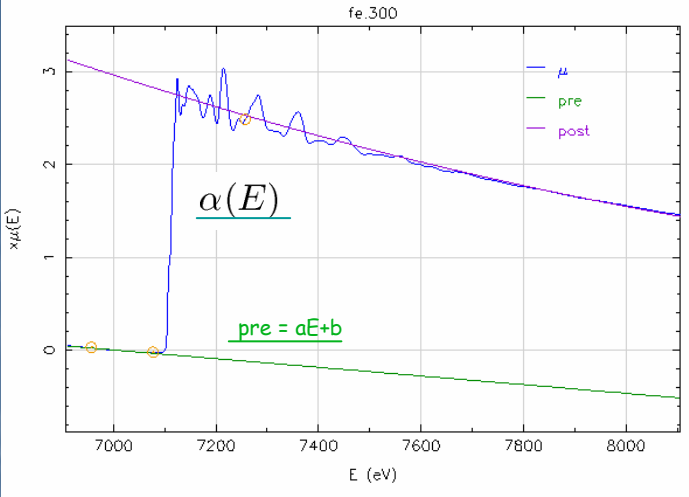
μ_o = free atom absorption
μ = embedded atom absorption
pre = all but the absorber

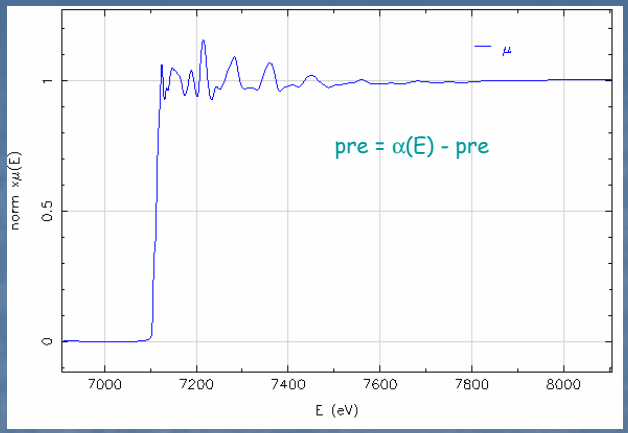
$$\alpha'(E) = \alpha(E) - \alpha_{pre}(E)$$

XAFS structural signal

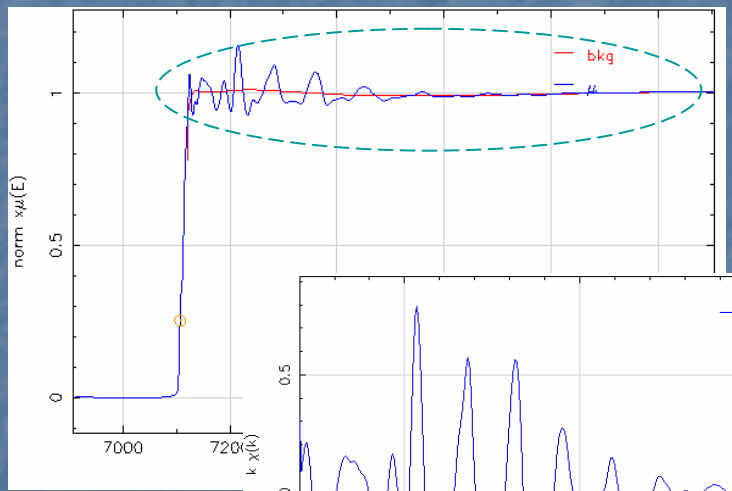
$$\chi^{exp}(k) = \frac{\alpha'(k) - \alpha_o(k)}{\alpha_o(k)} J$$

a Background subtraction

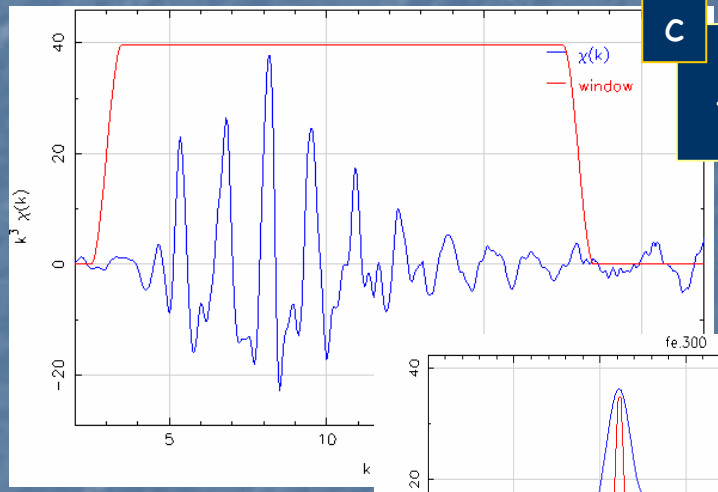


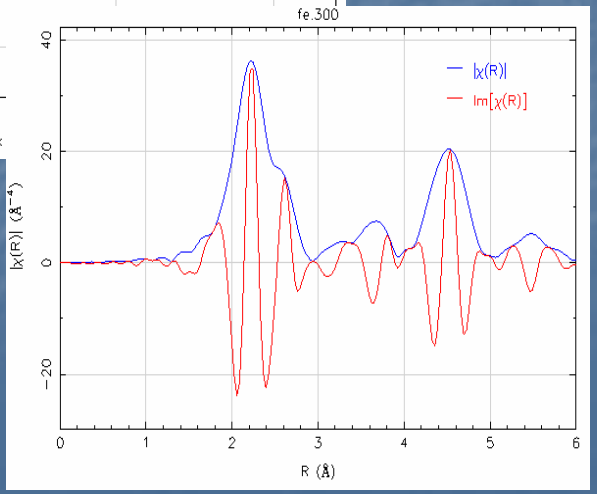


b calculate μ_o and $\chi(k)$



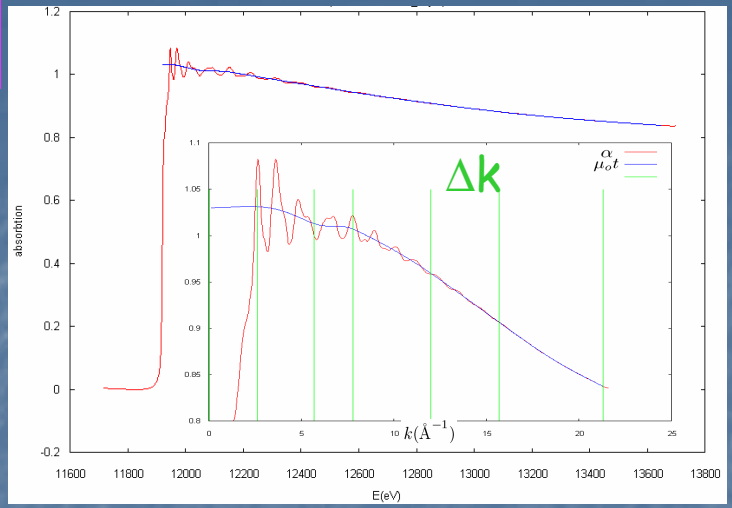
c Fourier Transform



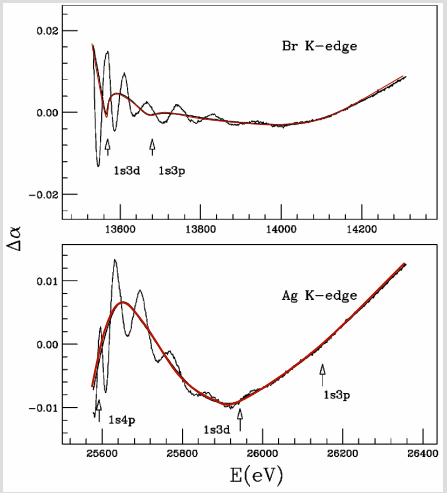


Structural signal

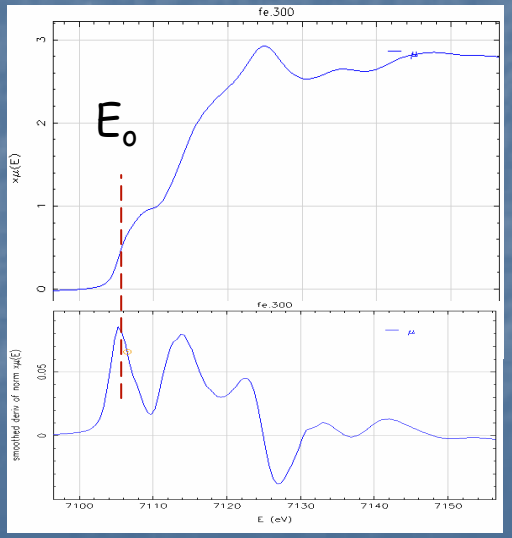
- Define E_o
- Calculate k
- Define μ_o
- Calculate $\chi(k)$
- Check FT



Note: Multiple excitations my affect the background with (small) discontinuities



A. Di Cicco et Al. Phys. Rev. B 62, 12001 (2000)



μ_o = represents the bare atom absorption.

It is calculated **empirically** as a smooth curve across the data.

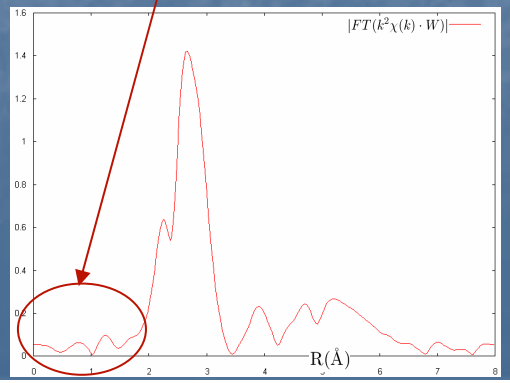
Different XAFS data analysis software apply different (generally equivalent) methods

Requirements for μ_o:

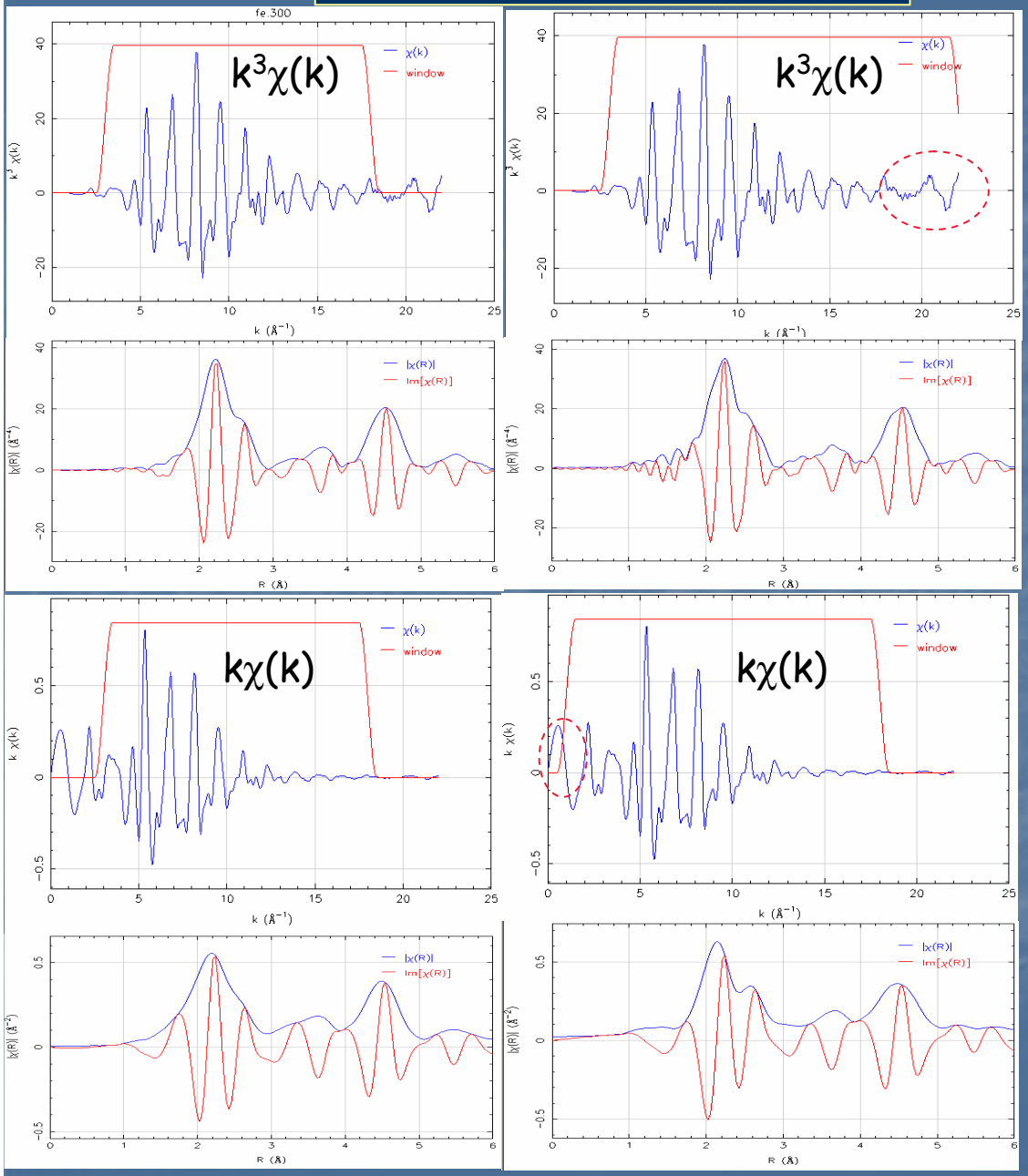
1) Smooth enough to not remove true structural features

2) Structured enough to remove background structures

Large |FT| contributions at low (unphysical) distances may signify "wrong μ_o"



Fourier Transform



Shape of FT widely changes as a function of:

- FT window
- k^w weight
- data range

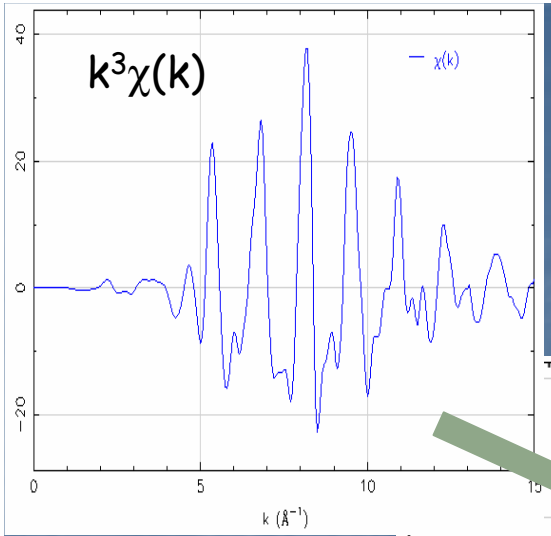
FT shows more intuitively the main structural features in the real space: the FT modulus represent a pseudo-radial distribution function modified by the effct of amplitude, phase and mean free path parameters:

|FT| peaks point out interatomic correlations

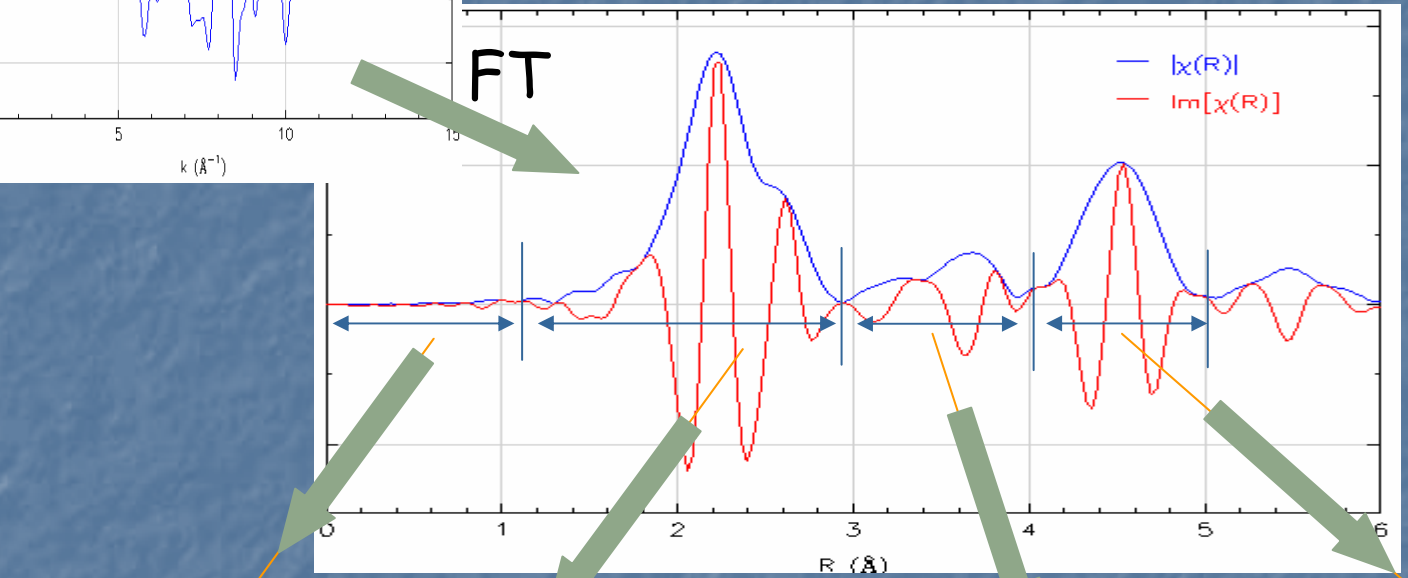
Peak positions are not the true distances due to the photoelectron phase shift

Fourier Filtering

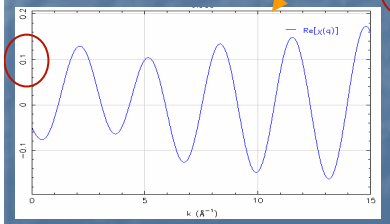
Fourier filtering allows isolating contributions of selected regions of the FT



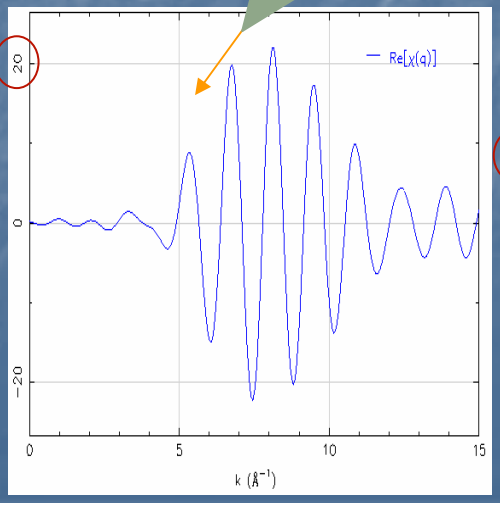
FT

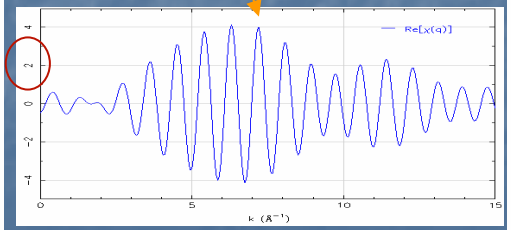


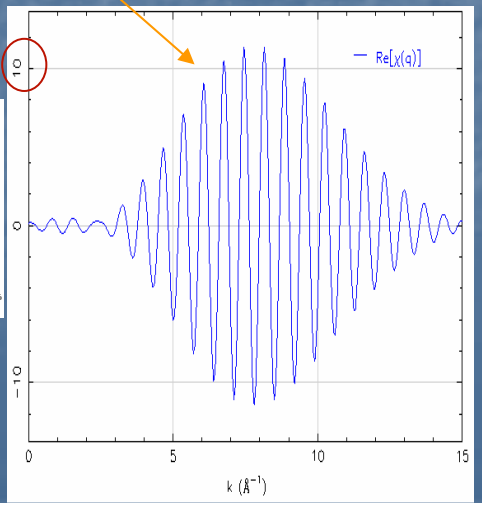
Background contribution

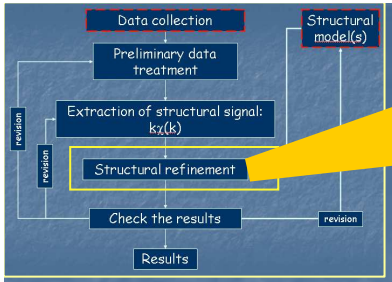


Back Fourier transform (BFT)







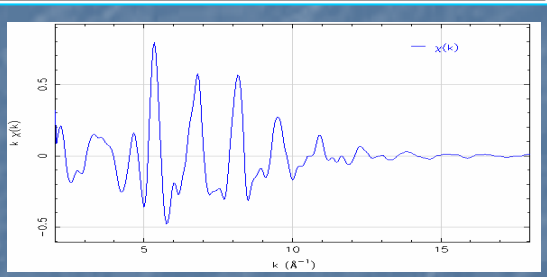


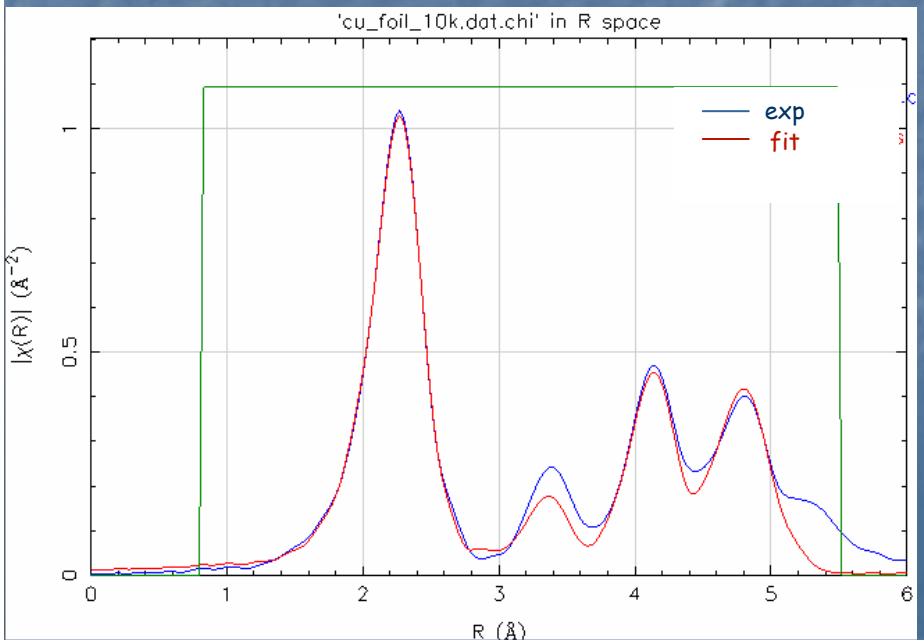
data refinement

Theoretical χ(k)

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

Experimental χ(k)





Exp. χ(k)

Choose a model

Select the relevant structural contributions

Refine the structural parameters: N, R, σ²

add new contributions?

y

n

Change the model?

y

n

Revise your data extraction?

