



# Artemis 软件应用

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北京同步辐射装置EXAFS谱分析讲习班，2011年12月7-8日，北京

# 主要内容



- ◆ 软件简介
- ◆ 数据处理
  - a 单壳层拟合
  - b 多壳层拟合
  - c 多权重拟合
  - d 多Feff拟合
  - e 多数据拟合



# Artemis 简介:



Artemis:阿尔忒弥斯,狩猎女神,阿波罗的妹妹;

- 由Bruce.Ravel开发,利用设定的晶体(团簇)模型通过**Feff**软件的计算,得到理论的散射振幅、相移函数、平均自由程;加上一定的未知结构参数,代入EXAFS理论表达式,对EXAFS振荡函数 $\chi(K)$ 进行Levenberg-Marquardt非线性最小二乘法拟合,得到所求拟合参数的值。
- 本身不进行数据处理,通常应用于拟合经过**athena**处理后的**EXAFS**实验振荡函数 $\chi(K)$ ,得到这些数据的配位数,配位键长,无序度因子等结构参数;

# Artemis 简介：主界面



选项栏

操作细节  
显示与控制, 数据与路径框图中不同部分的详细参数;

信息反馈  
显示artemis反馈的信息、提示;

Fit键

绘图  
绘图界面的参数

数据与路径  
显示拟合参数、数据、拟合结果与路径目录; 单击任一后在操作细节显示;

13 independent points data points (Nyquist): (1 data set) (4 variables)

- 三个主要部分：数据与路径、操作细节与绘图;