y

END

Choose a structural model

How to find a model structure

How to visualize the structure

How to calculate distances and geometries

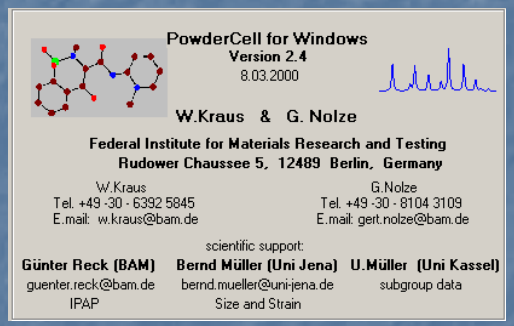
NEUTRONS FOR SCIENCE

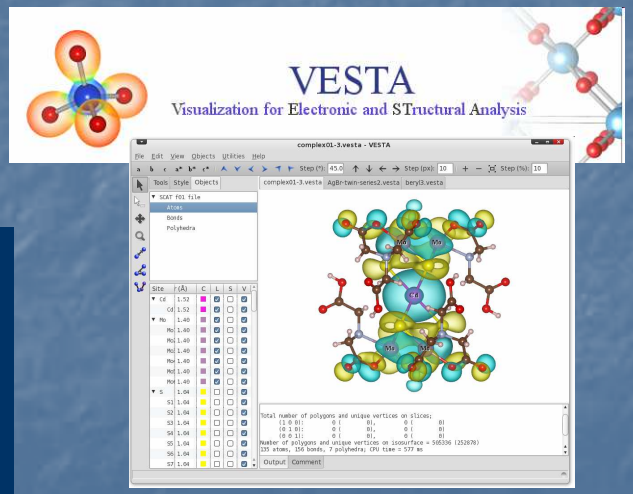
Barns.ill.fr

http://database.iem.ac.ru/mincryst/

Full inorganic structure database (ICSD) (registration fees)

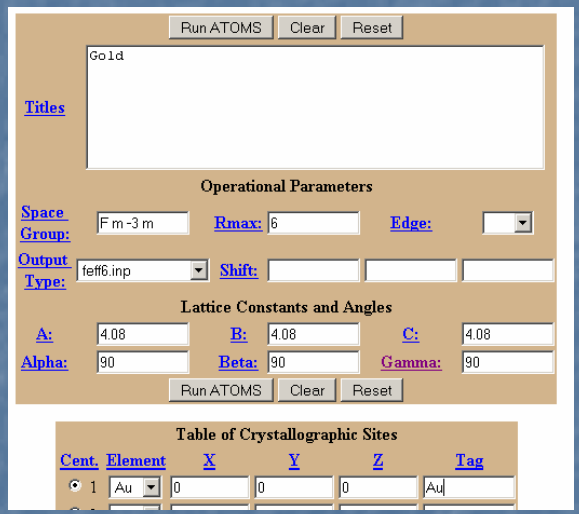
Protein Data Base (Free)



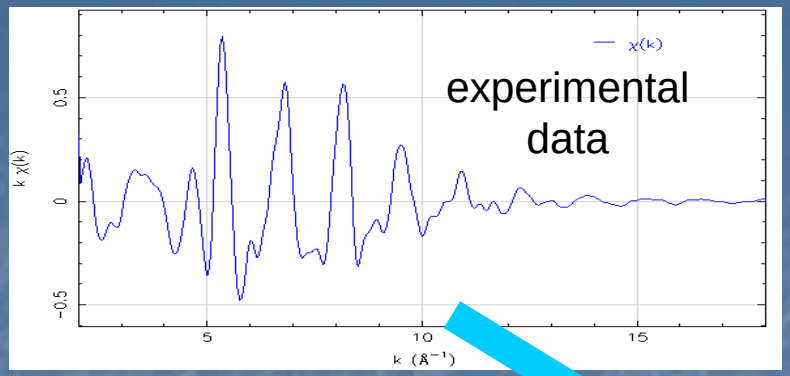


ATOMS on the Web

http://millenia.cars.aps.anl.gov/cgi-bin/atoms/atoms.cgi



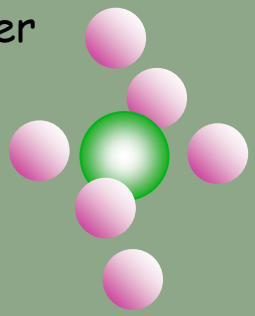
Search on the web !



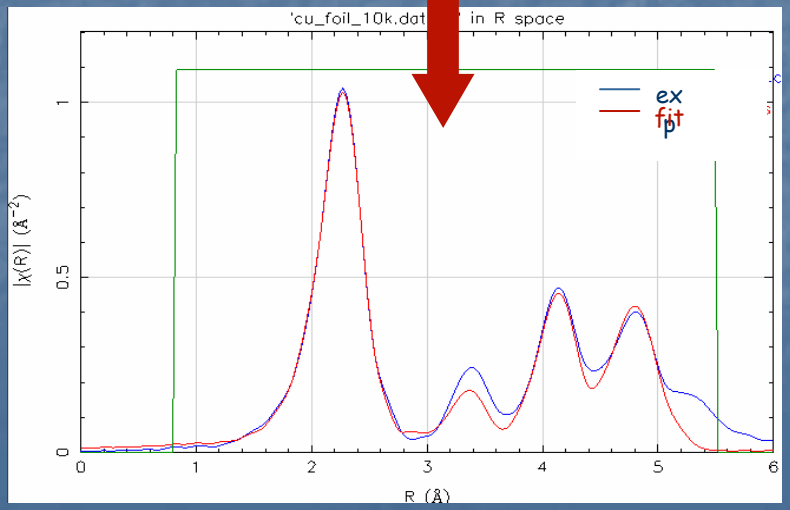
Theoretical formula

$$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

Amplitude and phase functions from atomic cluster models



How a data refinement program works



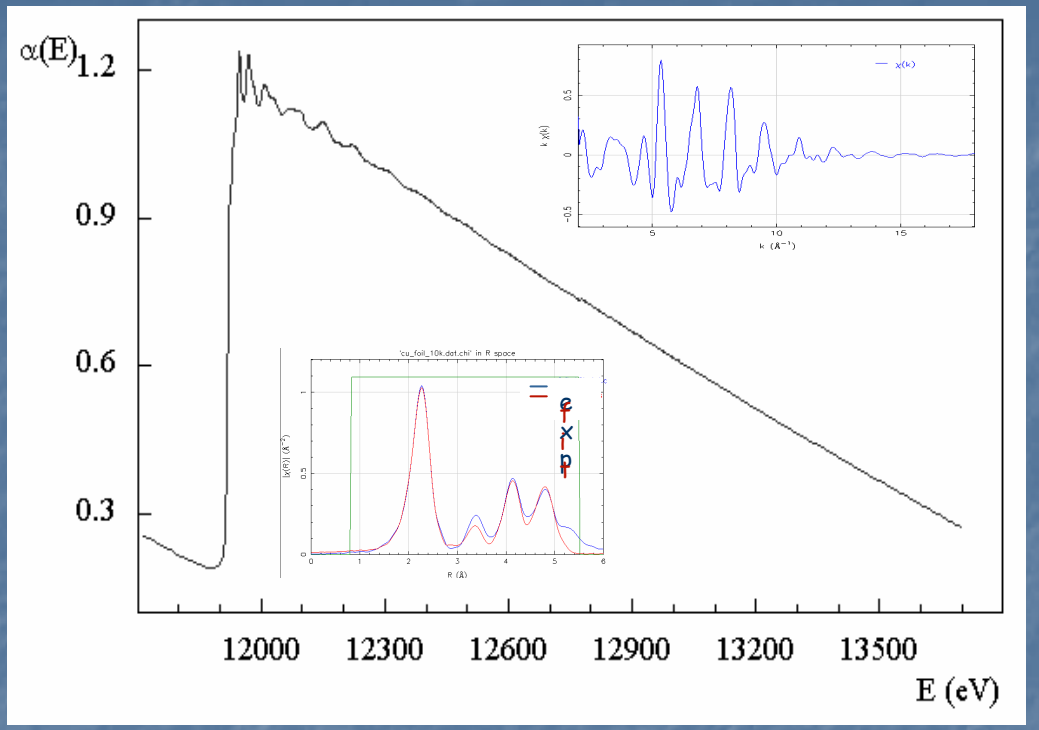
XAFS data analysis software

XAFS organizations

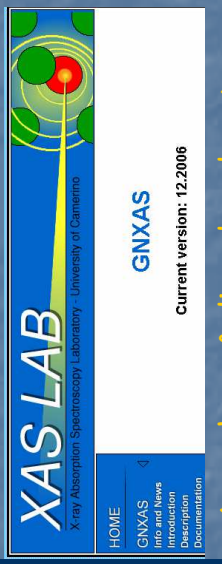
IXS Welcome to the International XAFS Society Home Page www.i-x-s.org

xafs.org

- XAFS
- RecentNews
- Applications
- TheoryAnalysis
- Experiment
- RelatedTechniques
- Community
- Resources
- Software
- Help



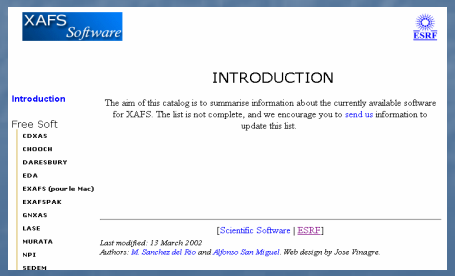
GNXAS home-page



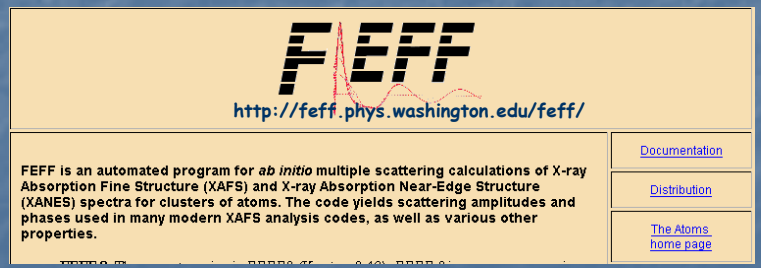
Amorphous & disordered systems

http://gnxas.unicam.it

XAFS data analysis



http://www.esrf.eu/computing/scientific/exafs/



FEFF home-page

http://cars9.uchicago.edu/ifeffit/

advantages:
- Freeware, multiplatform (Win, Mac, Linux)
- easy to handle,
- semi-automatic procedures

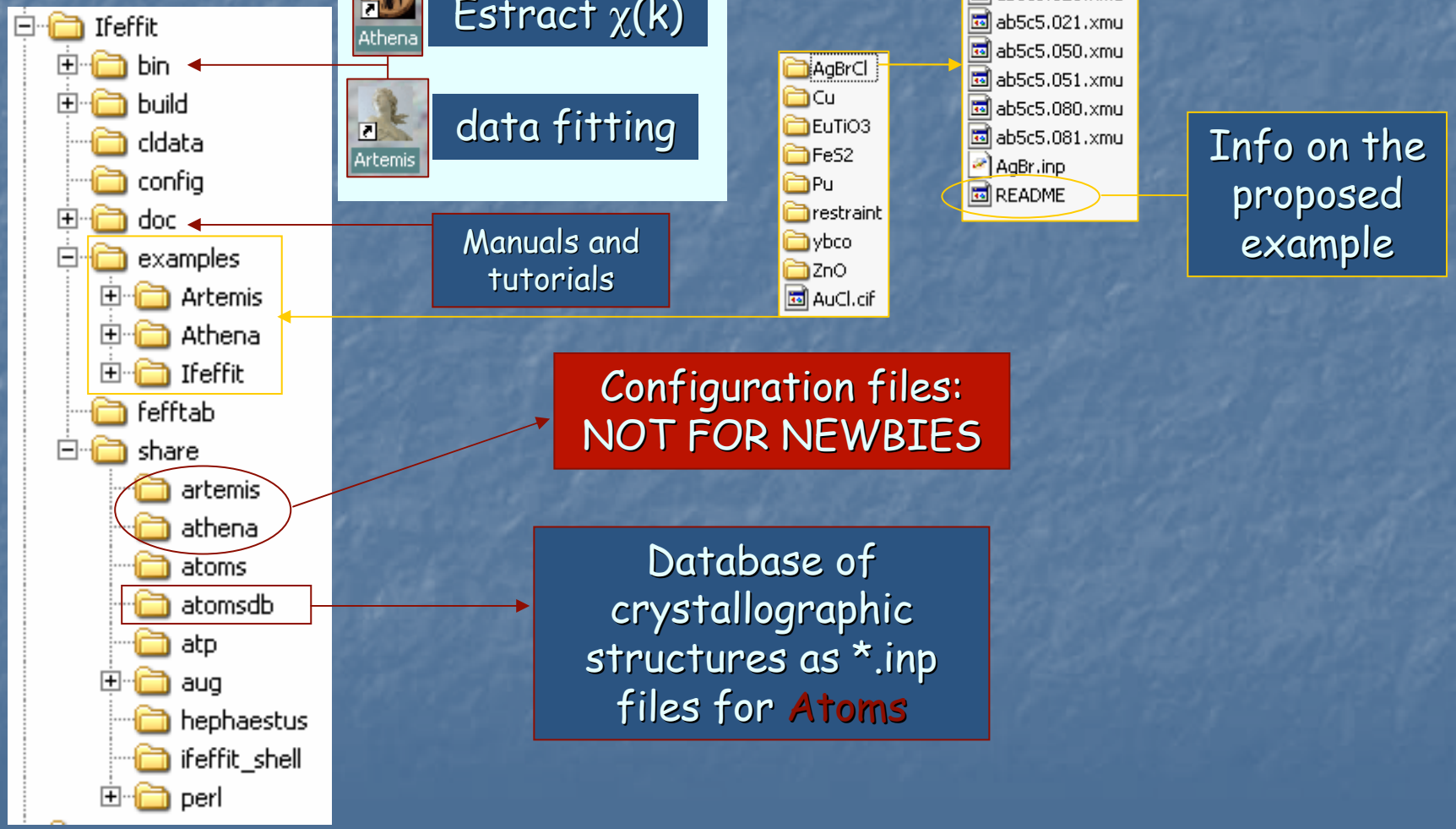
Ifeffit.exe

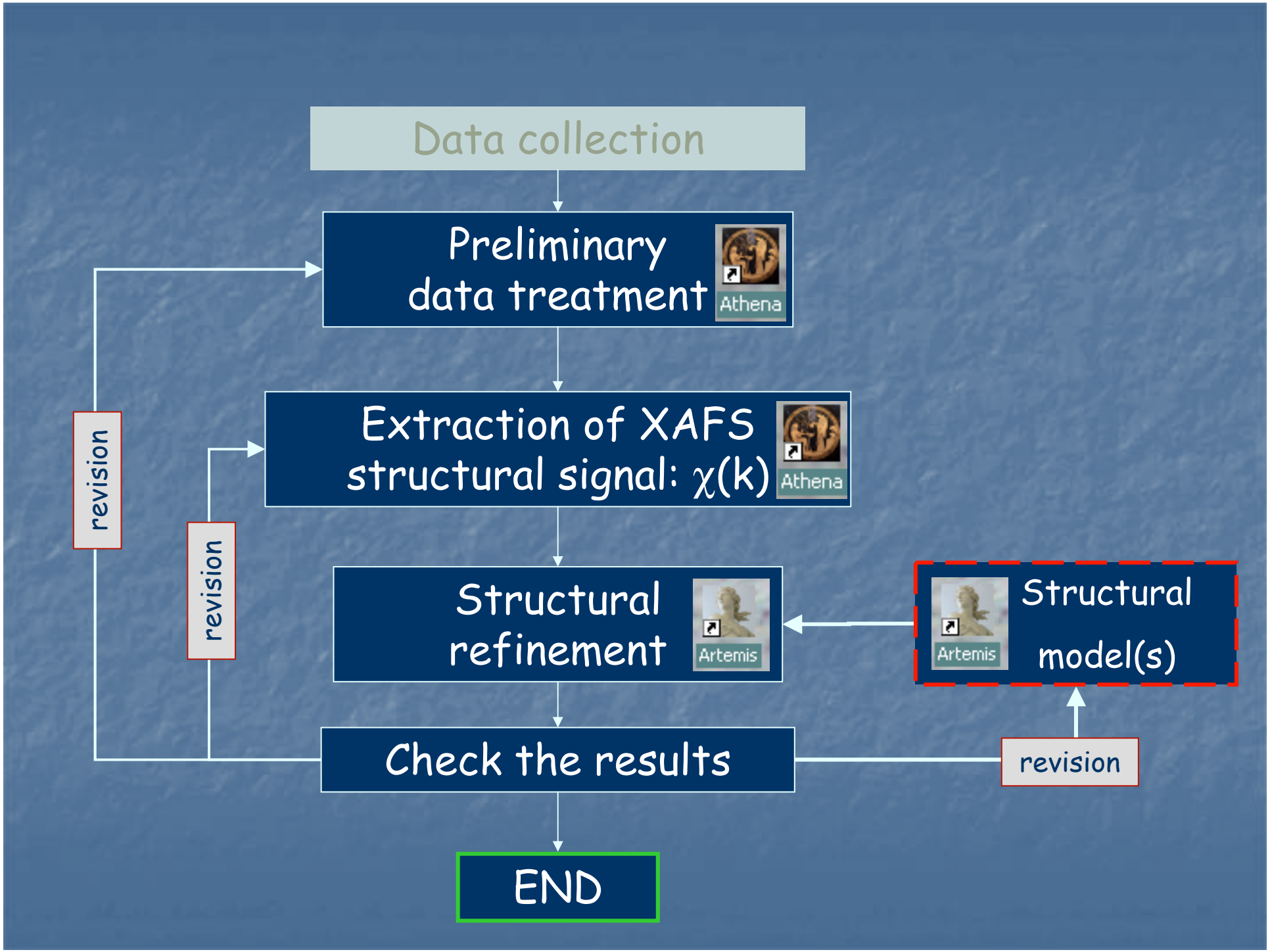
drawbacks:
- easy to handle,
- semi-automatic procedures

Install Ifeffit.exe

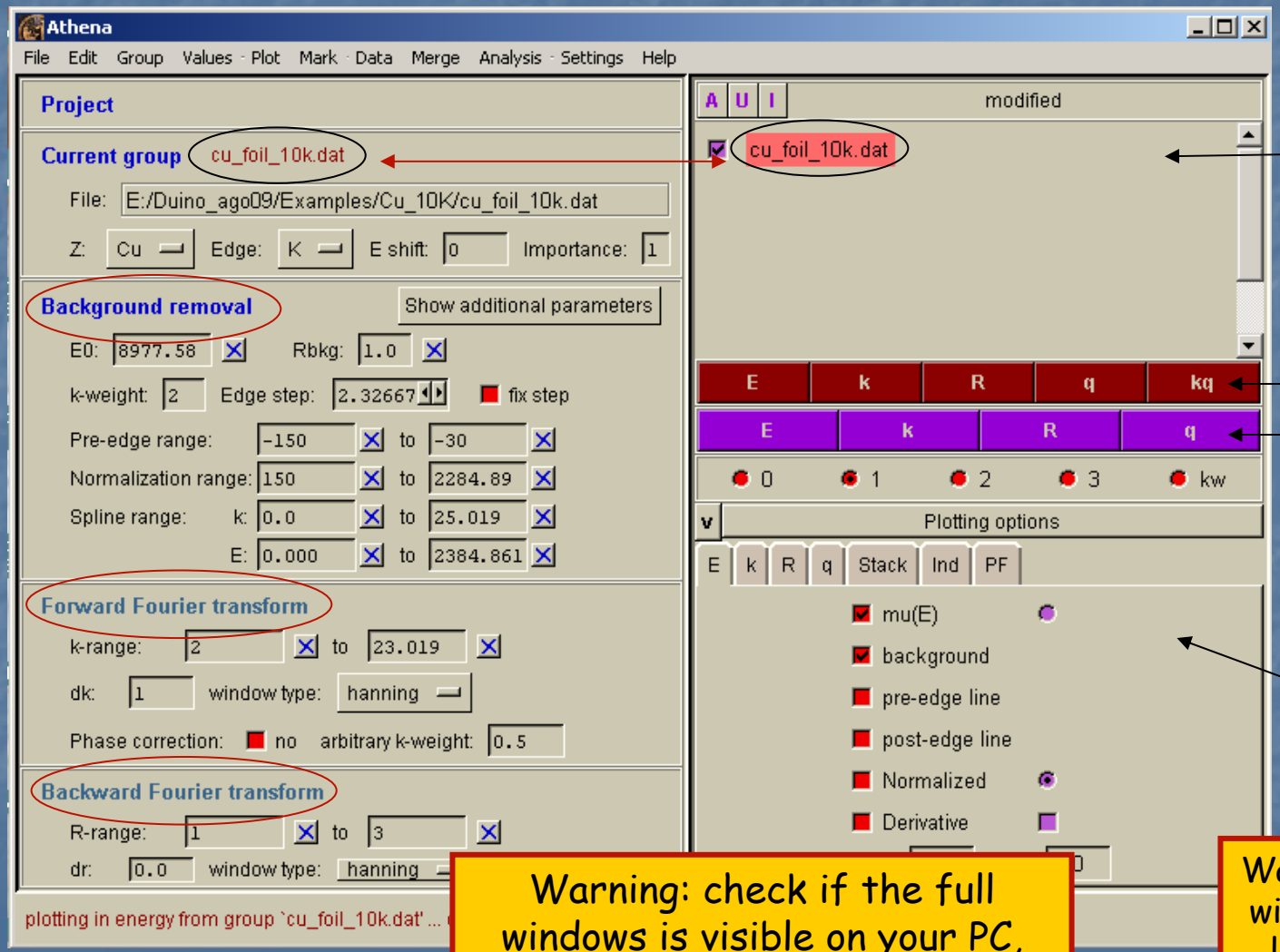
1.	athena	GUI for Data Processing with Ifeffit
2.	artemis	GUI for XAFS Fitting with Ifeffit
3.	hephaestus	GUI for general x-ray properties of the elements
4.	sixpack	GUI for XAFS Processing and Fitting with Ifeffit
5.	feff6L	Stand-alone program for ab inito EXAFS calculations
6.	atoms	Stand-alone, command line crystallography->feff.inp
7.	autobk	Stand-alone background removal program
8.	feffit	Stand-alone FEFF fitting program
9.	ifeffit	command-line version of Ifeffit

Inside the Ifeffit directory




Data collection
Preliminary data treatment
Athena
Extraction of XAFS structural signal: χ(k)
Athena
Structural refinement
Artemis
Structural model(s)
Artemis
Check the results
END
revision
revision
revision

Preliminary data treatment & Extraction of XAFS structural signal: χ(k)



List of files (group) opened into Athena

Plot highlighted files

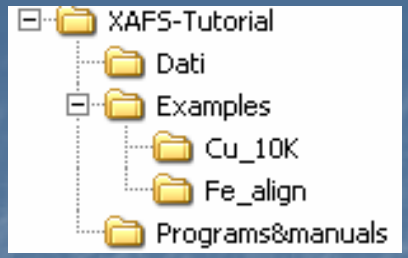
Plot (several) marked files

Options for plot

Warning: check if the full windows is visible on your PC, **smal screens (i.e. e-pc) may cut the lower part**

Warning: check the graphic windows and never close it leaving Athena/Artemis open… sometime the PC crashes