# Artemis 简介：信息显示界面



调色板（信息显示界面）

**lffeffit:** 显示artemis的操作；

**Results:** 显示拟合后的结果；

**Files :** 查看数据文件；  
(点击Browse, 引入数据查看)

**Messages:** 显示Feff的输出和报错；

**Echo:** 显示完整的信息反馈；

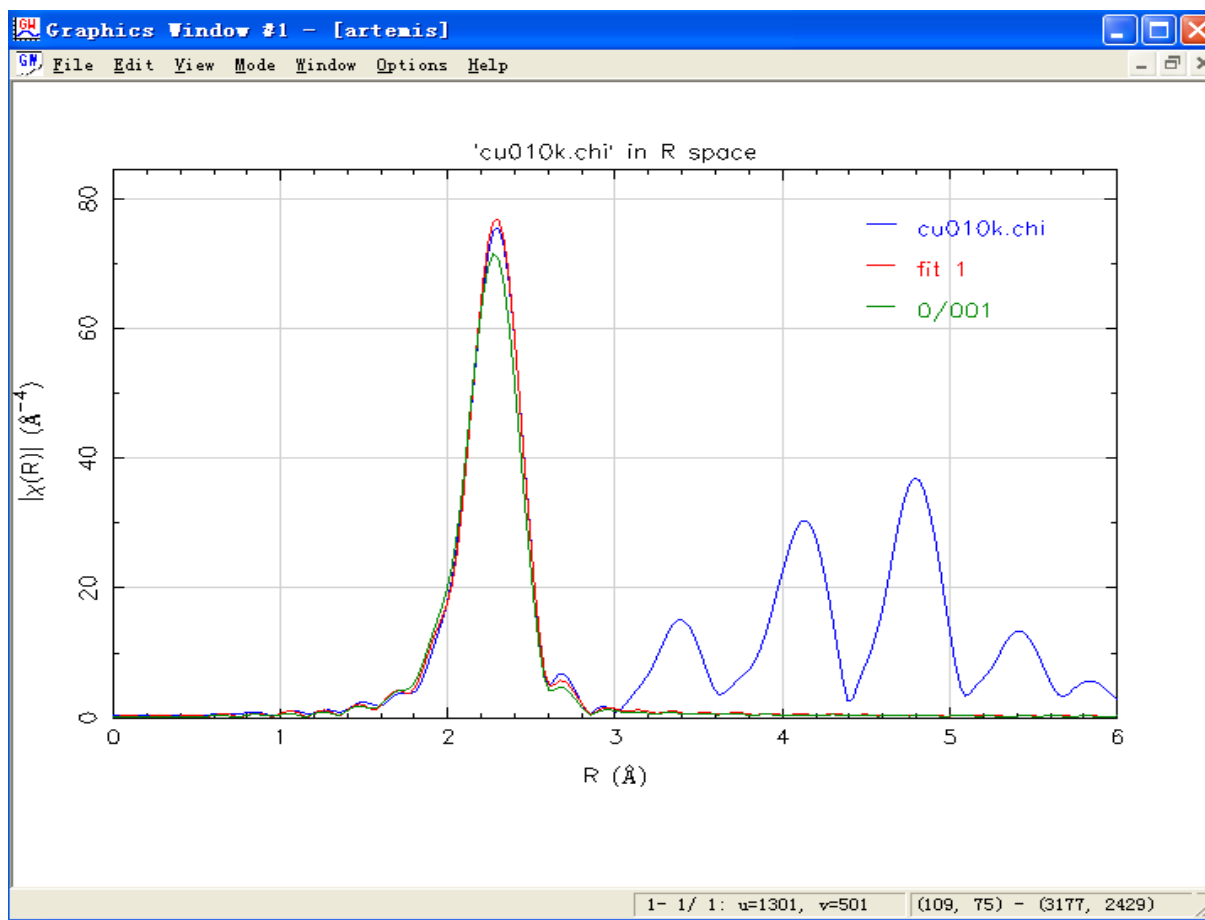
**Journal:** 拟合日志；

**Properties:** 文件信息；

```
Artemis palettes
lffeffit Results Files Messages Echo Journal Properties
lffeffit interaction buffer Save buffer to file Dismiss
read_data(file="C:\Documents and Settings\new\Application Data\hor:
      type=chi, group=data0_fit_1)
fftf(data0_fit_1.chi, k=data0_fit_1.k, kweight=3, rmax_out=10,
      kmin=2.5, kmax=18, dk=1, kwindow=kaiser-bessel)
plot(data0_fit_1.r, "data0_fit_1.chir_mag+0", style=solid,
      color="red", key="fit 1")
## Path #1
path(1, label = "feff0001.dat")
path(1, feff = "C:\Documents and Settings\new\Application Data\hor:
path(1, degen = 12)
path(1, s02 = amp)
path(1, e0 = enot)
path(1, delr = delr)
path(1, sigma2 = sigsqr + signor)
path(1, force_read = true)
path(1, ei=0, third=0, fourth=0)
ff2chi(1, group=feff0_1)
fftf(feff0_1.chi, k=feff0_1.k, kweight=3, rmax_out=10, kmin=2.5,
      kmax=18, dk=1, kwindow=kaiser-bessel)
plot(feff0_1.r, "feff0_1.chir_mag+0", style=solid,
      color="green4", key="0/001")
set &status = 0
Iffeffit>
```



# Artemis 简介：绘图界面



- 绘图界面

# 数据处理



## 前期数据处理

## 构建模型

导入EXAFS 振荡函数 $X(k)$

理论散射路径参数 ( 振幅、键长、配位数等 )

输入晶体结构参数 (  $a$   $b$   $c$   $\alpha$   $\beta$   $\gamma$  )  
运行ATOMS  
feff.inp  
运行Feff

设置拟合参数及其初始值

反复调整参数

输出拟合结果

接受

重新构建模型，重复上述过程；

修改Athena参数，重复上述过程。



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  - d 多Feff拟合
  - e 多数据拟合





# 单壳层拟合(以Cu 10k为例)



The screenshot shows the Artemis software interface with the following components:

- Titles:** Cu foil at 10K, cu10k.dat, data taken at NSLS beamline X-11A Sept 1992, by M Newville, B Ravel, and Y Zhang, foil of 99.999 Cu rolled and annealed to ~12 micr.
- Data file:** cu010k.chi
- Data controls:**  Include in the fit,  Plot after the fit,  Fit background.
- Fourier and fit parameters:** k-range: 2 to 22.95, 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.
- Fit weights:**  kw=1,  kw=2,  kw=3,  other k weight.
- Fit panel:** Plot selected groups in k, R, q. Plotting options: 0, 1, 2, 3, kw. Plot in R:  Magnitude,  Real part,  Imaginary part. Plot in q:  Magnitude,  Real part,  Imaginary part.  Window,  Background,  Residual. kmin: 0, kmax: 15, Rmin: 0, Rmax: 6, qmin: 0, qmax: 15.
- Graphics Window #1:** Plot of  $|k(R)|$  ( $\text{\AA}^{-3}$ ) vs  $R$  ( $\text{\AA}$ ) for 'cu010k.chi' in R space. The plot shows a sharp peak at approximately 2.2  $\text{\AA}$  and several smaller peaks at higher  $R$  values.

数据文件抬头



傅里叶变换参数



拟合参数



现有傅里叶变换参数下的自由节点数

拟合权重

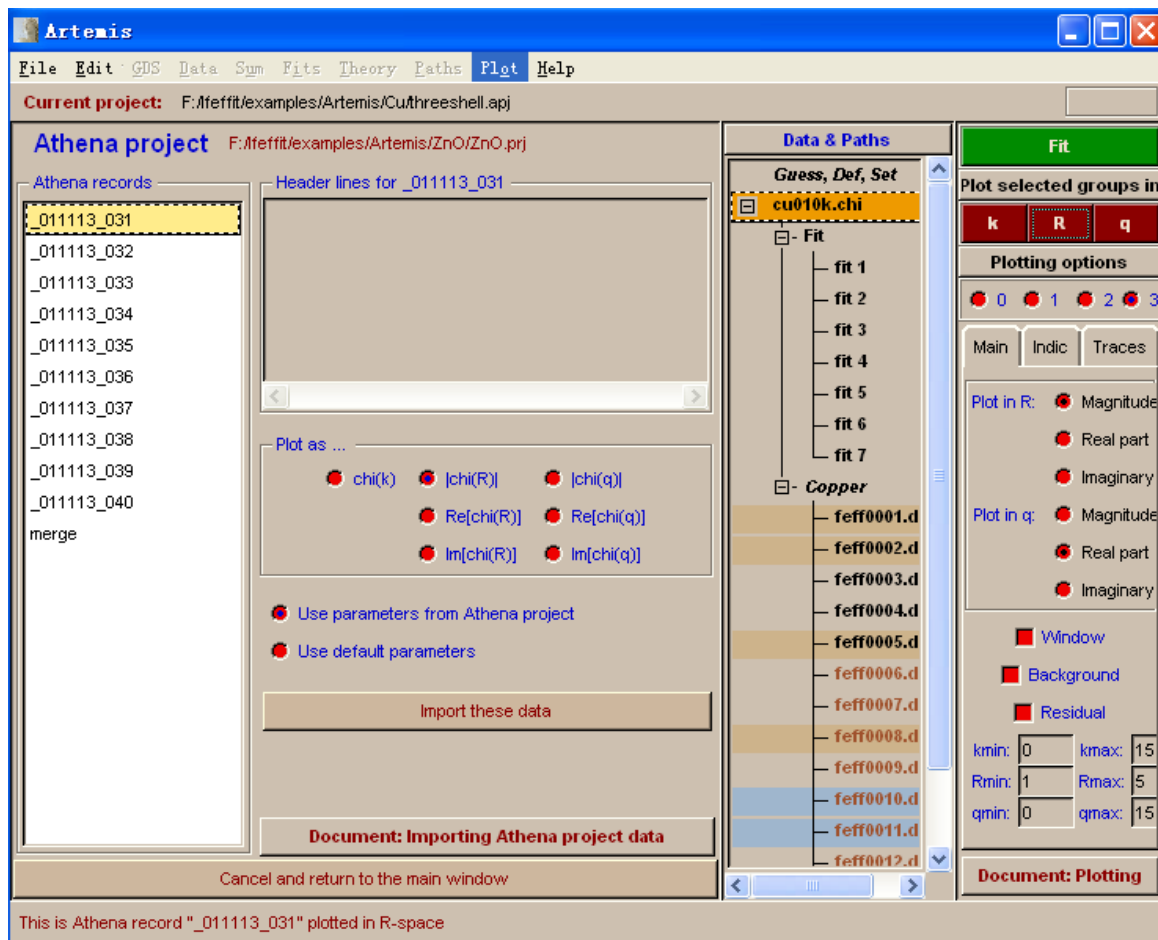
- 数据导入: File/open file



# 单壳层拟合(以Cu 10k为例)



prj文件中的数据

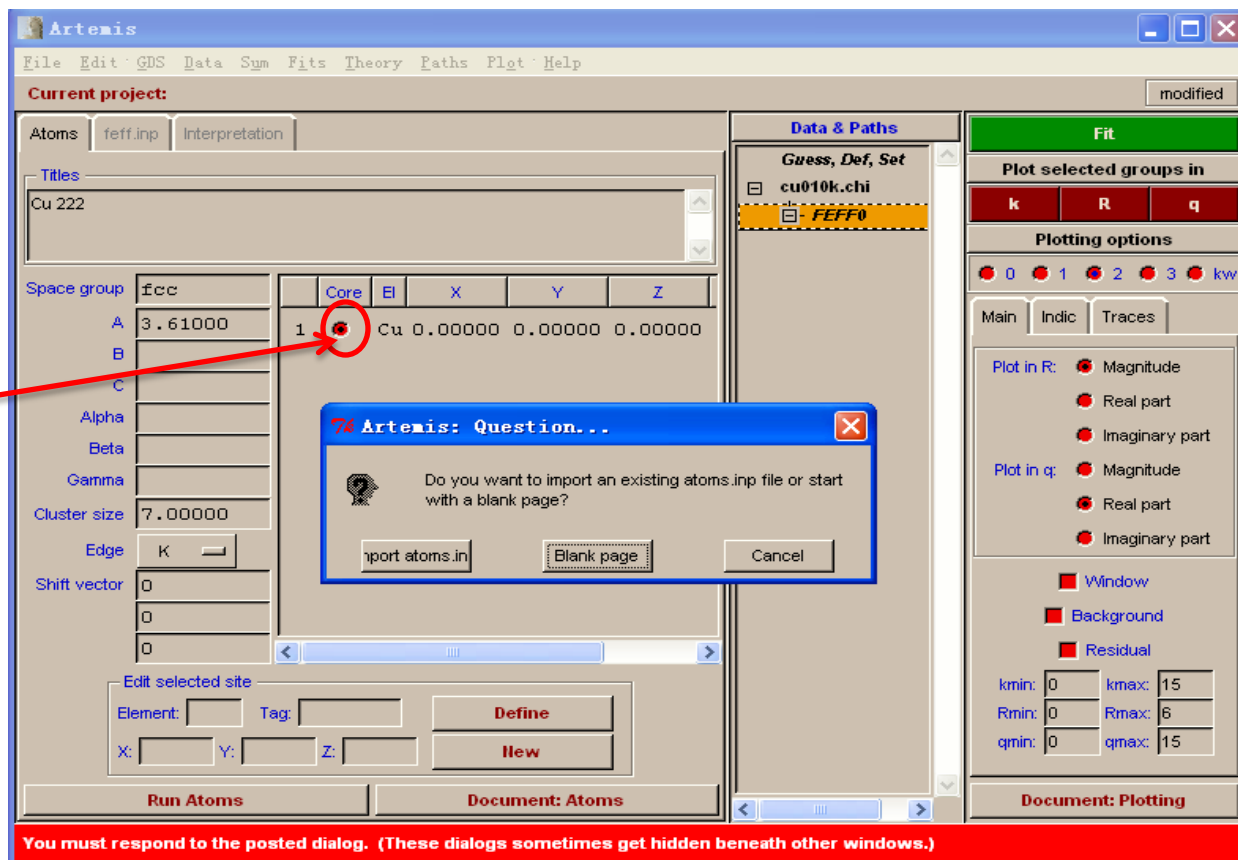


- 数据导入: File/open file



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# 单壳层拟合(以Cu 10k为例)



晶体结构参数



标记为吸收原子



原子占位信息



- 构建模型: Theory/New atom page /blank page;  
输入所需参数(空间群、晶体学参数、原子占位);  
shift victor(部分空间群需要, 点击Run Atoms后, 注意信息显示窗口, 按提示输入);