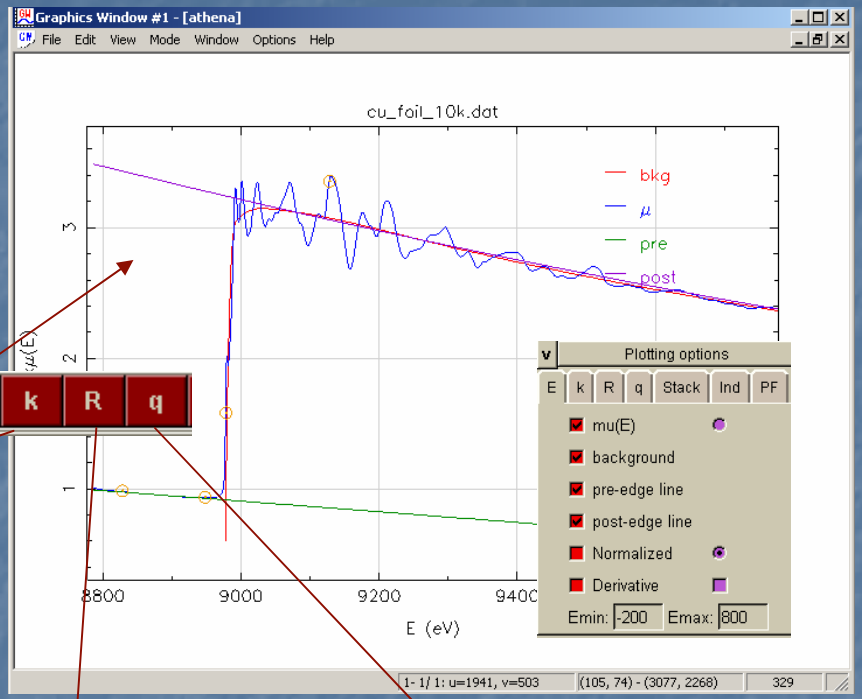
Example 1: Cu 10 K

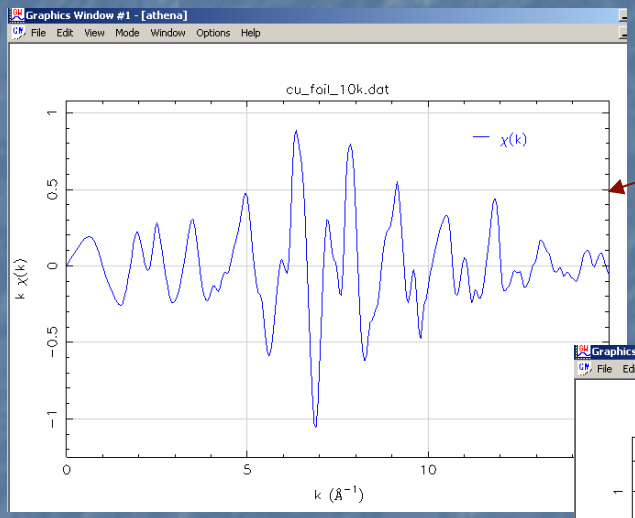


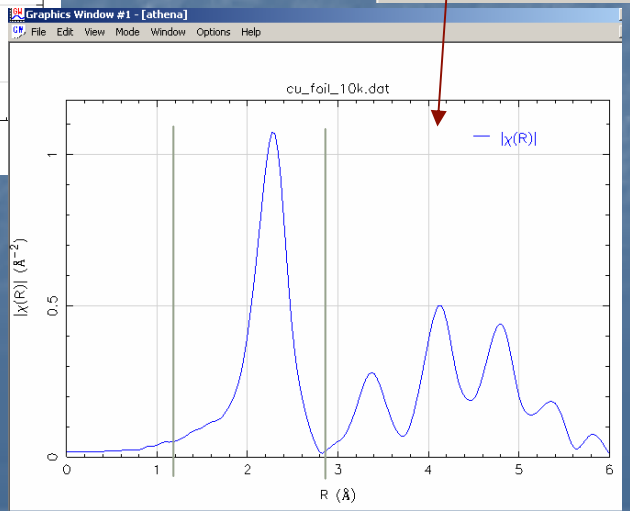
Open cu_foil_10k.dat into Athena

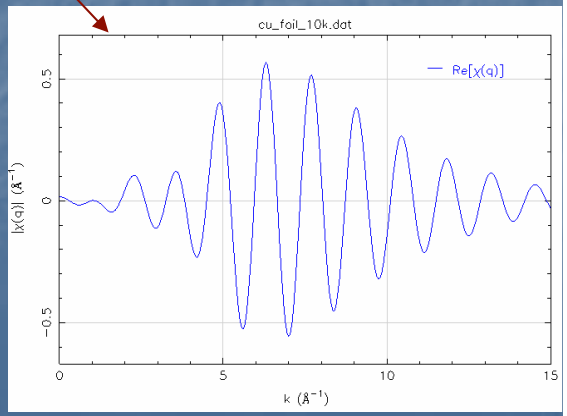
Exercise 1:

Look at the results obtained using the automatic extraction playing with plot options



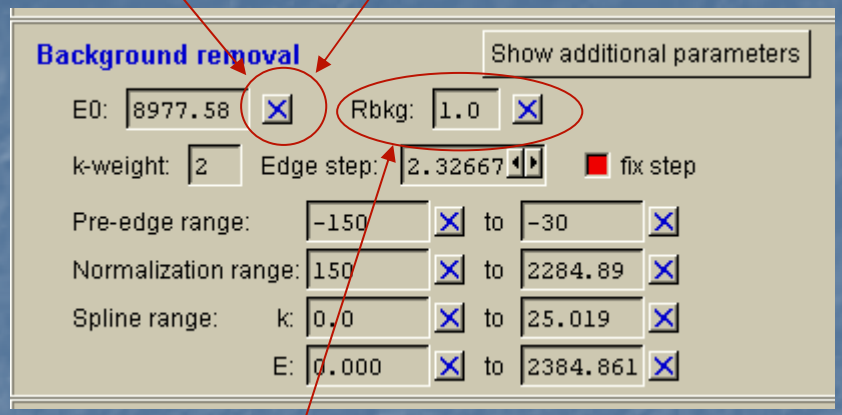






Select Eo

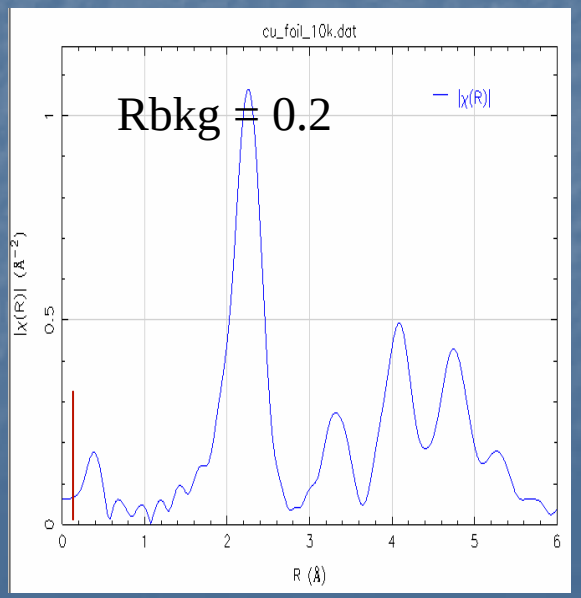
Takes the value from the cursor on the graph window

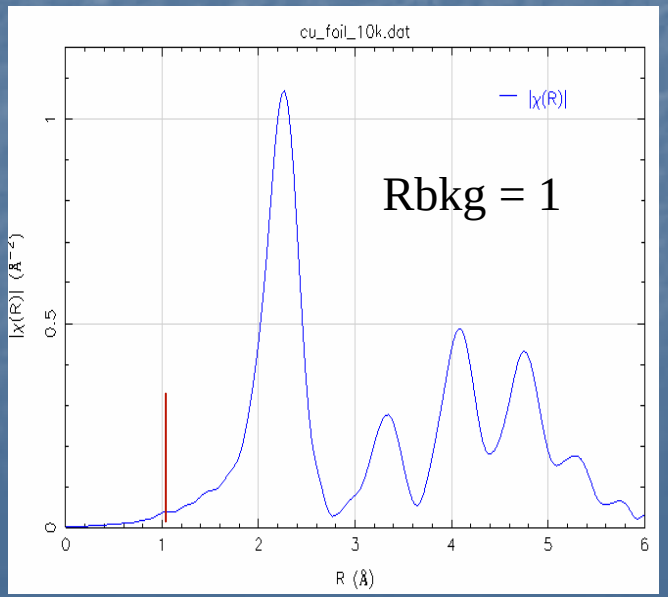


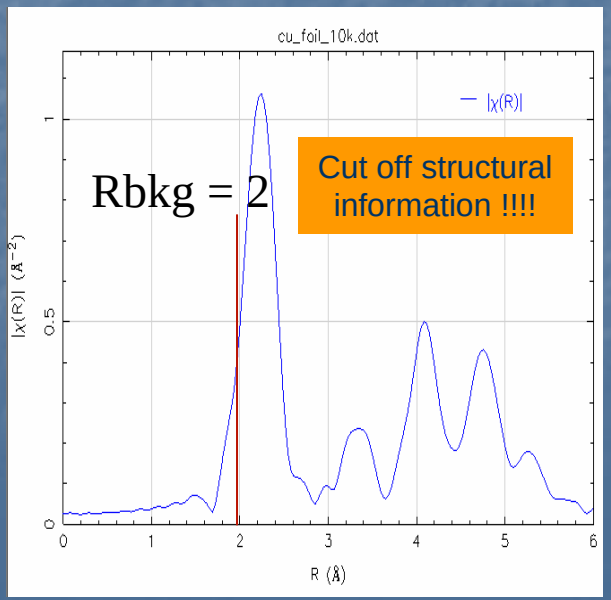
R cut off for automatic background calculation

Exercise 2: Look at the effects of changing background subtraction parameters

- Change Eo
- Change R_{bkg}
- ....







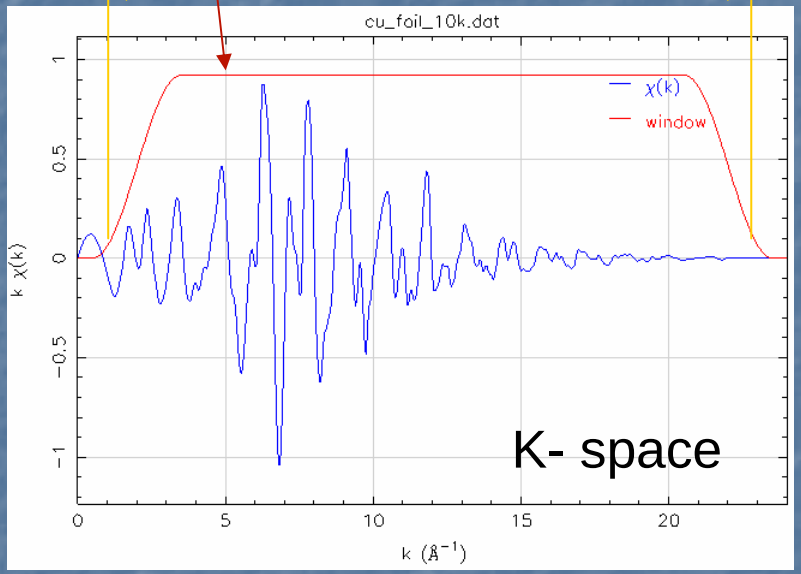
Forward Fourier transform

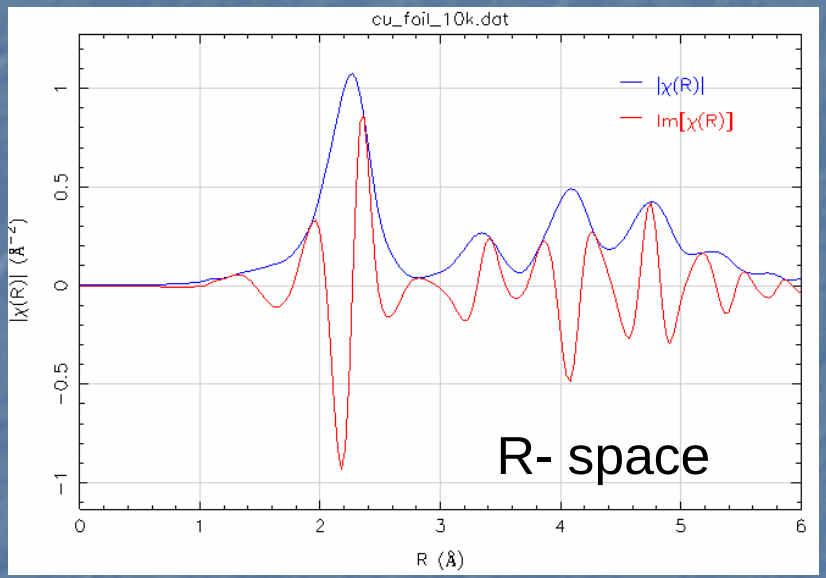
k-range: 2 to 23.019

dk: 1 window type: hanning

Phase correction: no arbitrary k-weight: 0.5

Exercise 3: in Real space look at the effects of changing extraction and FT parameters





0 1 2 3 kw

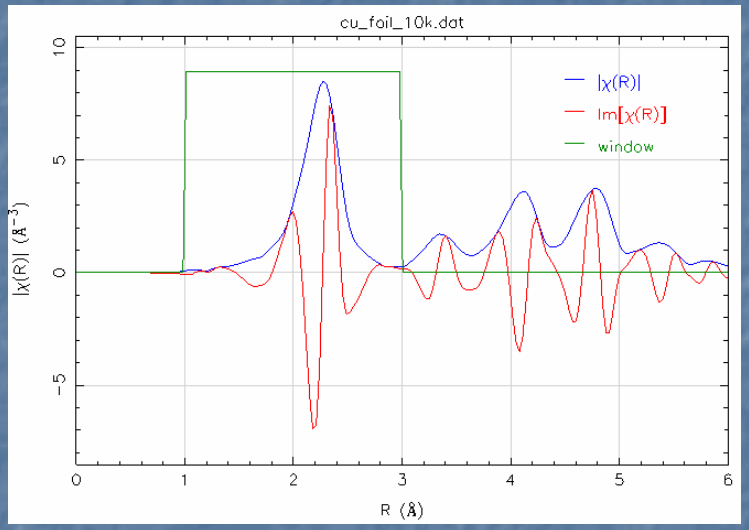
FT of: $k^{kw}\chi$ (k)

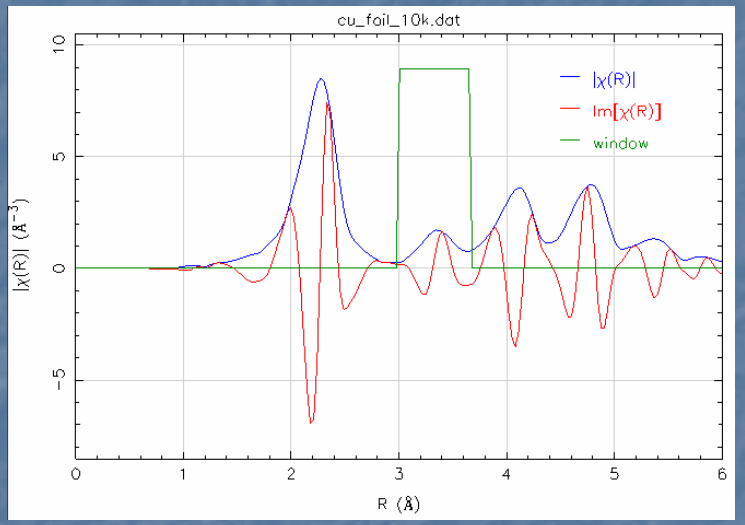
Backward Fourier transform

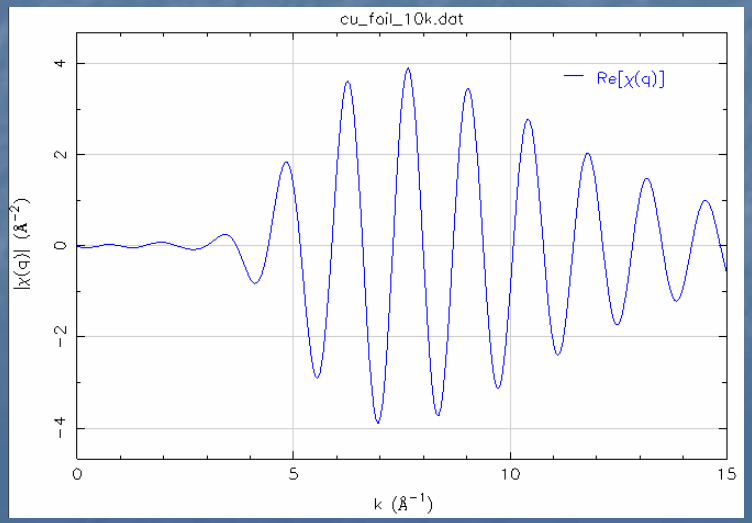
R-range: 1 to 3

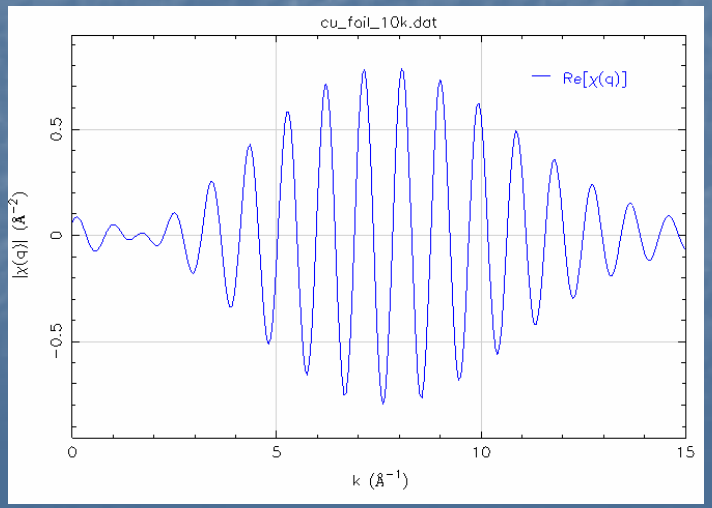
dr: 0.0 window type: hanning

Exercise 4: in q (Back Fourier) space look at the effects of changing BF parameters and regions

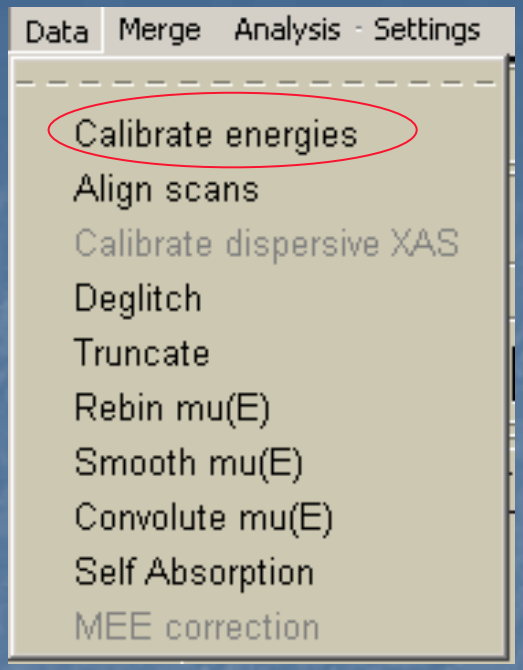




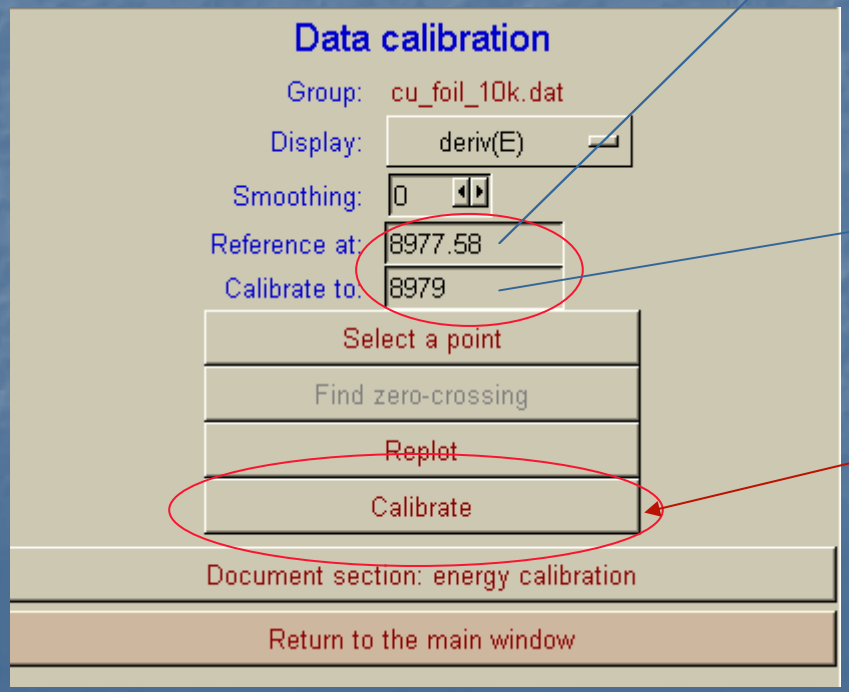


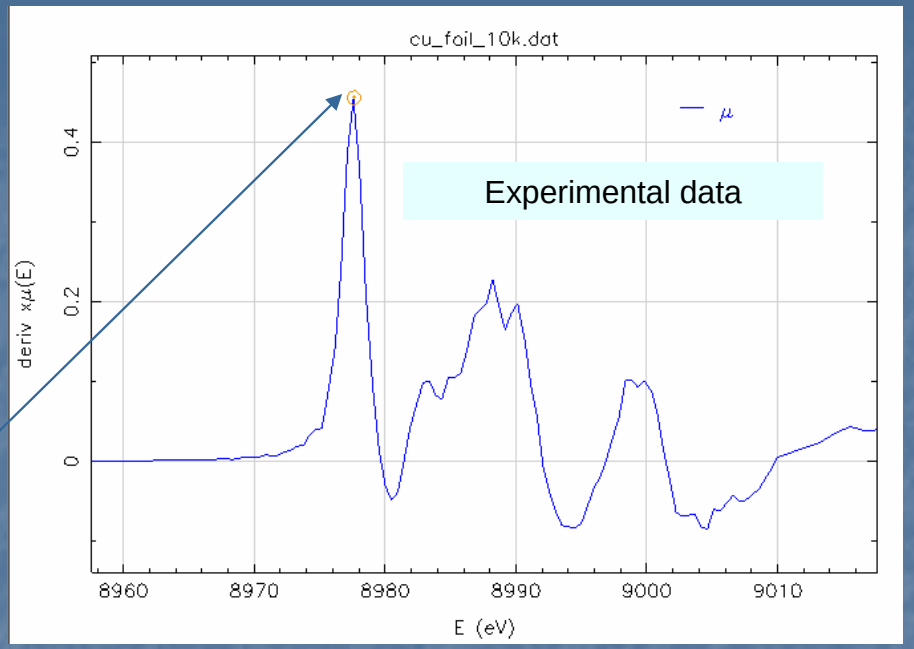


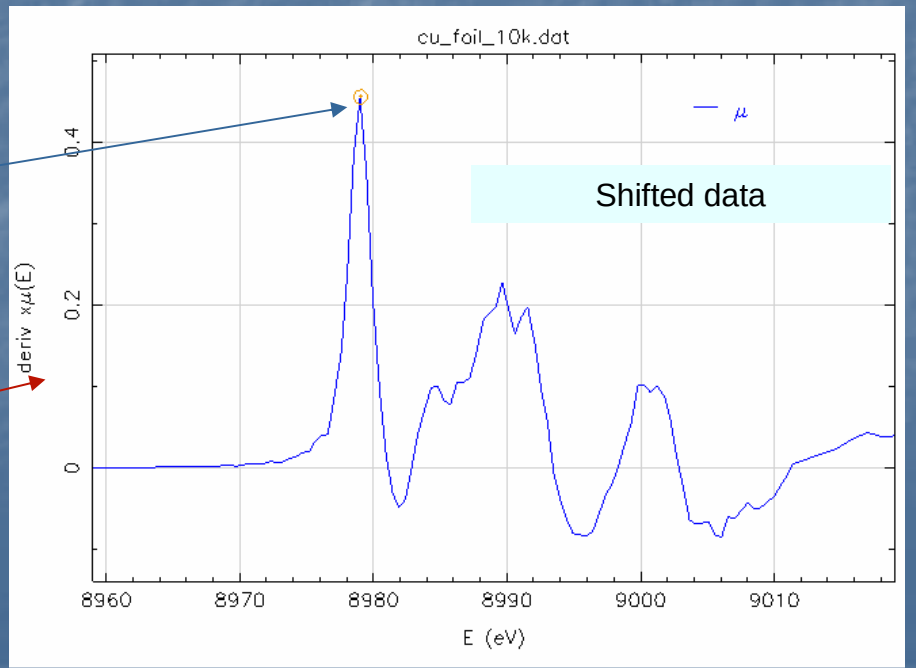
Exercise 5: Data treatment

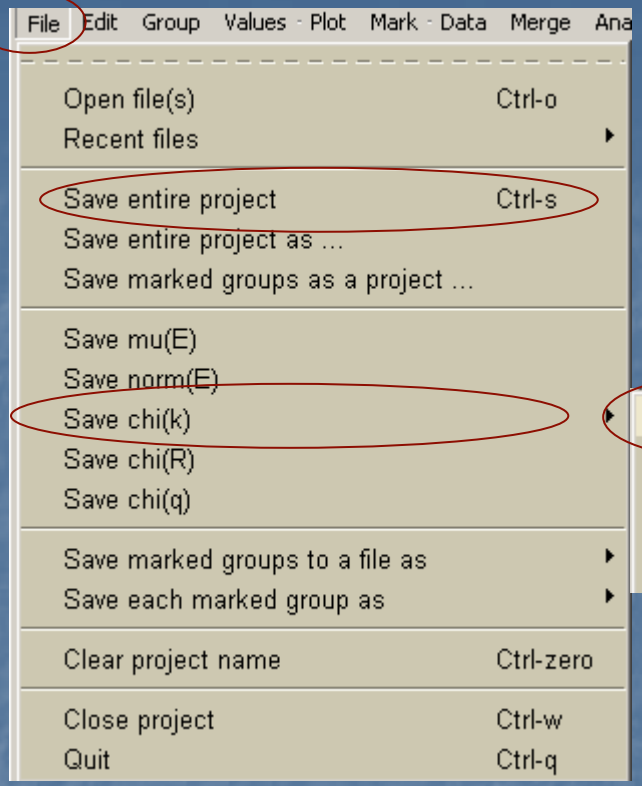


Shifts the spectrum to have selected point (reference at) at the calibration energy (calibrate to)