# 单壳层拟合(以Cu 10k为例)



Feff文件信息



```
TITLE Cu 222
HOLE 1 1.0 * Cu K edge (8979.0 eV), second nu
*
*      mphase,mpath,mfeff,mchi
CONTROL 1 1 1 1
PRINT 1 0 0 0
RMAX 7.0
*CRITERIA curved plane
*DEBYE temp debye-temp
NLEG 4
POTENTIALS
*      ipot Z element
      0 29 Cu
      1 29 Cu
ATOMS * this list contains
*      x y z ipot tag
      0.00000 0.00000 0.00000 0 Cu
      1.80500 1.80500 0.00000 1 Cu_1
      -1.80500 1.80500 0.00000 1 Cu_1
```

- 点击Run Atoms; 检查路径是否正确 (原子间距合适); 右键保存 feff.inp



# 单壳层拟合(以Cu 10k为例)



**Degen:** 简并度(独立散射路径数/配位原子数);

**reff:** 有效散射路径长度;

**amp:** 散射振幅强度(相对于最近邻路径);

**fs:** 前散射事件(多重散射中影响较大的部分);

**scattering path:** 散射中参与的原子, +表示吸收原子;

#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00	[+]	Cu_1 [+]
2	6	3.610	22.98	[+]	Cu_2 [+]
3	48	3.829	10.59	[+]	Cu_1 Cu_1 [+]
4	48	4.358	8.65	[+]	Cu_2 Cu_1 [+]
5	24	4.421	55.40	[+]	Cu_3 [+]
6	48	4.763	10.62	[+]	Cu_1 Cu_1 [+]
7	96	4.763	21.84	[+]	Cu_3 Cu_1 [+]
8	12	5.105	18.93	[+]	Cu_4 [+]
9	12	5.105	8.46	[+]	Cu_1 Cu_1 [+]
10	24	5.105	43.72	1	Cu_4 Cu_1 [+]
11	12	5.105	8.20	1	Cu_1 [+]
12	12	5.105	3.56	[+]	Cu_1 [+]
14	12	5.105	32.79	2	Cu_1 Cu_4 Cu_1 [+]

- 选择需要的路径(通常为前10条);



# 路径参数



路径信息描述



拟合参数设定



The screenshot shows the Artemis software interface with the following components:

- Current project:** FEFF1: Path 1: [Cu\_1]
- Fit panel:** Includes checkboxes for "Plot after the fit" and "Include in the fit" (circled in red). Below are "Plot selected groups in" (k, R, q) and "Plotting options" (0, 1, 2, 3, kw).
- Data & Paths panel:** Shows a tree view with "Path 1: [Cu\_1]" selected.
- Path parameter math expressions panel:** Contains a table for defining parameters:

label:	
N:	12 X S02: amp_1
delE0:	enot_1
delR:	delr_1
sigma^2:	ss_1
E:	
3rd:	
4th:	
- Document:** Paths and path parameters (left) and Plotting (right).

- 设定某一路径所需拟合的参数;

artemis有内部参量, 通常命名时建议后缀\_n, 以减少程序警告的可能;



# EXAFS的理论表达式:



$$\chi(K) = \sum_j \frac{N_j S_0^2 F_j(K)}{KR_j^2} \int g(R) e^{-2R_j/\lambda(K)} \text{Sin}[2KR_j + \delta_j(K)] dR$$

$g(R)$ :原子对分布函数

$$\chi(K) = \sum_j \frac{N_j S_0^2 F_j(K) e^{-2R_j/\lambda(K)} e^{-2K^2\sigma_j^2}}{KR_j^2} \text{Sin}[2KR_j + \delta_j(K)]$$

晶体等有序体系或弱无序体系（高斯分布）

$$\chi(K) = \sum_j \frac{N_j S_0^2 F_j(K)}{KR_j^2} \exp\left[-2K^2\sigma_j^2 + \frac{2}{3} C_{4j} K^4\right] e^{-2R_j/\lambda(K)} \text{Sin}\left[2KR_j + \delta_j(K) - \frac{4}{3} C_{3j} K^3\right]$$