Save:

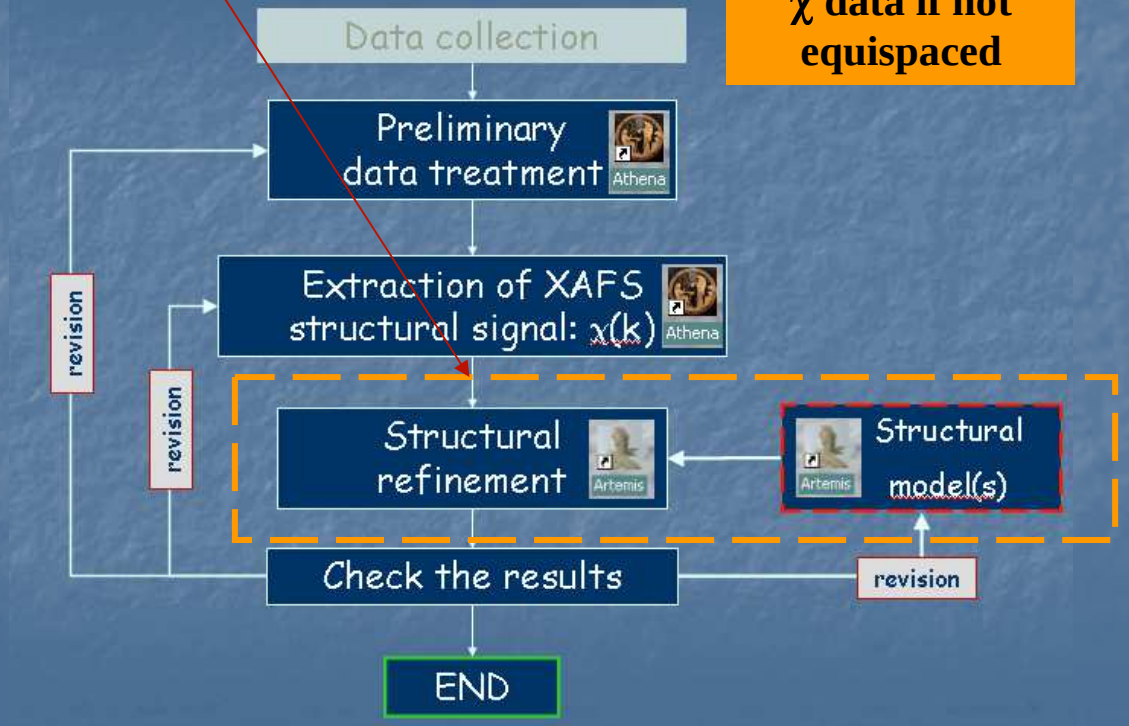
cu_foil_10k.dat.chi

χ(k) is required for ARTEMIS

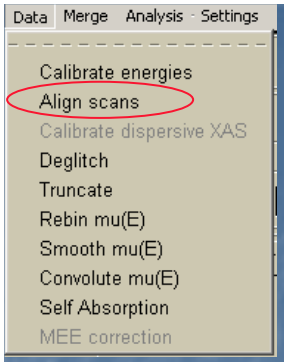
Note: Arthemis requires equispaced k data !!!

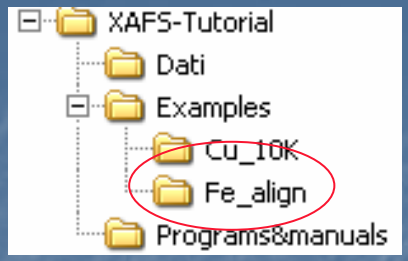
(i.e. δk = 0.05)

You cannot use χ data if not equispaced



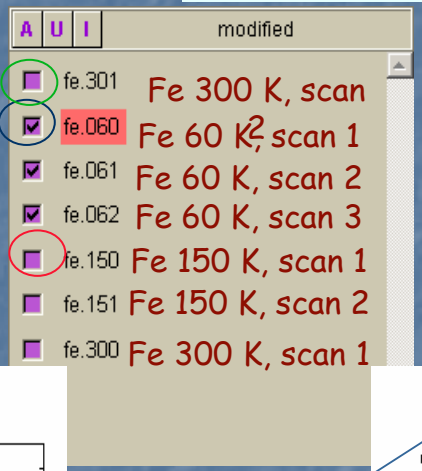
Working with several files

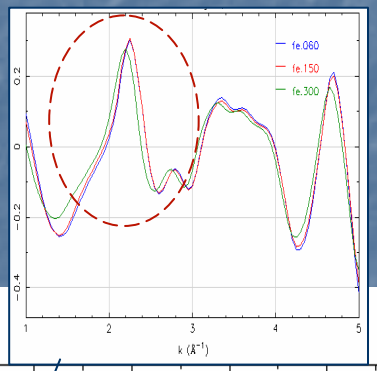




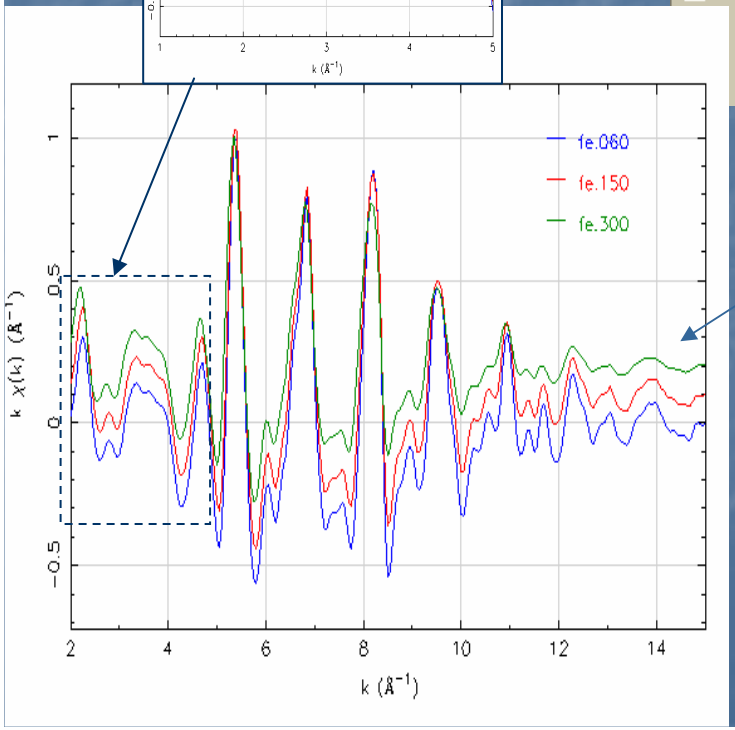
Go into the Fe_Align directory

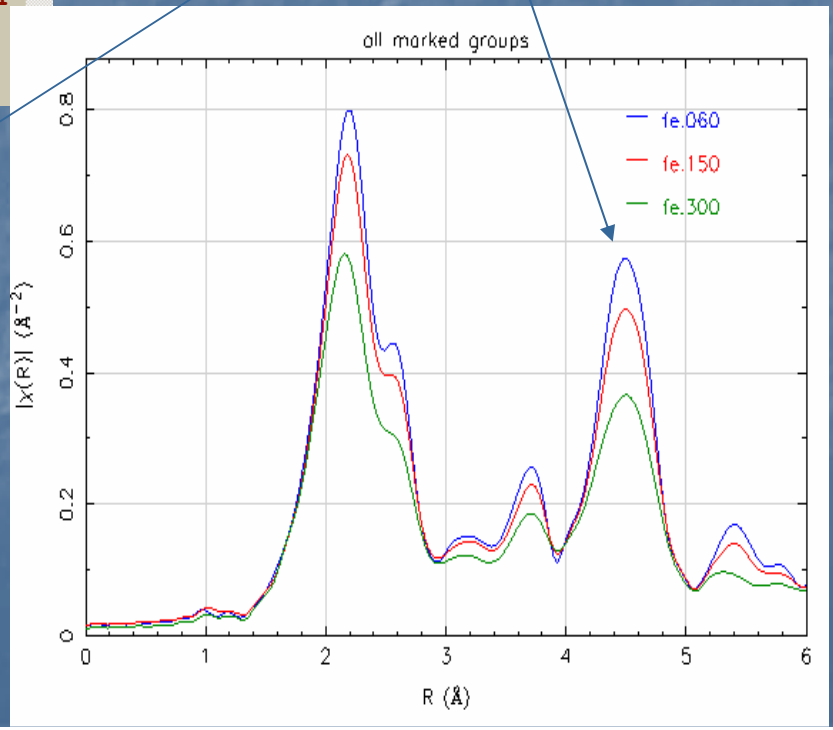
Open all Fe files into Athena



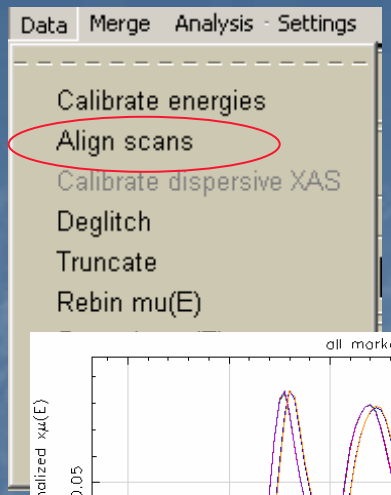


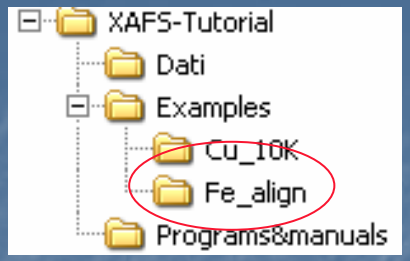
Temperature effect on EXAFS and FT data



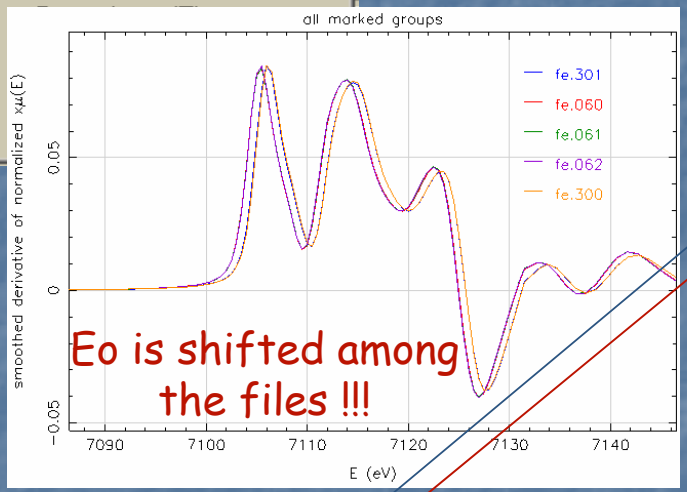


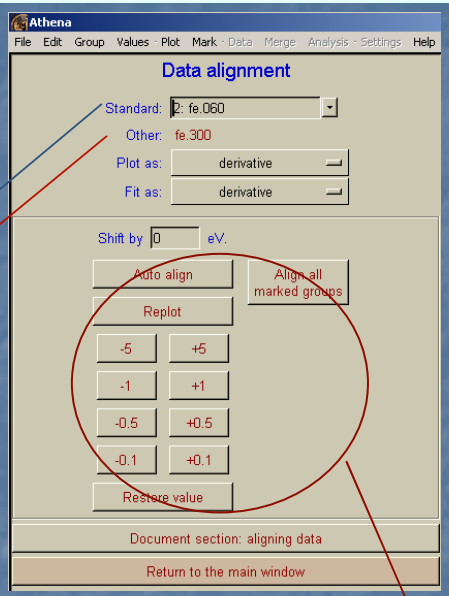
Exercise 6: align Eo

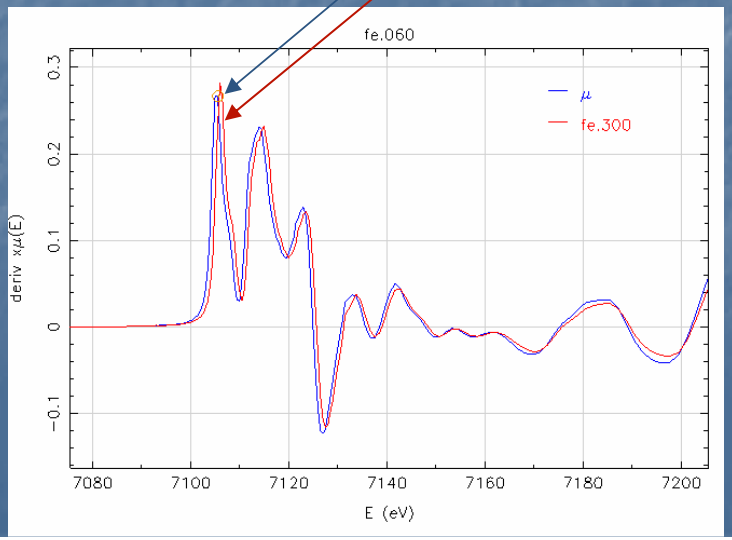


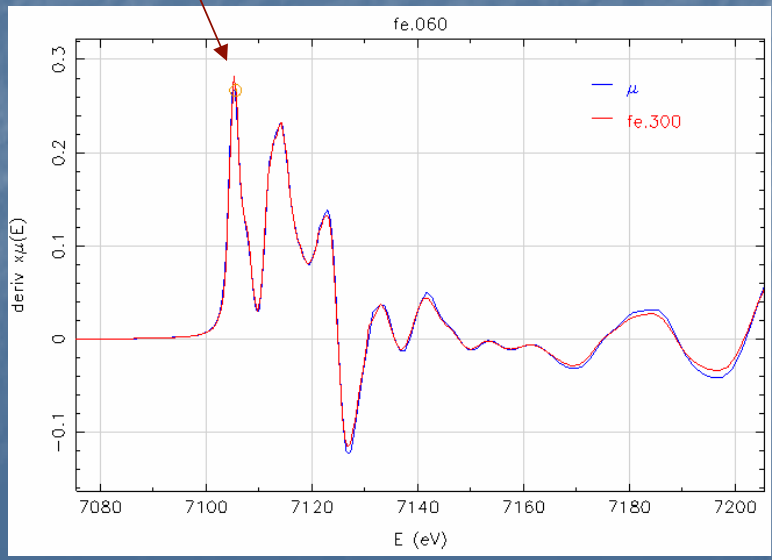


Open Fe files into Athena

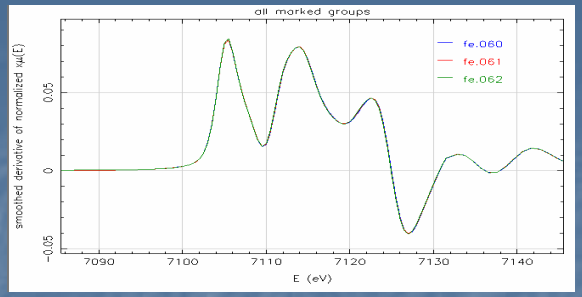


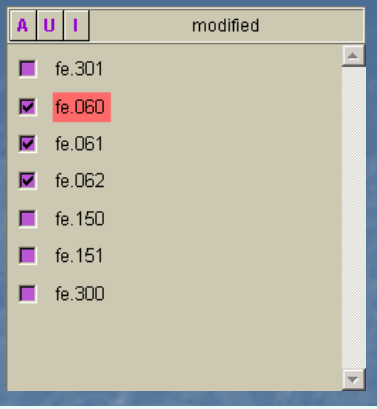


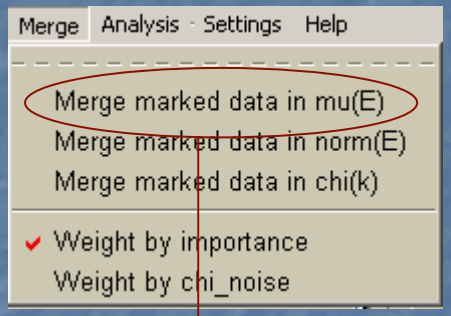


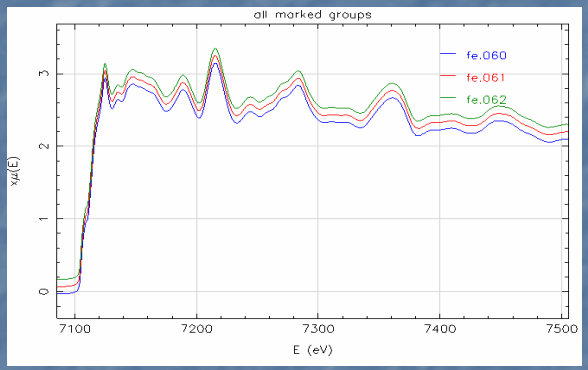


Exercise 7: Merge several files

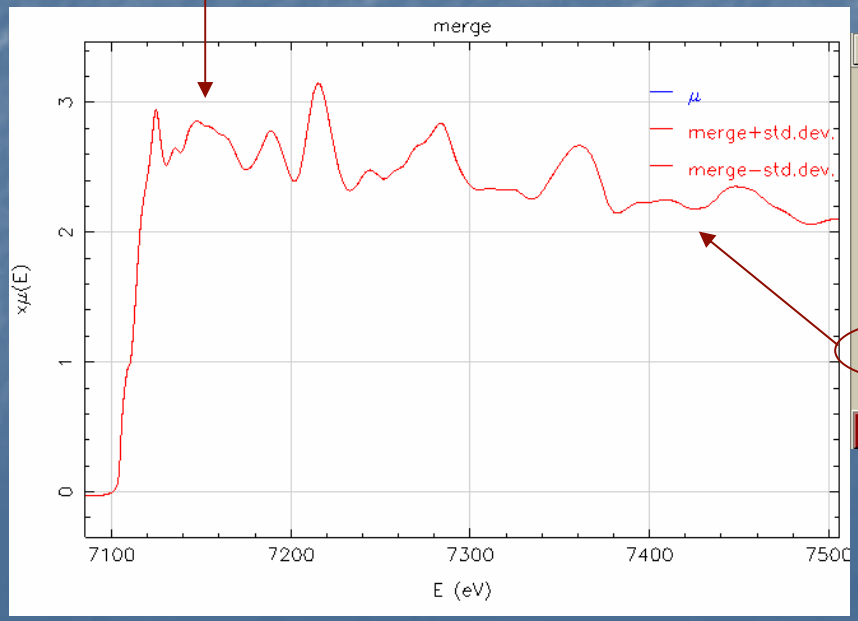


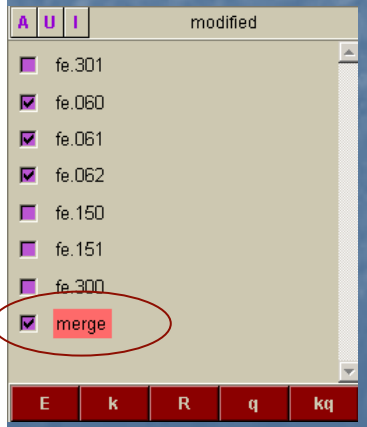


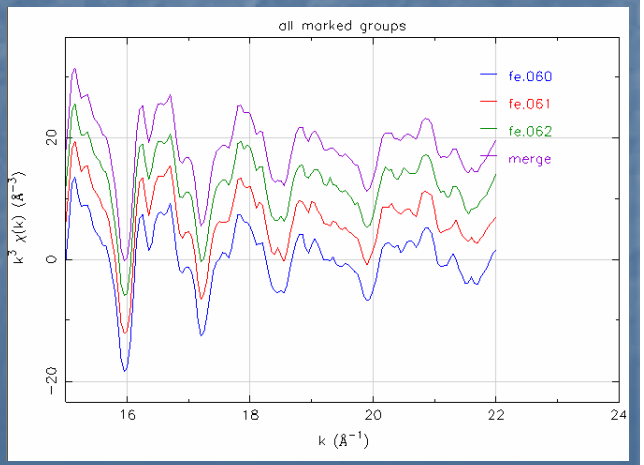




Fe 60 are now aligned

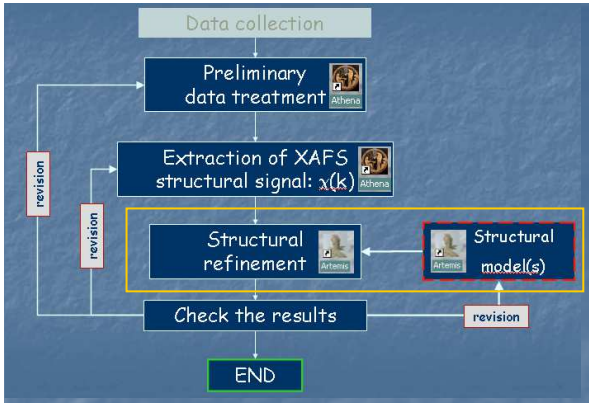






Full Exercise:

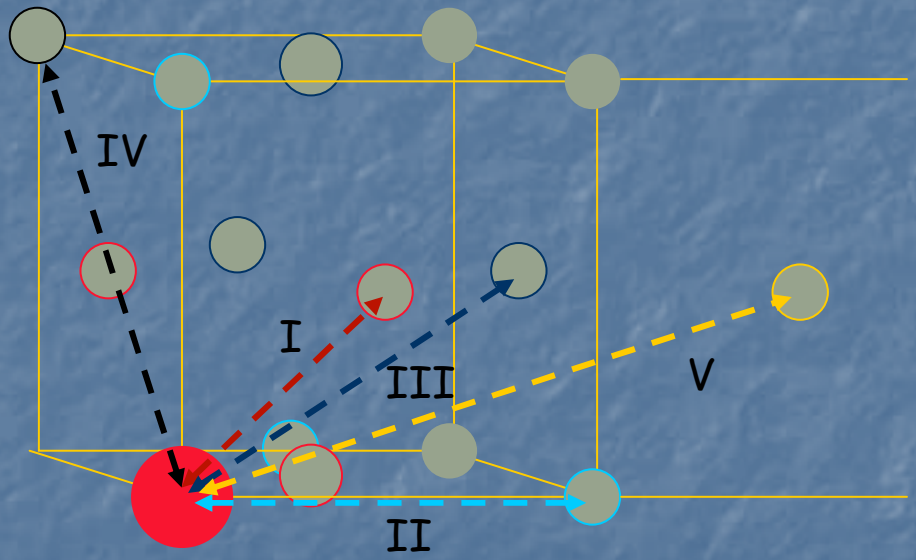
1. Read Fe Files
2. Align Fe files on order to have the same Eo
3. Merge files having the same T
4. Save $\chi(k)$ of merged files, to be used for the structural analysis



Structural model & Data refinement

Cu-fcc

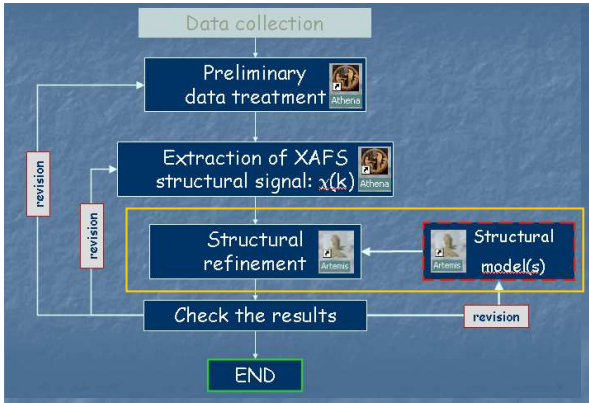
metal
SPG: fcc, f m 3 m (# 220)
a = 3.61 A
Cu 0.0 0.0 0.0



Sh	R	N	$R_{Cu}(A)$
I:	a/sqrt(2)	12	2.553
II:	a	6	3.610
III:	a·sqrt(1.5)	24	4.421
IV:	a·sqrt(2)	12	5.105
V:	a·sqrt(2.5)	24	5.708
....			

You can visualize the structure using VESTA program

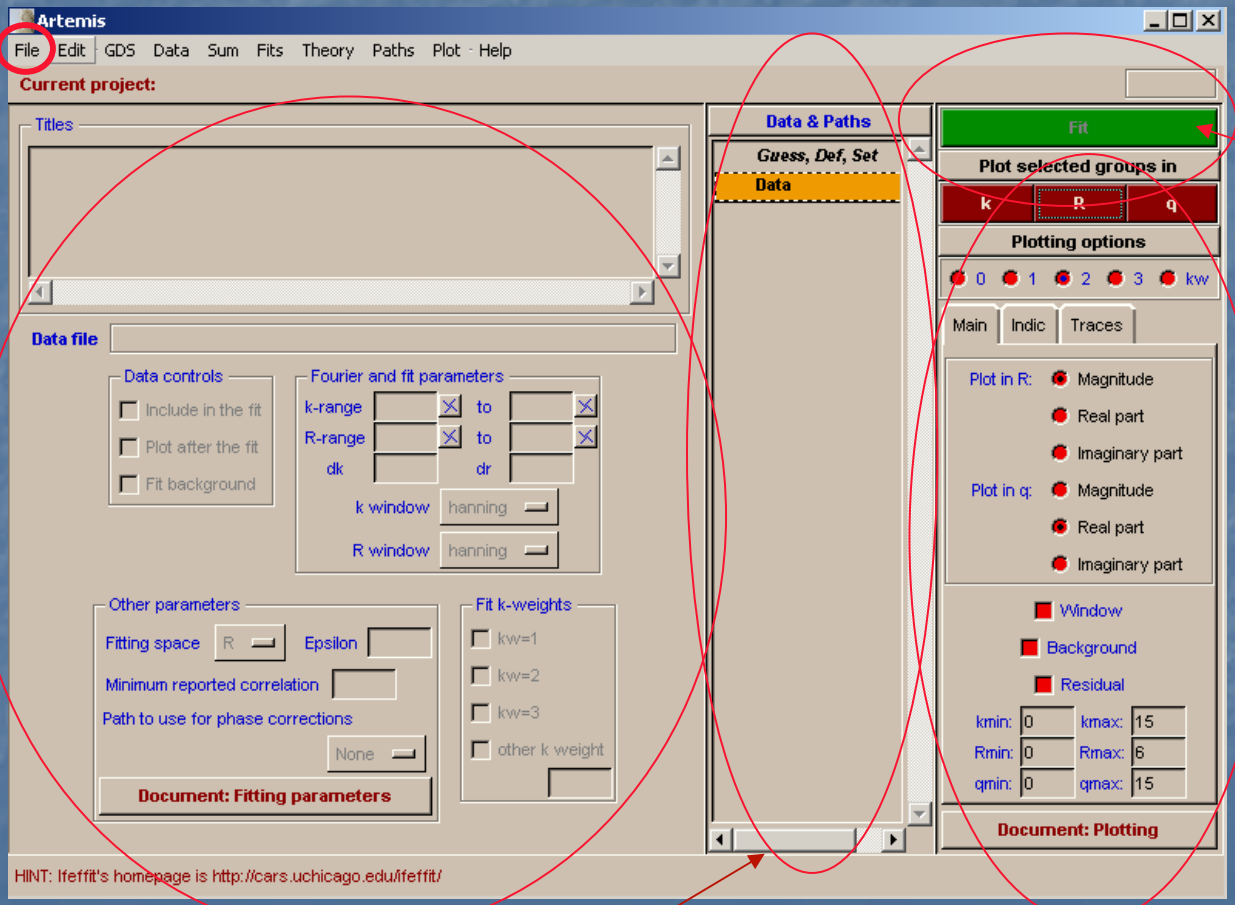
icsd_43493_Copper.cif



Structural model & Data refinement

Start the ARTEMIS program

The ARTEMIS panel



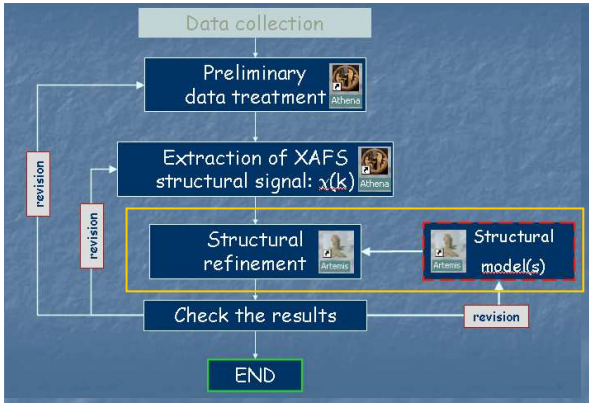
Start the refinement

Warning: check the full windows is visible on your PC, smaller screens may cut the lower part

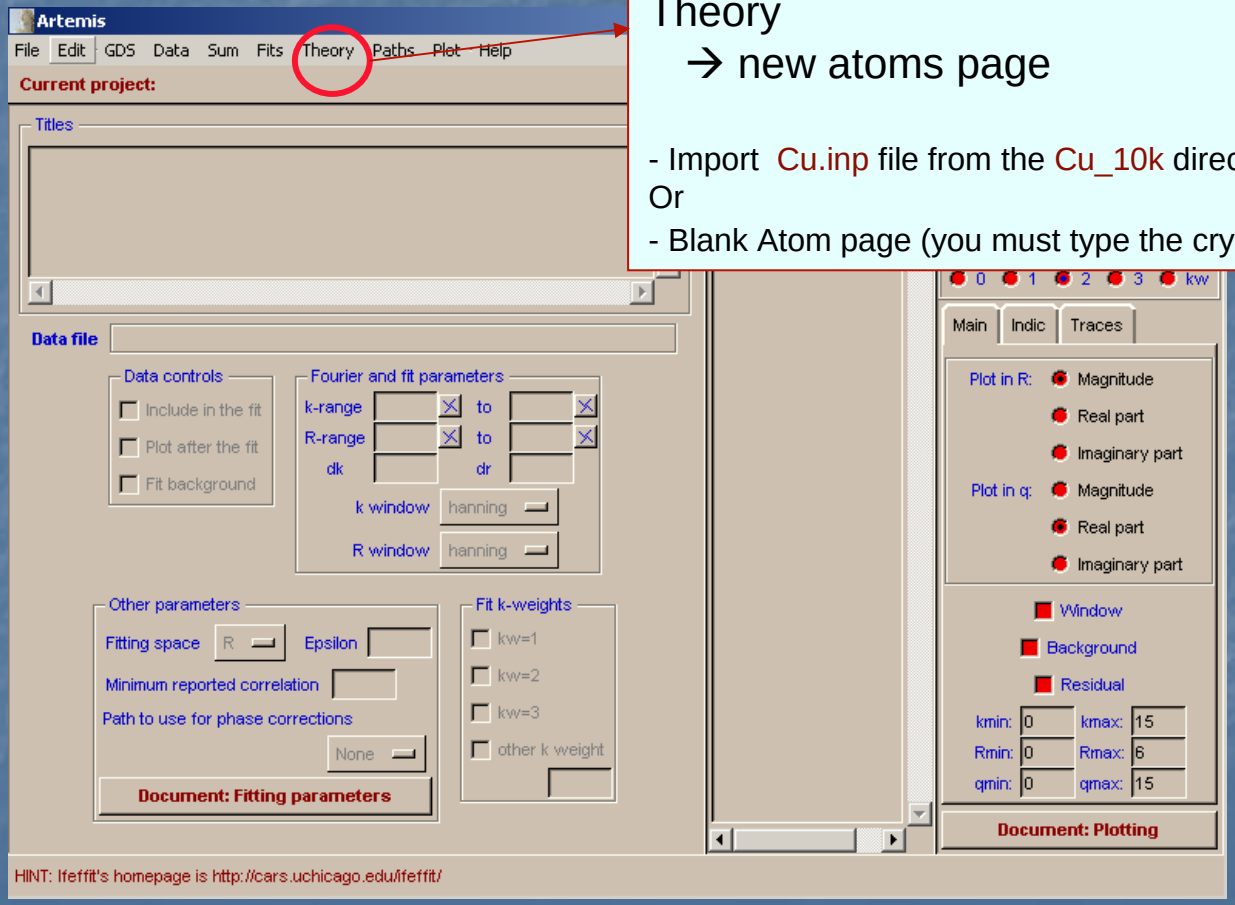
Warning: check the graphic windows and never close it leaving Athena/Artemis open… sometime the PC crashes

Depends on what is highlighted in the Data & Paths panel

Controls for plotting



Structural model & Data refinement



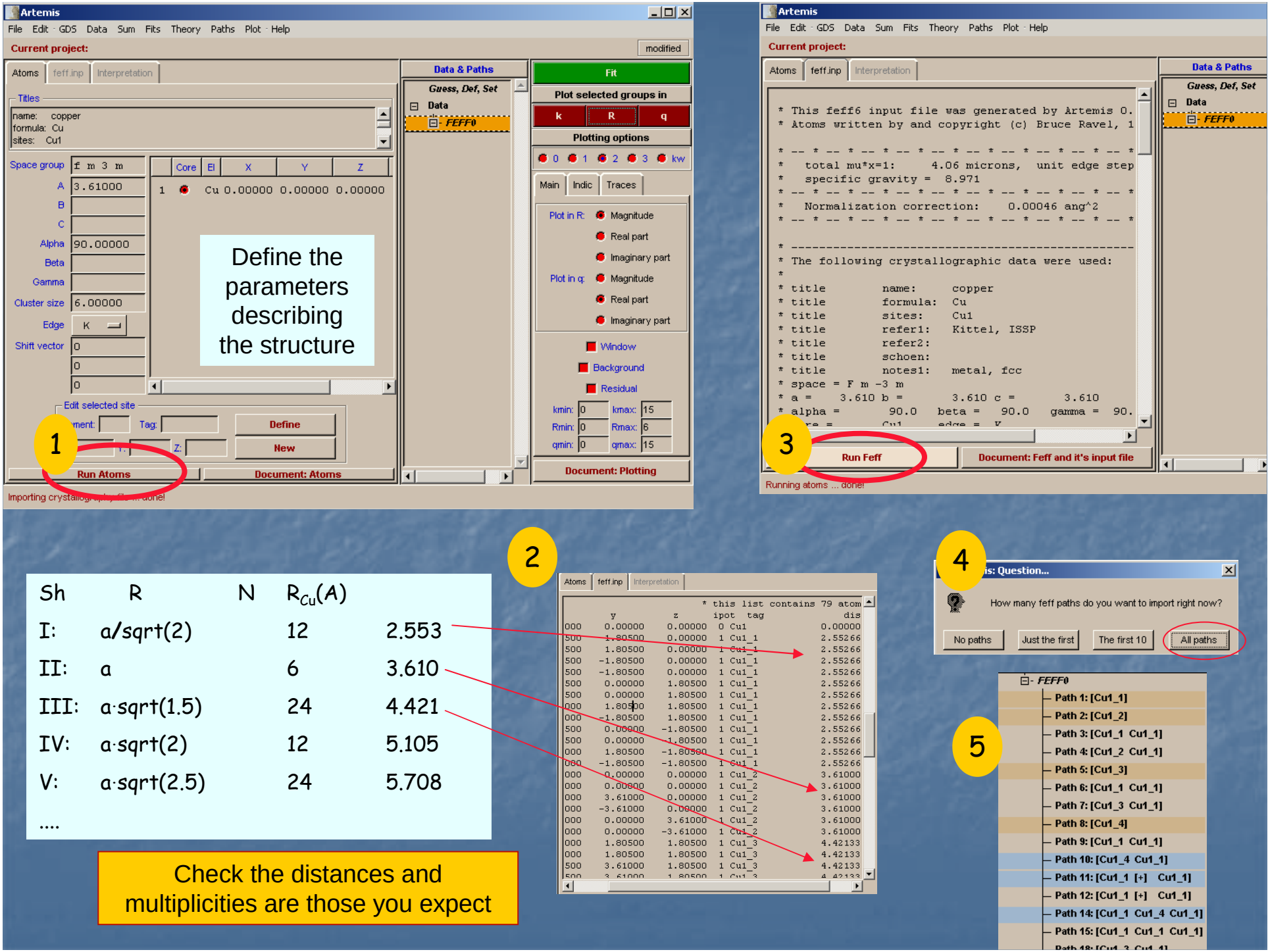
Theory
→ new atoms page

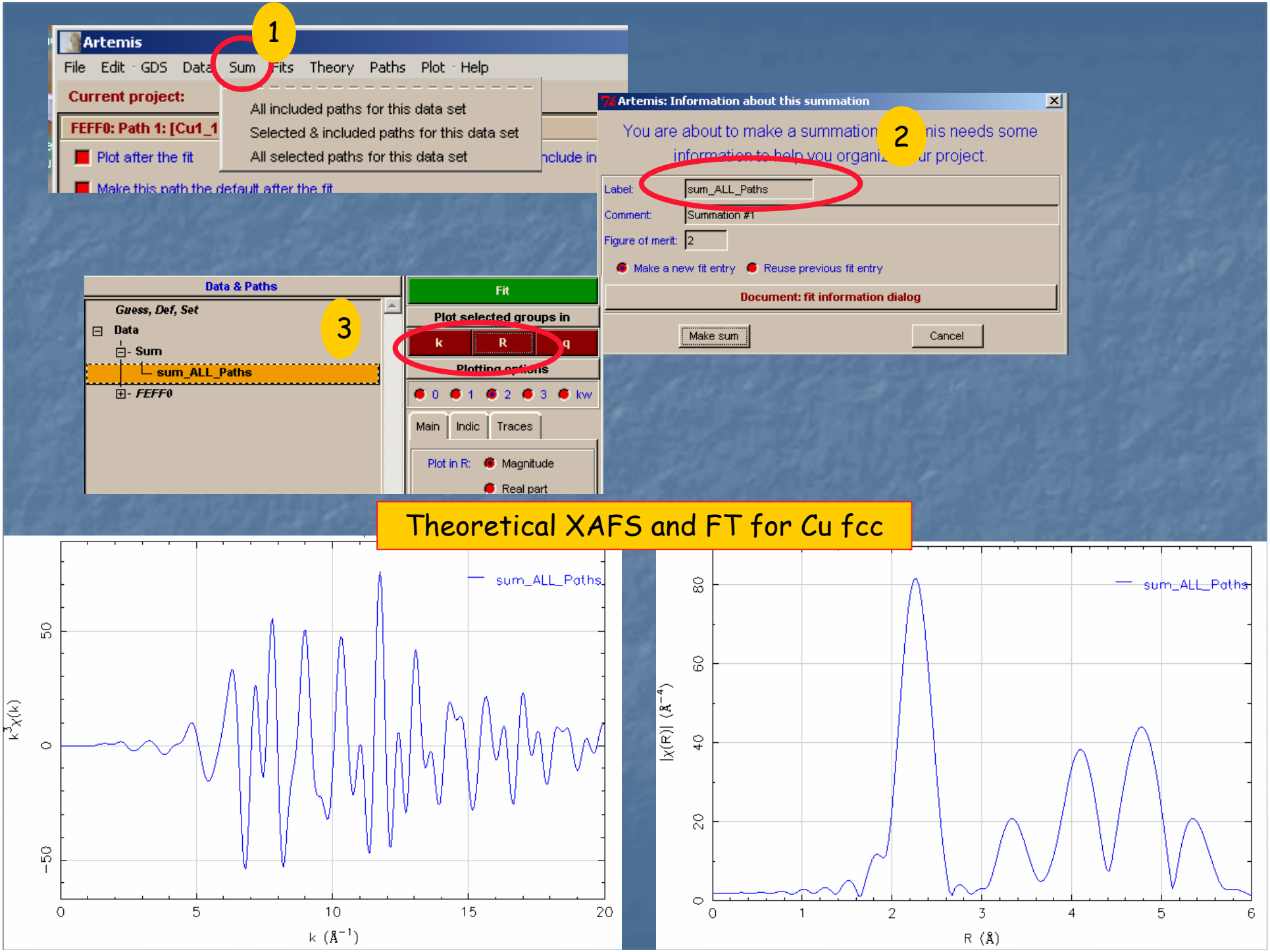
- Import Cu.inp file from the Cu_10k directory

Or

- Blank Atom page (you must type the crystallographic info)

Warning: check the full windows is visible on your PC, smaller screens may cut the lower part

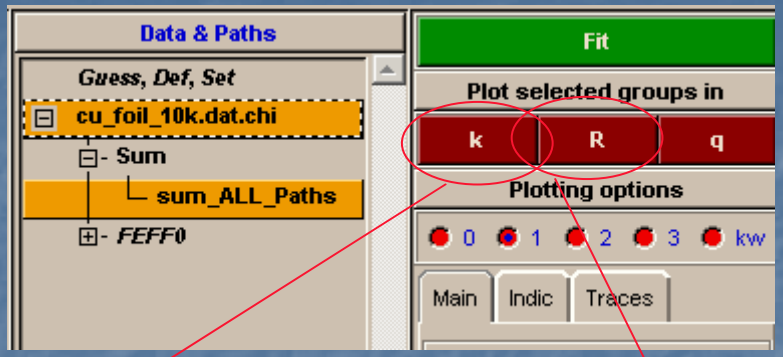

Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help
Current project:
modified
Atoms
feff.inp
Interpretation
Titles
name: copper
formula: Cu
sites: Cu1
Space group
A 3.61000
Alpha 90.00000
Cluster size 6.00000
Edge K
Shift vector
Core El X Y Z
1 Cu 0.00000 0.00000 0.00000
Define the parameters describing the structure
Edit selected site
Define
New
1
Run Atoms
Document: Atoms
Data & Paths
Guess, Def, Set
Data
FEFF0
Fit
Plot selected groups in
k R q
Plotting options
Main Indic Traces
Plot in R: Magnitude Real part Imaginary part
Plot in q: Magnitude Real part Imaginary part
Window
Background
Residual
kmin: kmax: 15
Rmin: Rmax: 6
qmin: qmax: 15
Document: Plotting
Importing crystallography file ... done!
Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help
Current project:
Atoms
feff.inp
Interpretation
* This feff6 input file was generated by Artemis 0.
* Atoms written by and copyright (c) Bruce Ravel, 1
* total mu*x=1: 4.06 microns, unit edge step
* specific gravity = 8.971
* Normalization correction: 0.00046 ang^2
* The following crystallographic data were used:
* title name: copper
* title formula: Cu
* title sites: Cu1
* title refer1: Kittel, ISSP
* title refer2:
* title schoen:
* title notes1: metal, fcc
* space = F m -3 m
* a = 3.610 b = 3.610 c = 3.610
* alpha = 90.0 beta = 90.0 gamma = 90.
3
Run Feff
Document: Feff and it's input file
Running atoms ... done!
Data & Paths
Guess, Def, Set
Data
FEFF0
Sh R N $R_{Cu}(A)$
I: a/sqrt(2) 12 2.553
II: a 6 3.610
III: a·sqrt(1.5) 24 4.421
IV: a·sqrt(2) 12 5.105
V: a·sqrt(2.5) 24 5.708
....
Check the distances and multiplicities are those you expect
2
Atoms
feff.inp
Interpretation
* this list contains 79 atom
y z ipot tag dis
000 0.00000 0.00000 0 Cu1 0.00000
500 1.80500 0.00000 1 Cu1_1 2.55266
500 1.80500 0.00000 1 Cu1_1 2.55266
500 -1.80500 0.00000 1 Cu1_1 2.55266
500 -1.80500 0.00000 1 Cu1_1 2.55266
500 0.00000 1.80500 1 Cu1_1 2.55266
500 0.00000 1.80500 1 Cu1_1 2.55266
000 1.80500 1.80500 1 Cu1_1 2.55266
000 -1.80500 1.80500 1 Cu1_1 2.55266
500 0.00000 -1.80500 1 Cu1_1 2.55266
500 0.00000 -1.80500 1 Cu1_1 2.55266
000 1.80500 -1.80500 1 Cu1_1 2.55266
000 -1.80500 -1.80500 1 Cu1_1 2.55266
000 0.00000 0.00000 1 Cu1_2 3.61000
000 0.00000 0.00000 1 Cu1_2 3.61000
000 3.61000 0.00000 1 Cu1_2 3.61000
000 -3.61000 0.00000 1 Cu1_2 3.61000
000 0.00000 3.61000 1 Cu1_2 3.61000
000 0.00000 -3.61000 1 Cu1_2 3.61000
000 1.80500 1.80500 1 Cu1_3 4.42133
000 1.80500 1.80500 1 Cu1_3 4.42133
500 3.61000 1.80500 1 Cu1_3 4.42133
4
Question...
How many feff paths do you want to import right now?
No paths
Just the first
The first 10
All paths
5
FEFF0
Path 1: [Cu1_1]
Path 2: [Cu1_2]
Path 3: [Cu1_1 Cu1_1]
Path 4: [Cu1_2 Cu1_1]
Path 5: [Cu1_3]
Path 6: [Cu1_1 Cu1_1]
Path 7: [Cu1_3 Cu1_1]
Path 8: [Cu1_4]
Path 9: [Cu1_1 Cu1_1]
Path 10: [Cu1_4 Cu1_1]
Path 11: [Cu1_1 [+] Cu1_1]
Path 12: [Cu1_1 [+] Cu1_1]
Path 14: [Cu1_1 Cu1_4 Cu1_1]
Path 15: [Cu1_1 Cu1_1 Cu1_1]