\*\*中等无序体系：累积量展开



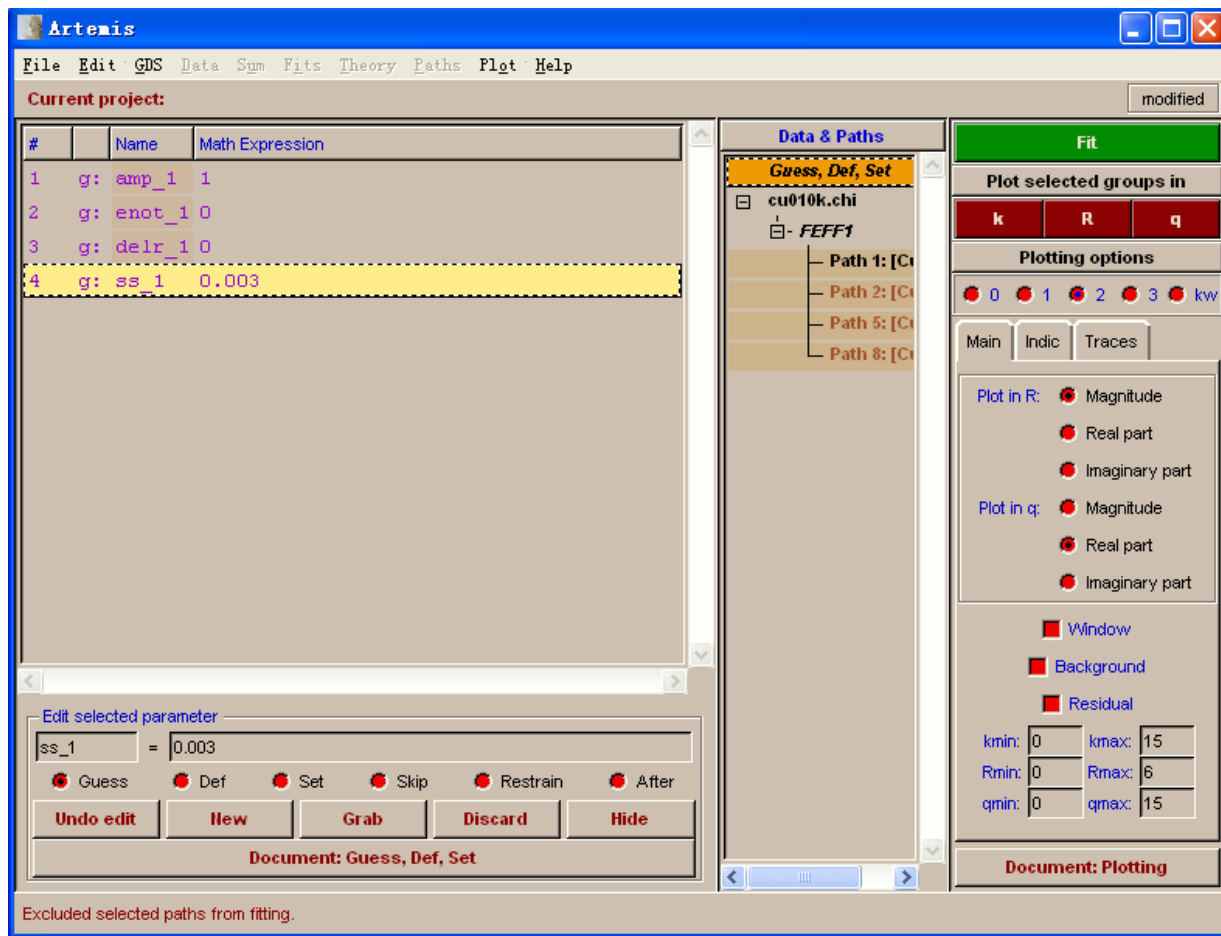
# 参数:



影响峰强	}	N: 配位数	
		S02: 振幅衰减因子	(0.7, 1)
		Sigma <sup>2</sup> : 无序度因子 (Debye-Waller factor)	(0.003, 0.02)
		C <sub>4</sub> : 4阶累积量	
影响峰位	}	R: 原子间距;	( $\Delta R < 0.5 \text{ \AA}$ )
		C <sub>3</sub> : 3阶累积量	
		E <sub>i</sub> : 能移展宽	
		$\Delta E_0$ : 能量零点偏移	( $\pm 10 \text{ eV}$ 以内)
拟合精度	}	N: +-20%	
		R: 0.01A	
		原子种类: +-4	



# 路径参数初始值设定



New: 新建拟合参数

Grab: 抓取拟合结果

Discard: 去除拟合参数

Hide: 隐藏编辑框

设定拟合变量初始值、采用固定、限制和定义等方式，调整拟合变量的值；（确认设定的参数名称正确，一一对应）





Guess: 设定初始值, 不做限制;

g enot=0

Def: 设定参数间的数学关系式;

d delr\_1= alfa\*reff

g alfa=0.01

Set: 设定成固定值, 不做改变;

s S02=0.85

Skip: 忽略该参数; (相当于程序语言中的注释符)

Restrain: 设定参数限定在固定值附近;

r delr\_res=(delr\_1-reff-0.1)\*factor

s factor=100;

g enot=0

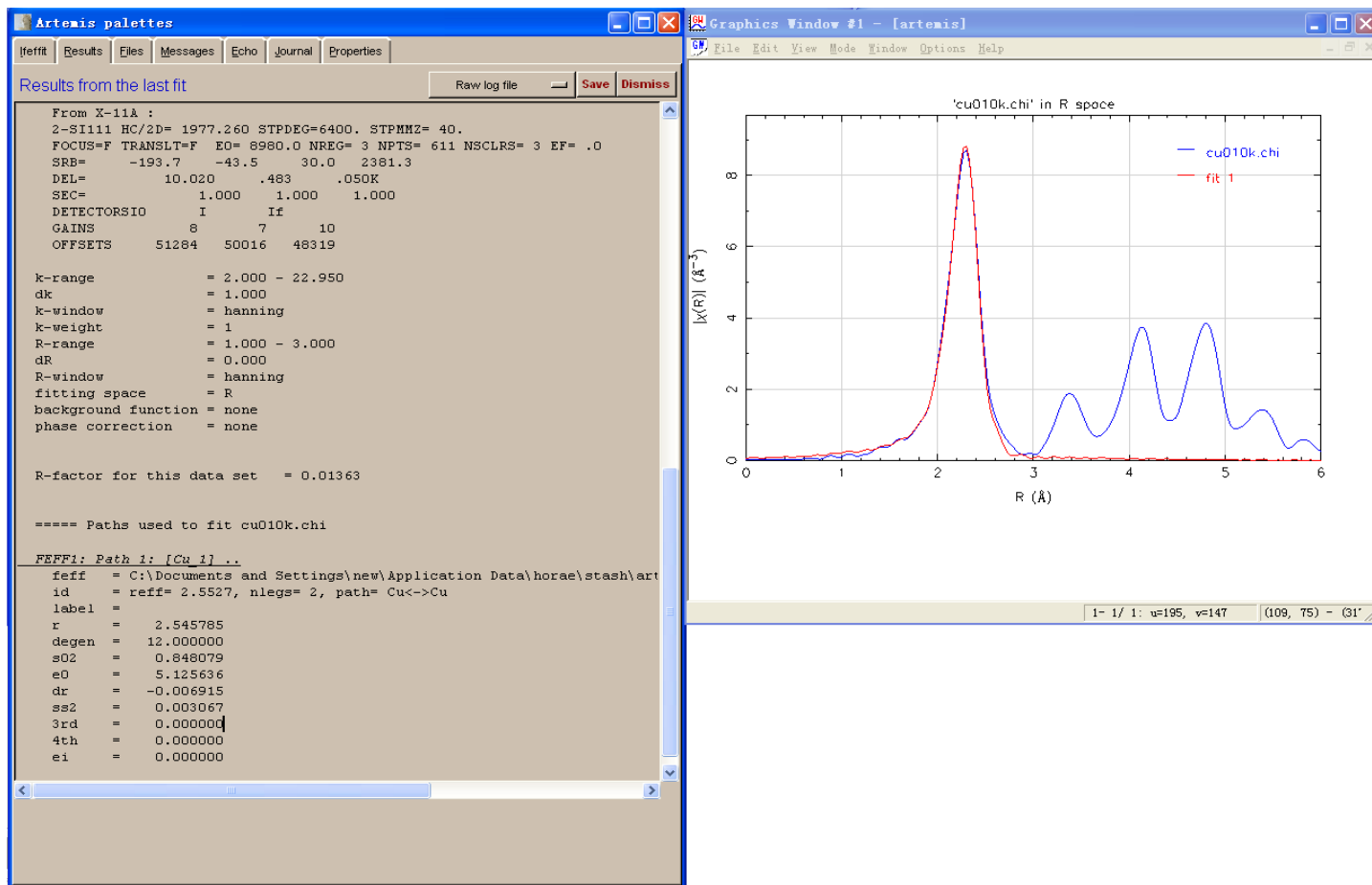
r enot\_res=scale\*penalty(enot,-5,5)