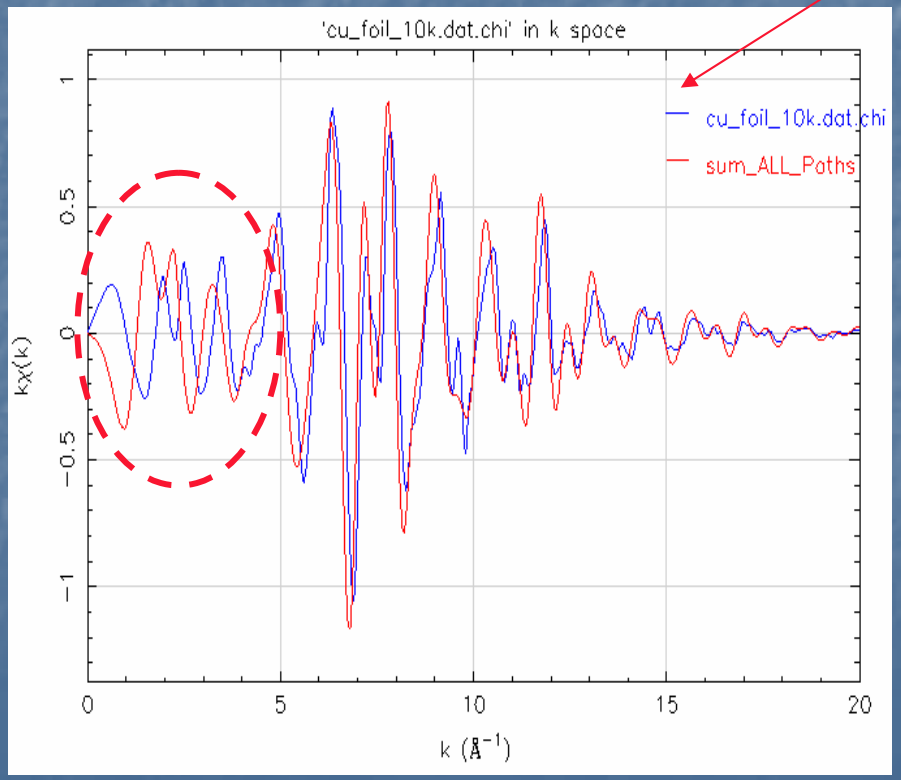

Artemis
File Edit GDS Data Sum Fits Theory Paths Plot Help
1
Current project:
FEFF0: Path 1: [Cu1_1
Plot after the fit
Make this path the default after the fit
All included paths for this data set
Selected & included paths for this data set
All selected paths for this data set
Artemis: Information about this summation
You are about to make a summation
2
Label: sum_ALL_Paths
Comment: Summation #1
Figure of merit: 2
Make a new fit entry
Reuse previous fit entry
Document: fit information dialog
Make sum
Cancel
Data & Paths
Guess, Def, Set
Data
Sum
sum_ALL_Paths
FEFF0
3
Fit
Plot selected groups in
k
R
q
0 1 2 3 kw
Main Indic Traces
Plot in R:
Magnitude
Real part
Theoretical XAFS and FT for Cu fcc
sum_ALL_Paths
k³χ(k)
k (Å⁻¹)
|χ(R)| (Å⁻⁴)
R (Å)

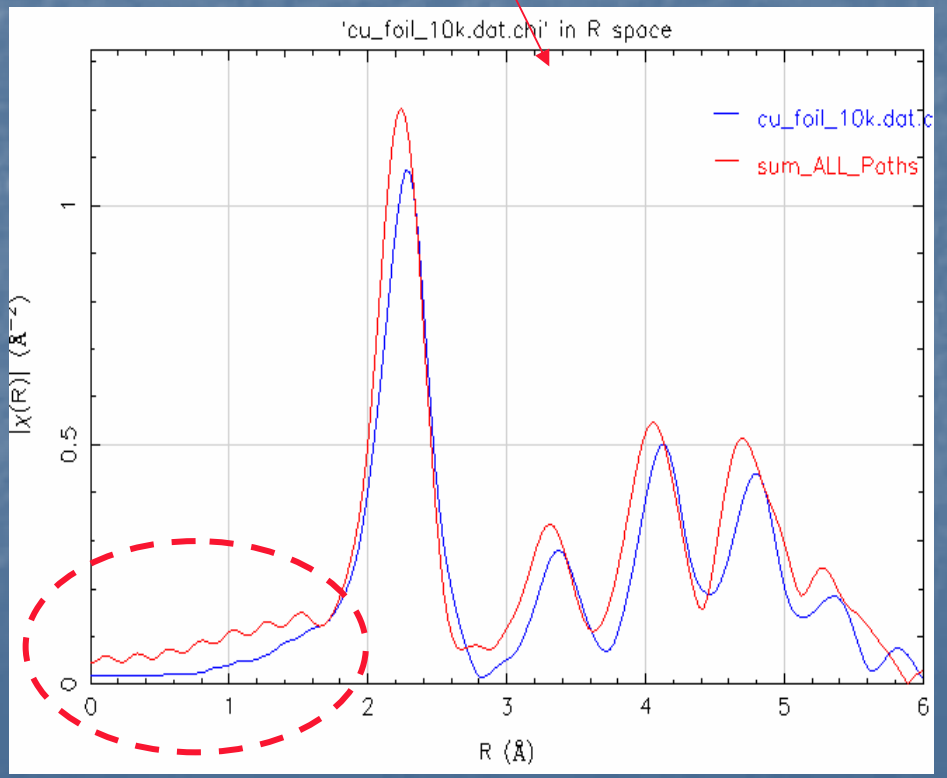
Compare model and experimental data

Open Cu_foil_10k.inp

Using CRTL key you can select groups for plot



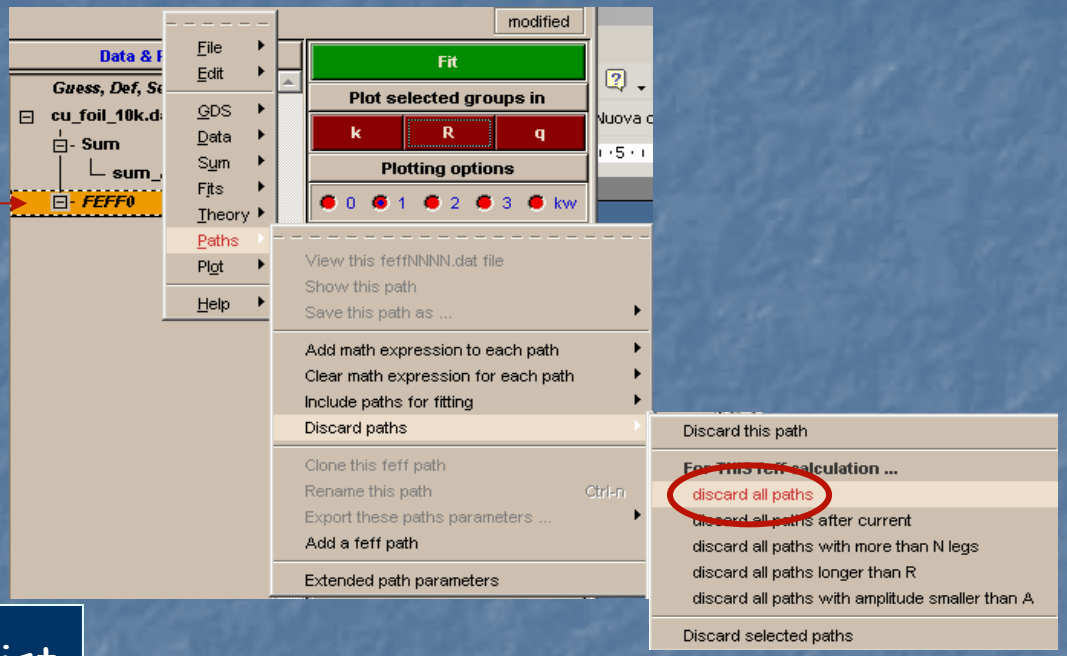




1st shell analysis

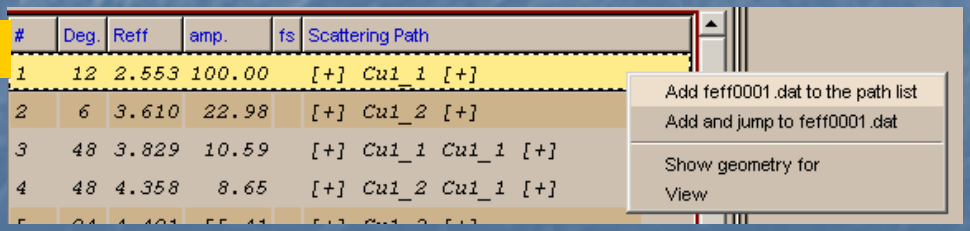
remove all paths or restart ARTEMIS

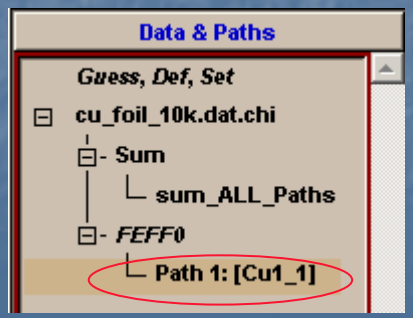
Right click

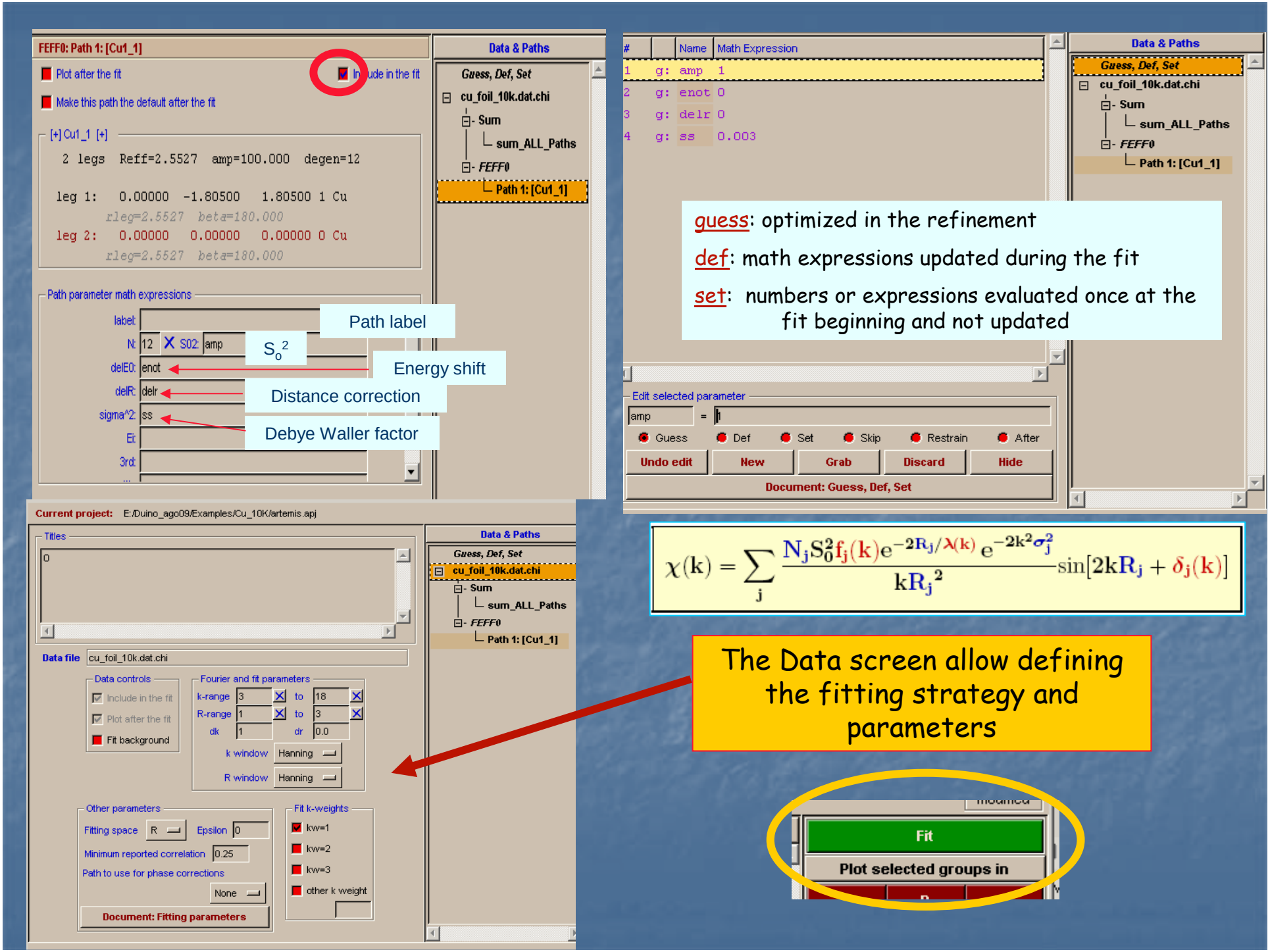


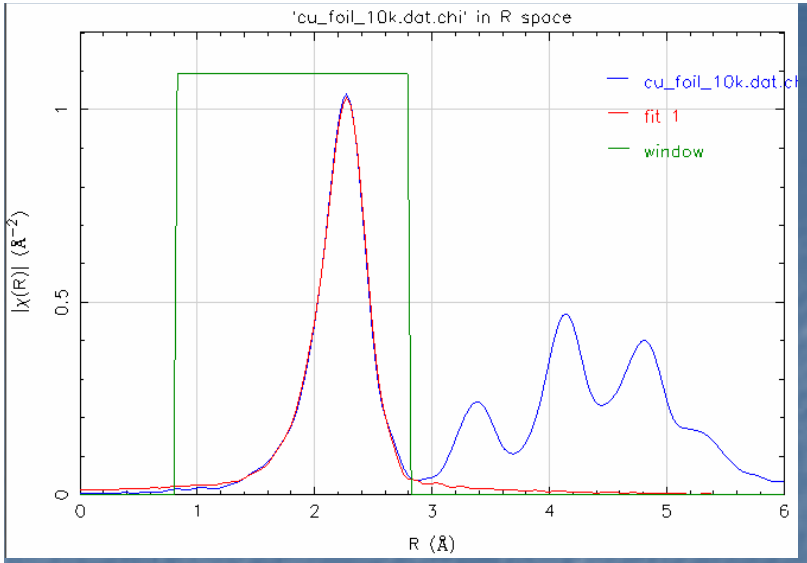
add 1st shell path to the list

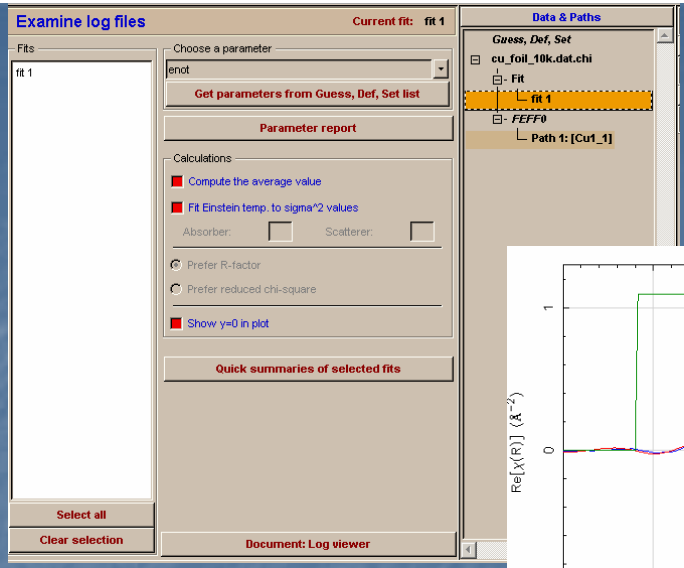
select and Right click

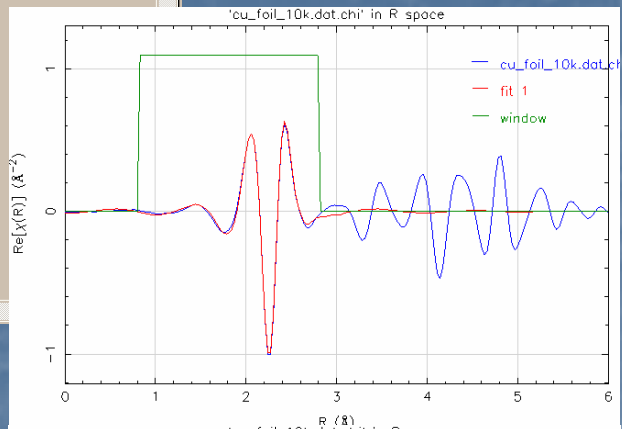


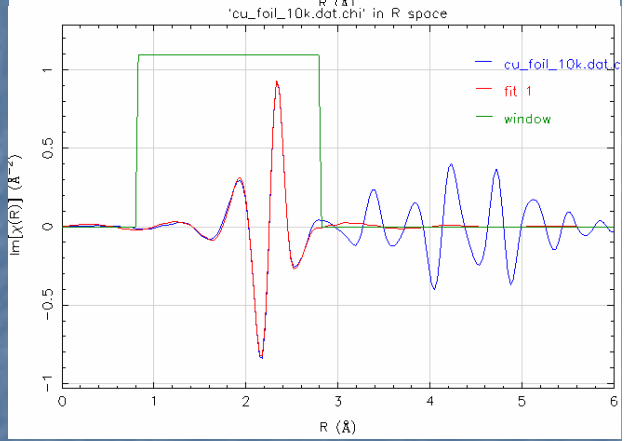



FEFF0: Path 1: [Cu1_1]
Plot after the fit
Include in the fit
Make this path the default after the fit
[+] Cu1_1 [+]
2 legs Reff=2.5527 amp=100.000 degen=12
leg 1: 0.00000 -1.80500 1.80500 1 Cu
releg=2.5527 beta=180.000
leg 2: 0.00000 0.00000 0.00000 0 Cu
releg=2.5527 beta=180.000
Path parameter math expressions
label:
N: 12 X S02: amp
delE0: enot
delR: delr
sigma^2: ss
Ei:
3rd:
Path label
S_o^2
Energy shift
Distance correction
Debye Waller factor
Data & Paths
Guess, Def, Set
cu_foil_10k.dat.chi
Sum
sum_ALL_Paths
FEFF0
Path 1: [Cu1_1]
Name Math Expression
1 g: amp 1
2 g: enot 0
3 g: delr 0
4 g: ss 0.003
Edit selected parameter
amp =
Guess Def Set Skip Restrain After
Undo edit New Grab Discard Hide
Document: Guess, Def, Set
guess: optimized in the refinement
def: math expressions updated during the fit
set: numbers or expressions evaluated once at the fit beginning and not updated
Current project: E:/Duino_ago09/Examples/Cu_10K/artemis.apj
Titles
0
Data file cu_foil_10k.dat.chi
Data controls
Include in the fit
Plot after the fit
Fit background
Fourier and fit parameters
k-range 3 to 18
R-range 1 to 3
dk 1 dr 0.0
k window Hanning
R window Hanning
Other parameters
Fitting space R Epsilon 0
Minimum reported correlation 0.25
Path to use for phase corrections
None
Document: Fitting parameters
Fit k-weights
kw=1
kw=2
kw=3
other k weight
$\chi(k) = \sum_j \frac{N_j S_0^2 f_j(k) e^{-2R_j/\lambda(k)} e^{-2k^2\sigma_j^2}}{kR_j^2} \sin[2kR_j + \delta_j(k)]$
The Data screen allow defining the fitting strategy and parameters
Fit
Plot selected groups in









$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left(\left(\Re e(\tilde{\chi}^{exp}(r_i) - \Re e\tilde{\chi}^{th}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) - \Im m\tilde{\chi}^{th}(r_i) \right)^2 \right)$$

$$\chi^2_\nu = \frac{\chi^2}{\nu}$$

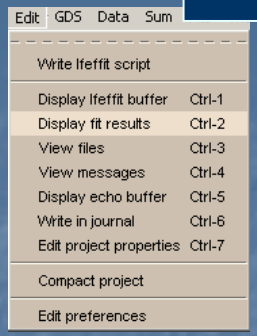
$\nu = N_{ind} - N_{var}$

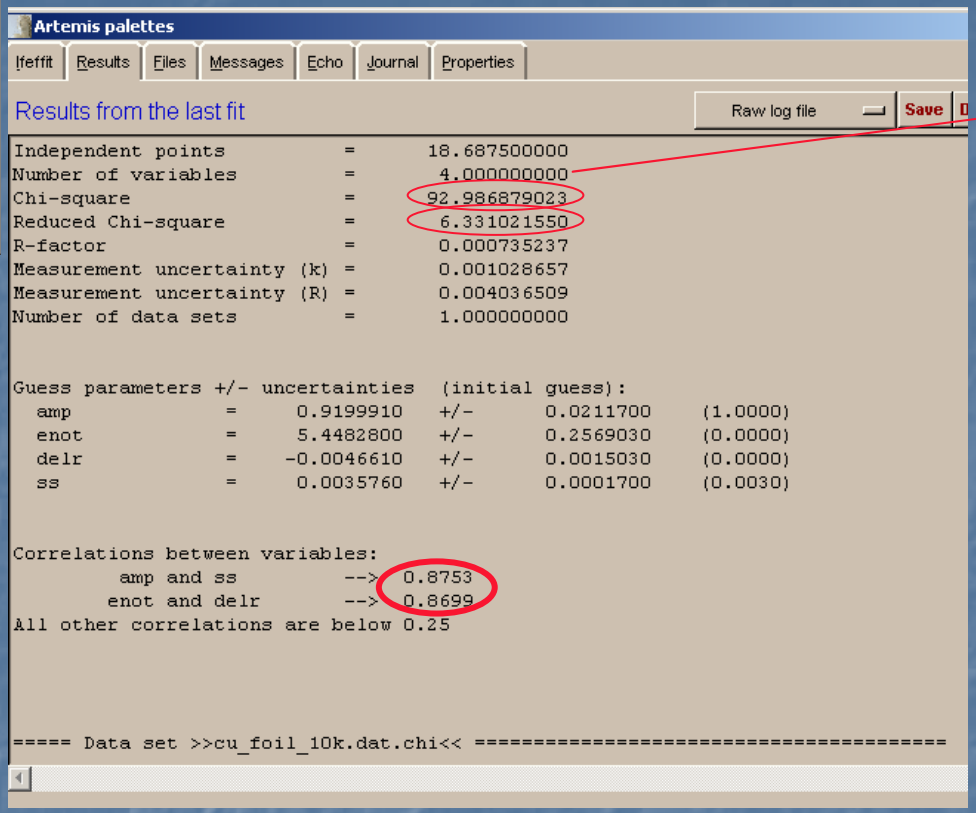
The refinement is performed in Real space, on the Real and Imaginary parts of the FT

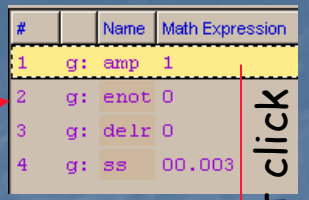
$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[\left(\Re e(\tilde{\chi}^{exp}(r_i) - \Re e\tilde{\chi}^{th}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) - \Im m\tilde{\chi}^{th}(r_i) \right)^2 \right]}{\sum_{i=1}^{N_{pts}} \left[\left(\Re e(\tilde{\chi}^{exp}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) \right)^2 \right]}$$

Absolute misfit between experimental data and theory

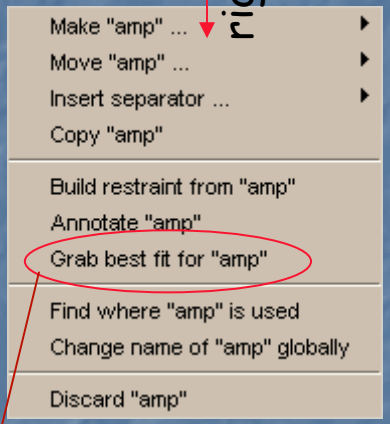
Structural results

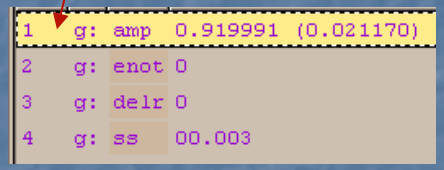






right click





$$\chi^2 = \frac{N_{ind}}{\epsilon N_{pts}} \sum_{i=1}^{N_{pts}} \left(\left(\Re e(\tilde{\chi}^{exp}(r_i) - \Re e\tilde{\chi}^{th}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) - \Im m\tilde{\chi}^{th}(r_i) \right)^2 \right)$$

$$R^2 = \frac{\sum_{i=1}^{N_{pts}} \left[\left(\Re e(\tilde{\chi}^{exp}(r_i) - \Re e\tilde{\chi}^{th}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) - \Im m\tilde{\chi}^{th}(r_i) \right)^2 \right]}{\sum_{i=1}^{N_{pts}} \left[\left(\Re e(\tilde{\chi}^{exp}(r_i) \right)^2 + \left(\Im m(\tilde{\chi}^{exp}(r_i) \right)^2 \right]}$$

Effects of Fitting parameters

Data file: cu_foil_10k.dat.chi

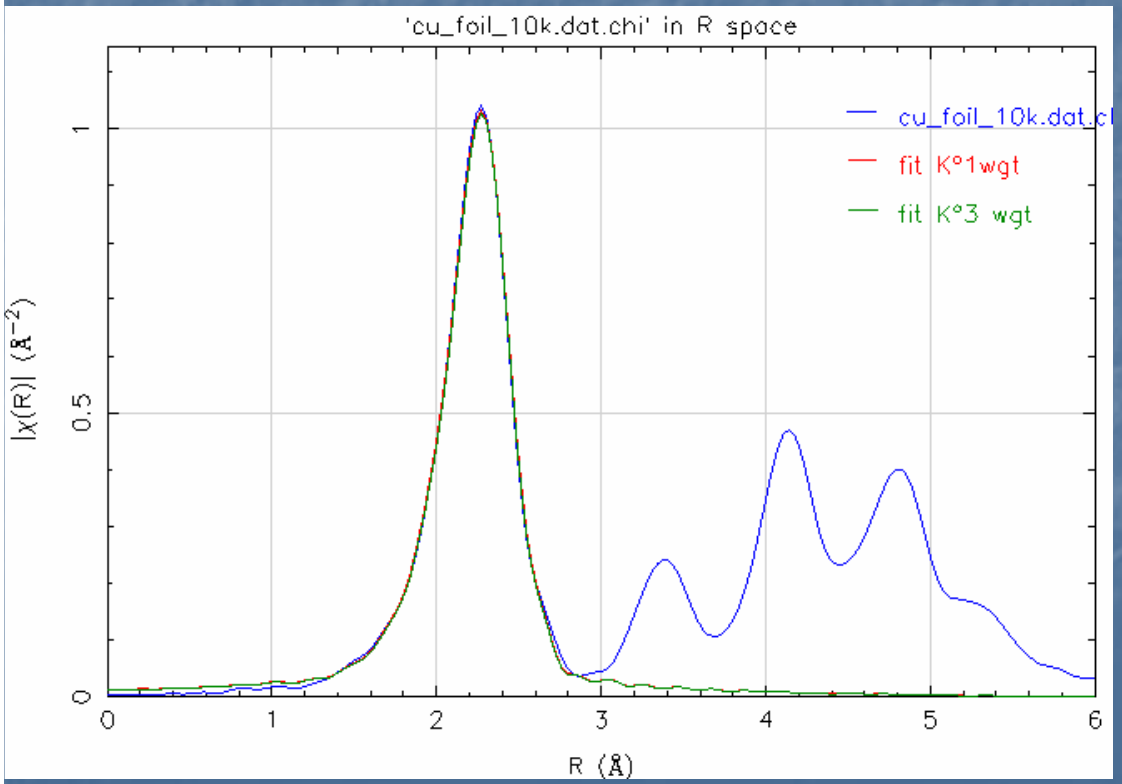
Data controls: Include in the fit; Plot after the fit; Fit background

Fourier and fit parameters: k-range 3 to 18; R-range 0.8 to 2.8; dk 1; dr 0.0; k window Hanning; R window Hanning

Other parameters: Fitting space R; Epsilon 0; Minimum reported correlation 0.25; Path to use for phase corrections: None

Document: Fitting parameters

Fit k-weights: kw=1; kw=2; kw=3; other k weight



Artemis palettes

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

Results from the last fit — Raw log file — Save

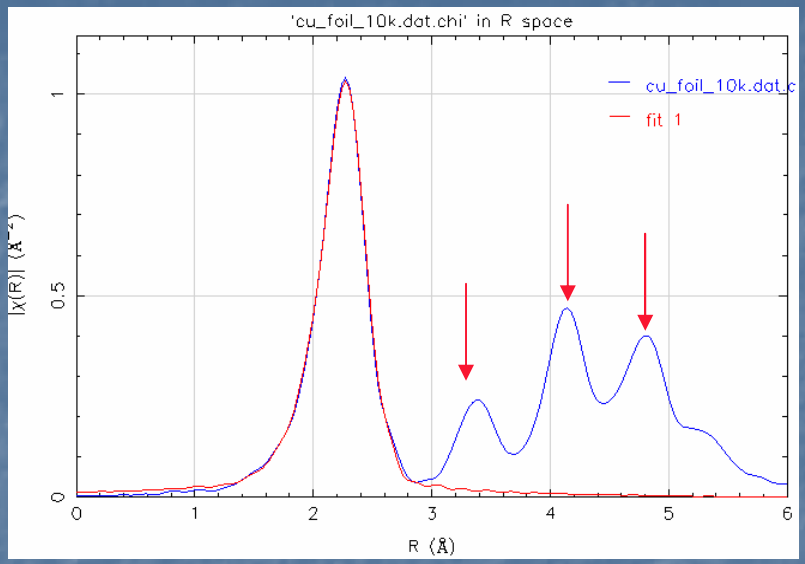
```
Independent points           =       18.687500000
Number of variables          =        4.000000000
Chi-square                   =       92.986879023
Reduced Chi-square           =        6.331021550
R-factor                     =        0.000735237
Measurement uncertainty (k)  =        0.001028657
Measurement uncertainty (R)  =        0.004036509
Number of data sets          =        1.000000000


Guess parameters +/- uncertainties  (initial guess):
  amp             =     0.9199910   +/-       0.0211700    (1.0000)
  enot            =     5.4482800   +/-       0.2569030    (0.0000)
  delr            =    -0.0046610   +/-       0.0015030    (0.0000)
  ss              =     0.0035760   +/-       0.0001700    (0.0030)


Correlations between variables:
        amp and ss          -->  0.8753
       enot and delr        -->  0.8699
All other correlations are below 0.25



===== Data set >>cu_foil_10k.dat.chi<< ========================================
```

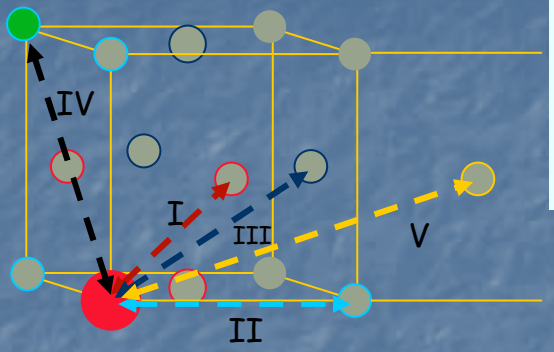
Kwt = 1

```
Independent points           =       18.687500000
Number of variables          =        4.000000000
Chi-square                   =      191.610462627
Reduced Chi-square           =       13.045818732
R-factor                     =    0.118453126E-05
Measurement uncertainty (k)  =        0.000533874
Measurement uncertainty (R)  =        0.445387356
Number of data sets          =        1.000000000


Guess parameters +/- uncertainties  (initial guess):
  amp             =     0.8886660   +/-       0.0263100    (0
  enot            =     5.4650780   +/-       0.4109850    (0
  delr            =    -0.0043940   +/-       0.0012080    (0
  ss              =     0.0033710   +/-       0.0001530    (0


Correlations between variables:
        amp and ss          -->  0.7805
       enot and delr        -->  0.7766
        amp and enot        --> -0.2833
All other correlations are below 0.25
```

Kwt = 3

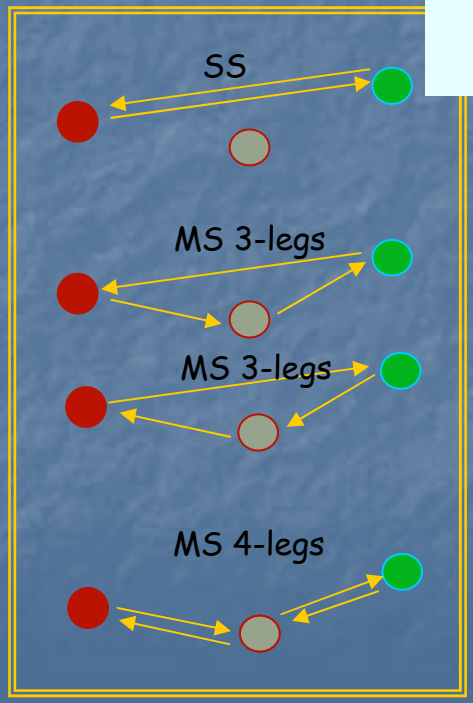
Add new contributions





Visualize the structure and understand the neighbour shells!

Take care about multiple scattering contributions



Atoms | feff.inp | Interpretation

Interpretation of the FEFF Calculation

```
# TITLE name:     copper
# TITLE formula:  Cu
# TITLE sites:    Cu1
# TITLE refer1:   Kittel, ISSP
# TITLE refer2:
```

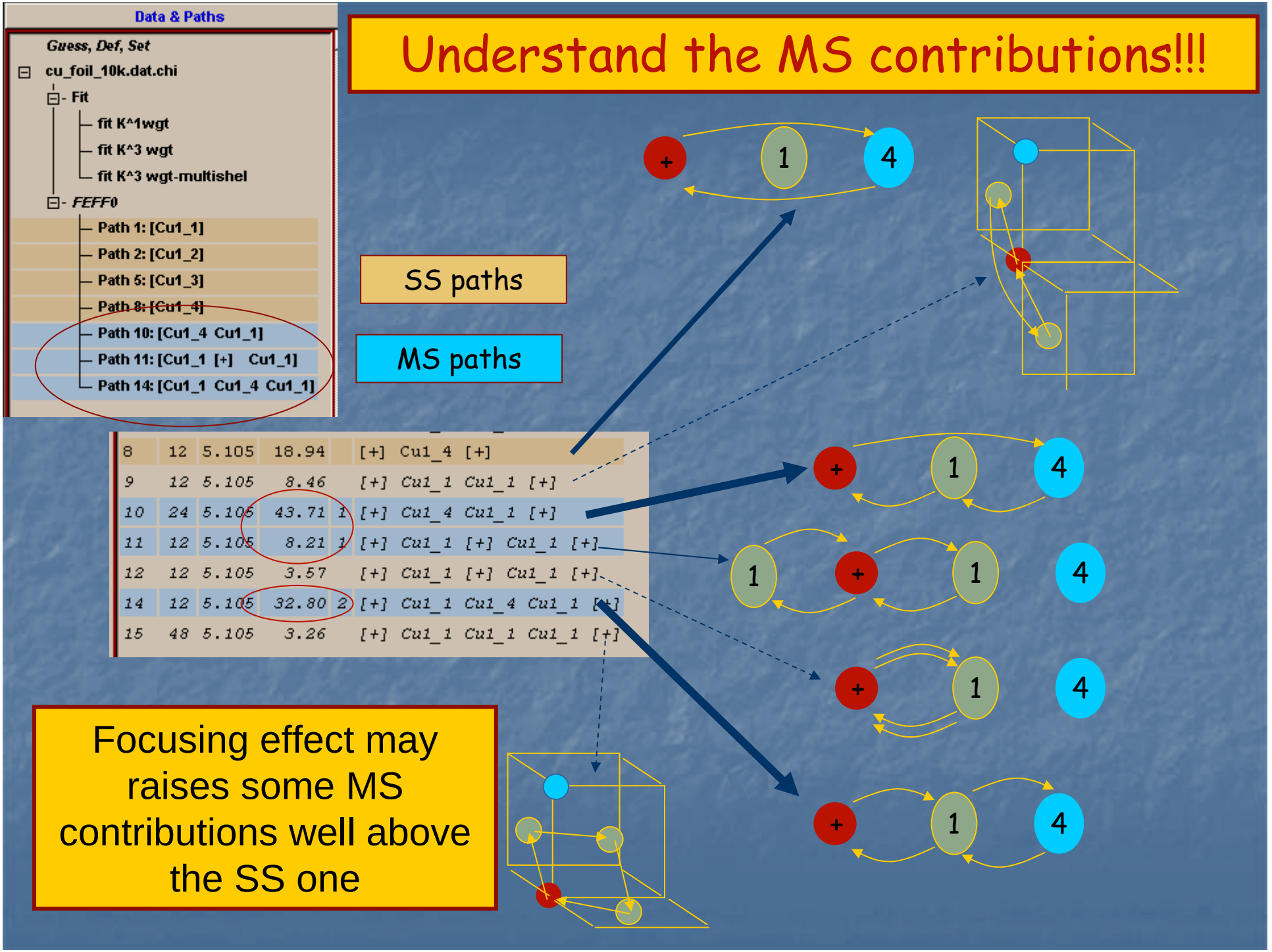
#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00		[+] Cu1_1 [+]
2	6	3.610	22.98		[+] Cu1_2 [+]
3	48	3.829	10.59		[+] Cu1_1 Cu1_1 [+]
4	48	4.358	8.65		[+] Cu1_2 Cu1_1 [+]
5	24	4.421	55.41		[+] Cu1_3 [+]
6	48	4.763	10.63		[+] Cu1_1 Cu1_1 [+]
7	96	4.763	21.81		[+] Cu1_3 Cu1_1 [+]
8	12	5.105	18.94		[+] Cu1_4 [+]
9	12	5.105	8.46		[+] Cu1_1 Cu1_1 [+]
10	24	5.105	43.71	1	[+] Cu1_4 Cu1_1 [+]
11	12	5.105	8.21	1	[+] Cu1_1 [+] Cu1_1 [+]
12	12	5.105	3.57		[+] Cu1_1 [+] Cu1_1 [+]

Document: Feff interpretation

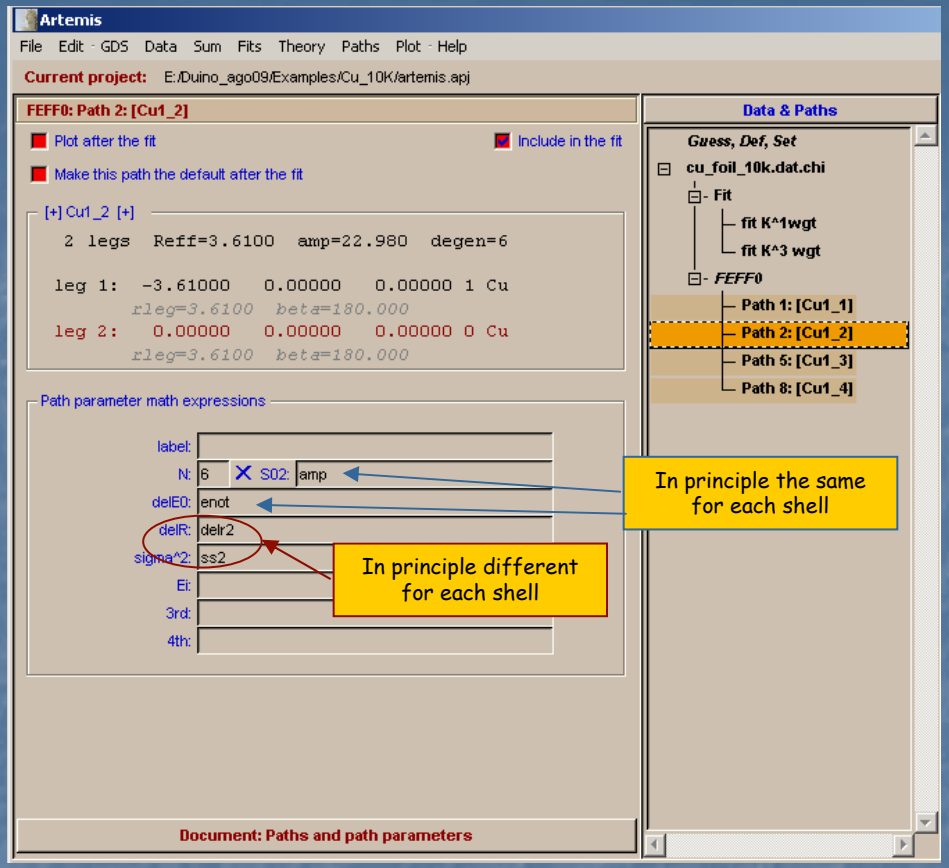
Single Scattering

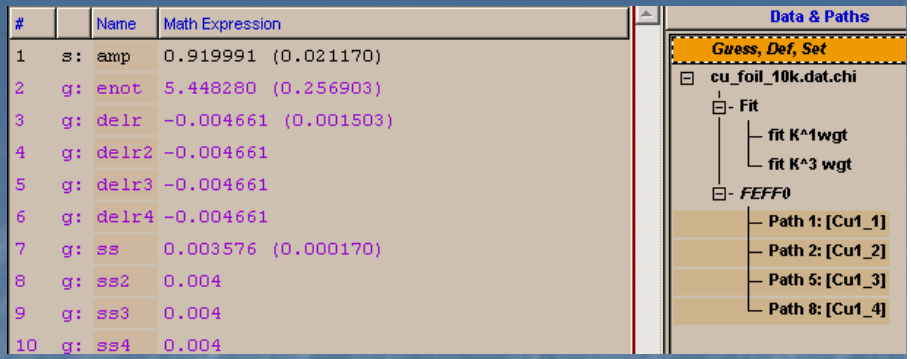
MS + Focusing

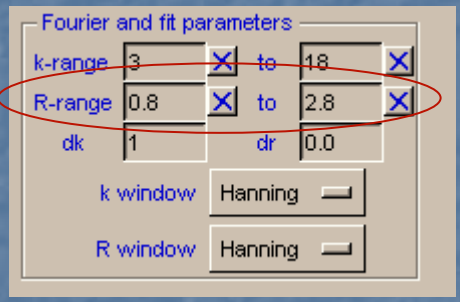
Understand the MS contributions!!!



Focusing effect may raises some MS contributions well above the SS one







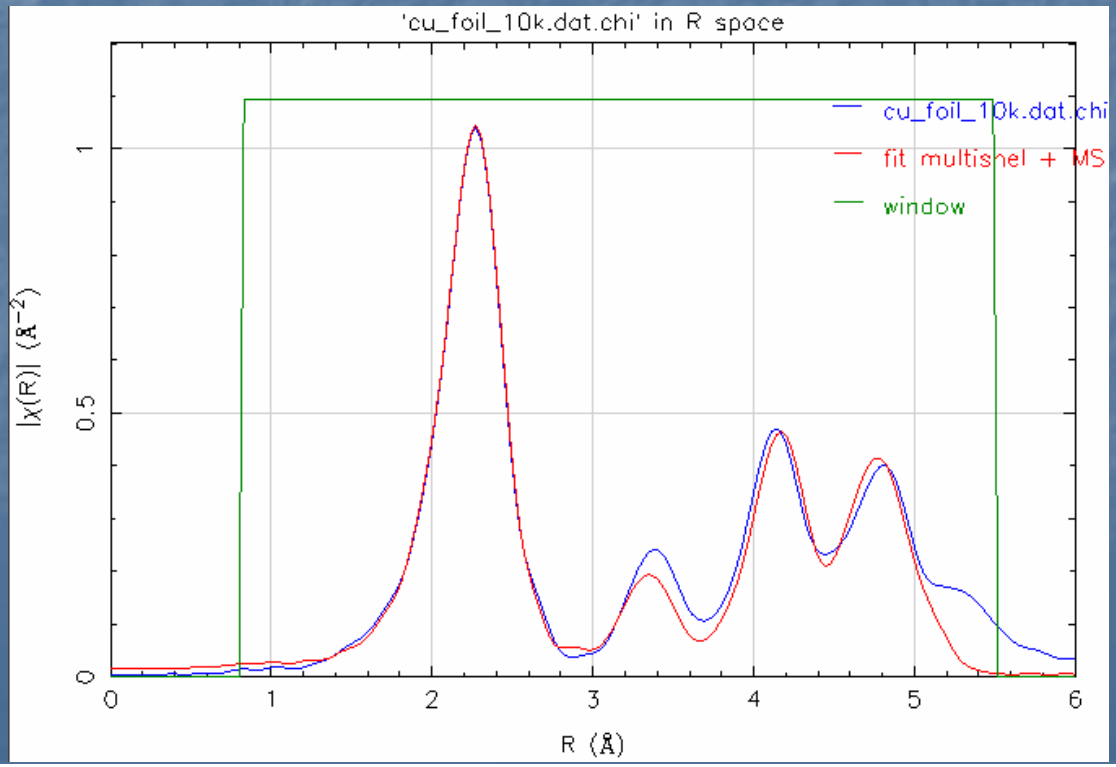
Warning:

The used path must be inside the fit range

#		Name	Math Expression
1	s:	amp	0.919991
2	g:	enot	5.448280
3	g:	delr	-0.004
4	g:	delr2	-0.004661
5	g:	delr3	-0.004
6	g:	delr4	-.004
7	g:	ss	0.003596 (0.000283)
8	g:	ss2	0.005123 (0.001735)
9	g:	ss3	0.004593 (0.000671)
10	g:	ss4	0.028058 (0.043714)
11	g:	ss5	0.004597 (0.000968)
12	g:	ss6	0.006

```
Independent points               =      44.382812500
Number of variables              =      12.000000000
Chi-square                       =    1816.763460636
Reduced Chi-square               =      56.102707590
R-factor                         =       0.011517825
Measurement uncertainty (k)      =       0.001028657
Measurement uncertainty (R)      =       0.004036509
Number of data sets              =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =      5.1036410   +/-       0.6089100
  delr             =     -0.0063660   +/-       0.0037480
  delr2            =     -0.0235000   +/-       0.0122330
  delr3            =      0.0189970   +/-       0.0075140
  delr4            =     -0.0359130   +/-       0.0098410
  ss               =      0.0035890   +/-       0.0002440
  ss2              =      0.0044530   +/-       0.0013020
  ss3              =      0.0045820   +/-       0.0005800
  ss4              =      0.3097740   +/-     132.3316580
  ss5              =      0.0151180   +/-       0.0062090
  ss6              =     -0.0003130   +/-       0.0019450
  ss7              =      0.0073710   +/-       0.0022950
```

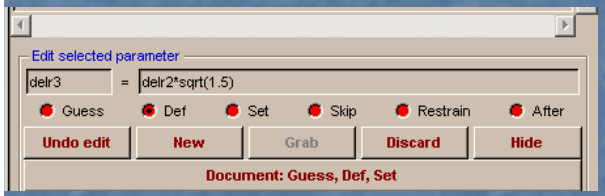
```
Correlations between variables:
          ss6 and ss7          -->  -0.8579
         enot and delr         -->   0.8206
        delr4 and ss5          -->  -0.6973
         enot and delr3        -->   0.6923
         delr and delr3        -->   0.5675
         enot and ss5          -->   0.4211
         enot and delr2        -->   0.3650
         delr and ss5          -->   0.3464
        delr3 and delr4        -->   0.3298
         delr and delr2        -->   0.2970
        delr4 and ss6          -->  -0.2649
         enot and ss7          -->   0.2521
All other correlations are below 0.25
```

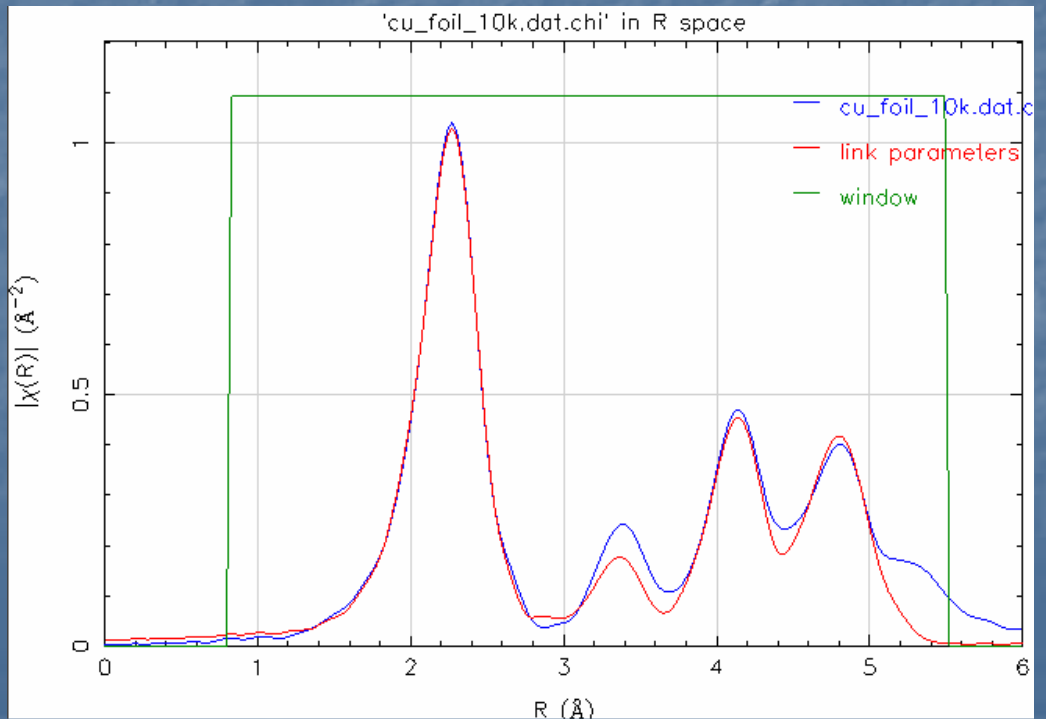


#		Name	Math Expression
1	s:	amp	0.919991
2	g:	enot	5.448280
3	d:	delr	delr2/sqrt(2)
4	g:	delr2	-0.004661
5	d:	delr3	delr2*sqrt(1.5)
6	d:	delr4	delr2*sqrt(2)
7	g:	ss	0.003596 (0.000283)
8	g:	ss2	0.005123 (0.001735)
9	g:	ss3	0.004593 (0.000671)
10	g:	ss4	0.028058 (0.043714)
11	g:	ss5	0.004597 (0.000968)
12	g:	ss6	0.006
13	g:	ss7	0.006964 (0.006210)

```
Independent points               =       44.382812500
Number of variables              =        9.000000000
Chi-square                       =     3499.926965502
Reduced Chi-square               =       98.916019339
R-factor                         =        0.022188660
Measurement uncertainty (k)      =        0.001028657
Measurement uncertainty (R)      =        0.004036509
Number of data sets              =        1.000000000


Guess parameters +/- uncertainties  (initial guess):
  enot             =      4.5727030   +/-       0.7133360
  delr2            =     -0.0051830   +/-       0.0061960
  ss               =      0.0036500   +/-       0.0003280
  ss2              =      0.0046410   +/-       0.0018030
  ss3              =      0.0047920   +/-       0.0007880
  ss4              =      0.0239730   +/-       0.0373920
  ss5              =      0.0057660   +/-       0.0014520
  ss6              =      0.0010460   +/-       0.0058090
  ss7              =      0.0060830   +/-       0.0044900
```

```
Correlations between variables:
          ss6 and ss7          --> -0.9544
         enot and delr2        -->  0.8598
          ss4 and ss5          -->  0.6684
          ss5 and ss7          -->  0.6517
          ss4 and ss7          -->  0.6019
          ss5 and ss6          --> -0.5675
          ss4 and ss6          --> -0.4966
```





Data & Paths

Guess, Def, Set

- cu_foil_10k.dat.chi
  - Fit
    - fit K^1wgt
    - fit K^3 wgt
    - link parameters
  - FEFF0
    - Path 1: [Cu1_1]
    - Path 2: [Cu1_2]
    - Path 5: [Cu1_3]
    - Path 8: [Cu1_4]
    - Path 10: [Cu1_4 Cu1_1]
    - Path 11: [Cu1_1 [+] Cu1_1]
    - Path 14: [Cu1_1 Cu1_4 Cu1
    - Path 22: [Cu1_5]

Current project: E:/Duino_ago09/Examples/Cu_10K/Cu_10

#		Name	Math Expression
1	g:	amp	0.907810 (0.096404)
2	g:	enot	5.448280
3	g:	delr	0.0
4	g:	delr2	-0.004661
5	d:	delr3	delr2*sqrt(1.5)
6	d:	delr4	delr2*sqrt(2)
7	d:	delr5	delr2*sqrt(2.5)
8	g:	ss	0.003596 (0.000283)
9	g:	ss2	0.005123 (0.001735)
10	g:	ss3	0.004593 (0.000671)
11	g:	ss4	0.028058 (0.043714)
12	g:	ss5	0.004597 (0.000968)
13	g:	ss6	0.006
14	g:	ss7	0.006964 (0.006210)
15	g:	ss8	0.006964 (0.006210)

```
Independent points               =      48.178710937
Number of variables              =      12.000000000
Chi-square                       =    8110.229963402
Reduced Chi-square               =     224.171335939
R-factor                         =       0.000045721
Measurement uncertainty (k)      =       0.000533874
Measurement uncertainty (R)      =       0.445387356
Number of data sets              =       1.000000000


Guess parameters +/- uncertainties  (initial guess):
  amp                =      0.9054050   +/-       0.0941340
  enot               =      3.7197170   +/-       0.3651800
  delr               =     -0.0094960   +/-       0.0028930
  delr2              =     -0.0009550   +/-       0.0034220
  ss                 =      0.0034400   +/-       0.0004310
  ss2                =      0.0048280   +/-       0.0005880
  ss3                =      0.0048200   +/-       0.0004620
  ss4                =      0.0355080   +/-       0.1148830
  ss5                =      0.0047690   +/-       0.0009910
  ss6                =      0.0022460   +/-       0.0040870
  ss7                =      0.0078980   +/-       0.0043780
  ss8                =      0.0052190   +/-       0.0006400
```

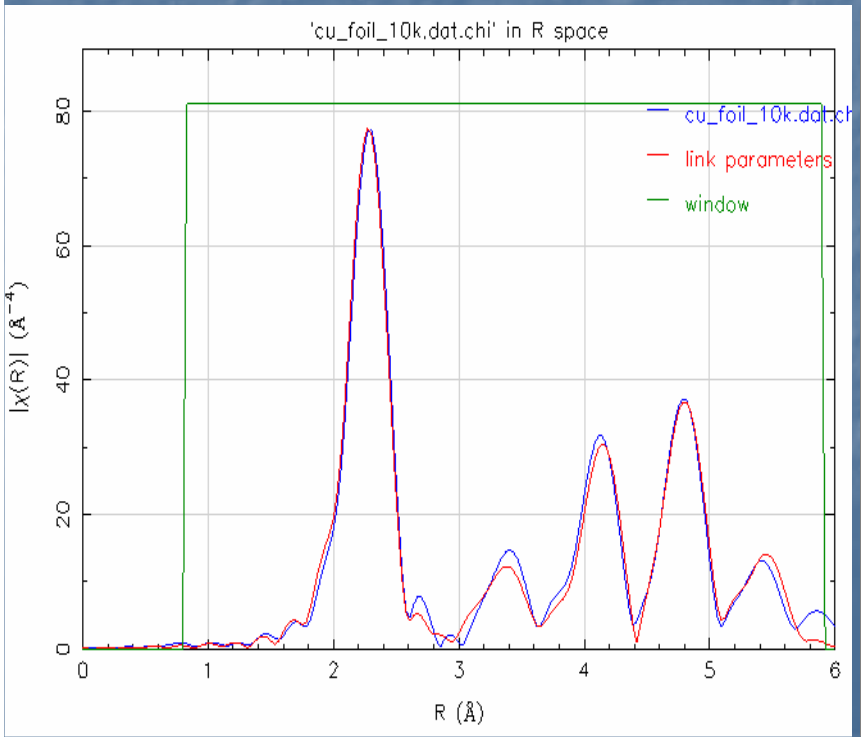
Data file: cu_foil_10k.dat.chi

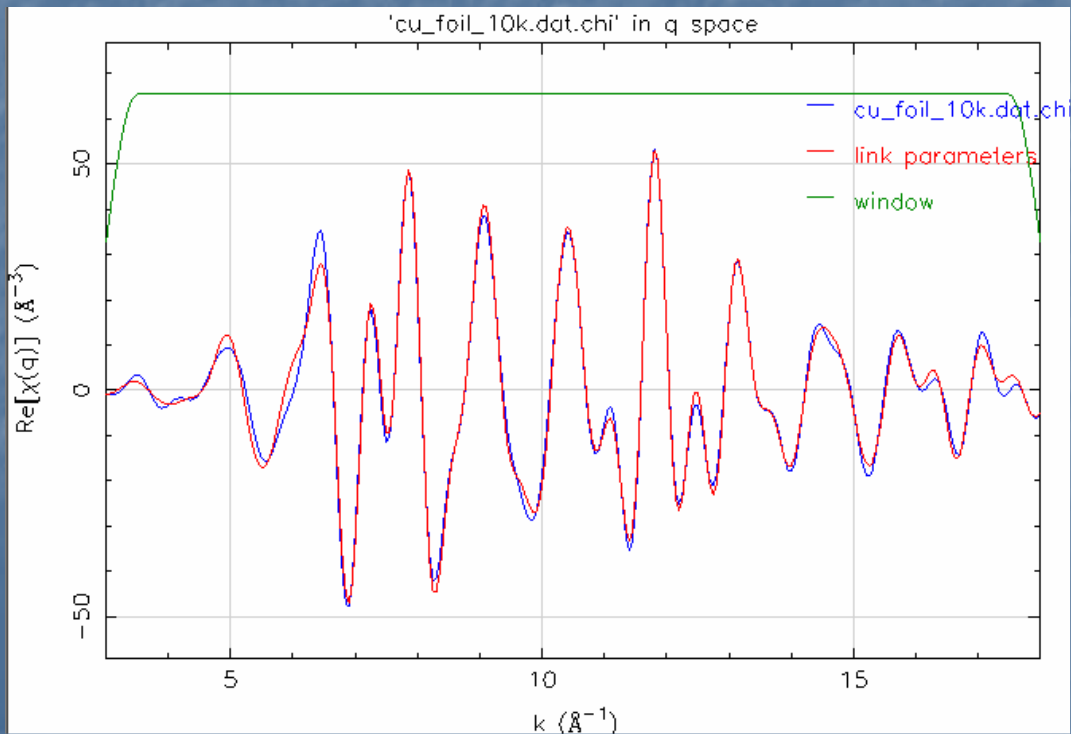
Data controls
- Include in the fit
- Plot after the fit
- Fit background

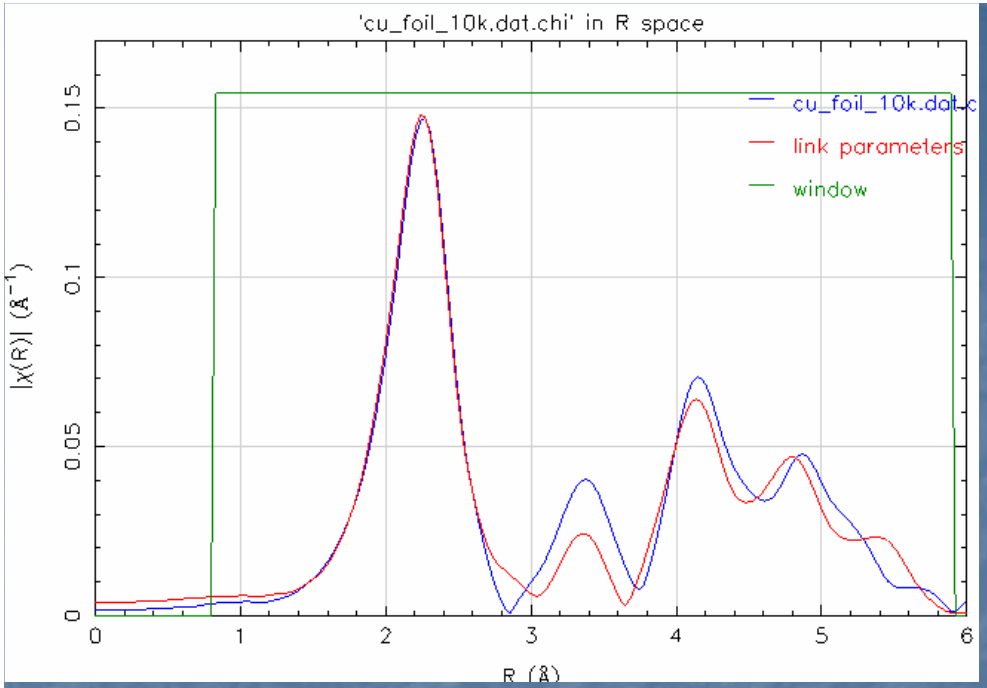
Fourier and fit parameters
- k-range: 3 to 18
- R-range: 0.8 to 5.9
- dk: 1 dr: 0.0
- k window: Hanning
- R window: Hanning

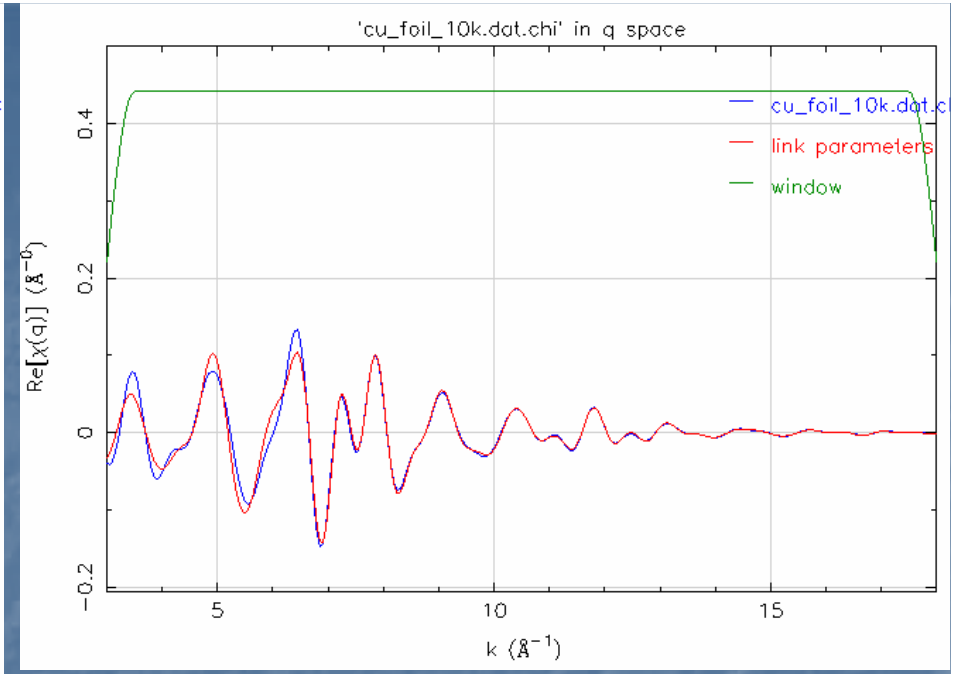
Other parameters
- Fitting space: R
- Epsilon: 0
- Minimum reported correlation: 0.25
- Path to use for phase corrections: None
- Document: Fitting parameters

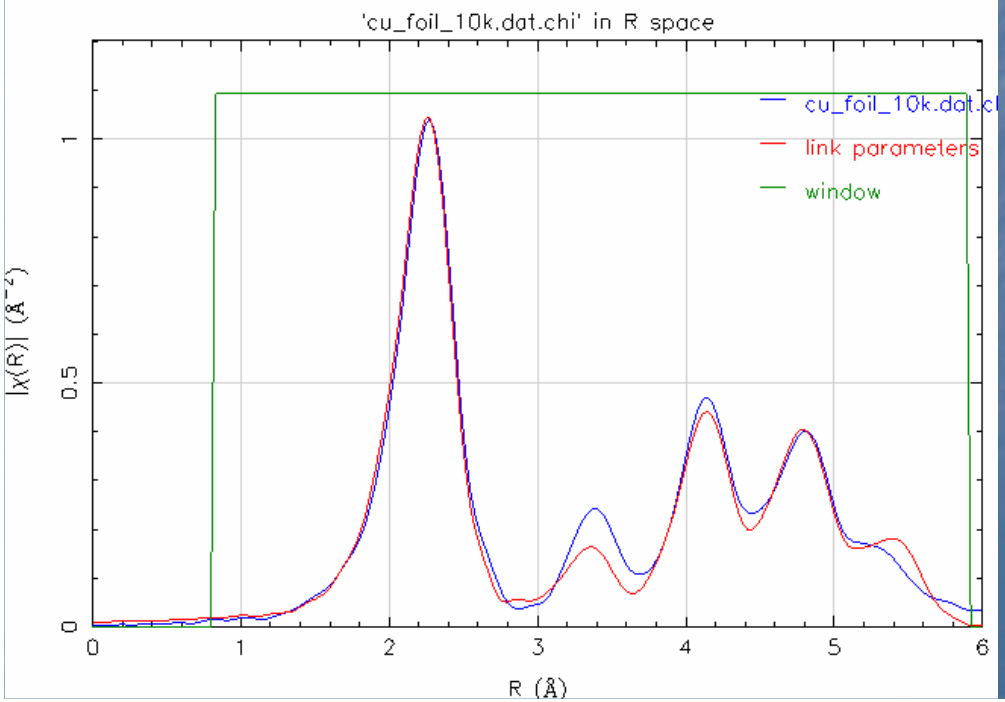
Fit k-weights
- kw=1
- kw=2
- kw=3
- other k weight

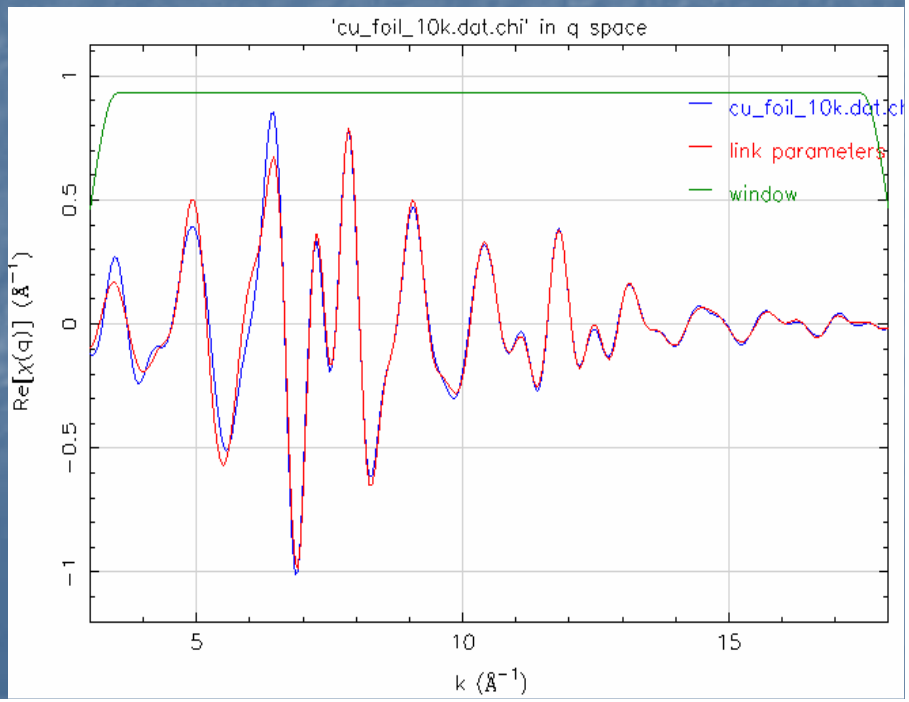





'cu_foil_10k.dat.chi' in R space
cu_foil_10k.dat.c
link parameters
window
|χ(R)| (Å⁻¹)
R (Å)


'cu_foil_10k.dat.chi' in q space
cu_foil_10k.dat.c
link parameters
window
Re[χ(q)] (Å⁻⁰)
k (Å⁻¹)


'cu_foil_10k.dat.chi' in R space
cu_foil_10k.dat.ch
link parameters
window
|χ(R)| (Å⁻²)
R (Å)


'cu_foil_10k.dat.chi' in q space
cu_foil_10k.dat.ch
link parameters
window
Re[χ(q)] (Å⁻¹)
k (Å⁻¹)

it's your work now!

a. Fe bcc

b. GeO

c. ...