s scale=2000;

After: 设定参数间的数学关系式;  
(拟合结束后, 用参数的最优值代入)



# 单壳层拟合



- 选定第一壳层进行拟合后



# Result解读



本次拟合的统计信息

拟合参数最优值与不确定度

拟合参数相关性

```

Artemis palettes
-----
View files
-----
Project title : Three shell copper foil demo
Comment      : 7path
Prepared by  : bruce@atropos
Contact      :
Started      : 15:28:45 on 9 December, 2003
This fit at  : 22:51:38 on 7 December, 2011
Environment  : Artemis 0.8.014 using Windows XP, perl 5.008008, Tk 804.027,
Data sets    : "cu010k.chi"
Fit label    : fit 1
Figure of merit : 1

-----
Independent points      = 25.669921875
Number of variables    = 4.000000000
Chi-square             = 5901.785121481
Reduced Chi-square     = 272.349164687
R-factor               = 0.025820817
Measurement uncertainty (k) = 0.001106115
Measurement uncertainty (R) = 0.004671217
Number of data sets    = 1.000000000

Guess parameters +/- uncertainties (initial guess):
amp      = 0.9557080 +/- 0.0668780 (1.0000)
enot     = 5.5166320 +/- 0.5263790 (0.0000)
alpha    = 0.0002770 +/- 0.0010820 (0.0000)
theta    = 292.0185790 +/- 34.0174990 (350.0000)

Set parameters:
temp     = 10
signor   = 0.00052

Correlations between variables:
amp and theta --> -0.8693
enot and alpha --> 0.7831
All other correlations are below 0.43

==== Data set >>cu010k.chi<< =====
file: C:\Documents and Settings\new\Application Data\horae\stash\artemis.proj
    
```

```

Artemis palettes
-----
Results from the last fit
-----
From X-11A :
2-S1111 HC/2D= 1977.260 STPDEG=6400. STPMZ= 40.
FOCUS=F TRANSLT=F EO= 8980.0 NREG= 3 NPTS= 611 NSCLRS= 3 EF= .0
SRB= -193.7 -43.5 30.0 2381.3
DEL= 10.020 .483 .050K
SEC= 1.000 1.000 1.000
DETECTOR SIO I If
GAINS 8 7 10
OFFSETS 51284 50016 48319

k-range = 2.000 - 22.950
dk = 1.000
k-window = hanning
k-weight = 1
R-range = 1.000 - 3.000
dR = 0.000
R-window = hanning
fitting space = R
background function = none
phase correction = none

R-factor for this data set = 0.01363

==== Paths used to fit cu010k.chi
FEFF: Path 1: [Cu 1] ..
feff = C:\Documents and Settings\new\Application Data\horae\stash\art
id = reff= 2.5527, nlegs= 2, path= Cu<->Cu
label =
r = 2.545785
degen = 12.000000
s02 = 0.848079
e0 = 5.125636
dr = -0.006915
ss2 = 0.003067
3rd = 0.000000
4th = 0.000000
ei = 0.000000
    
```

各壳层的拟合结果



# 统计信息的定义



Chi-square 
$$\chi^2 = \frac{N_{idp}}{\epsilon N_{data}} \sum_{i=min}^{max} \left[ \text{Re} (\chi_d(r_i) - \chi_t(r_i))^2 + \text{Im} (\chi_d(r_i) - \chi_t(r_i))^2 \right]$$

Reduced  
Chi-square 
$$\chi_\nu^2 = \frac{\chi^2}{\nu}$$

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

不确定度  $\epsilon = \text{measurement uncertainty}$

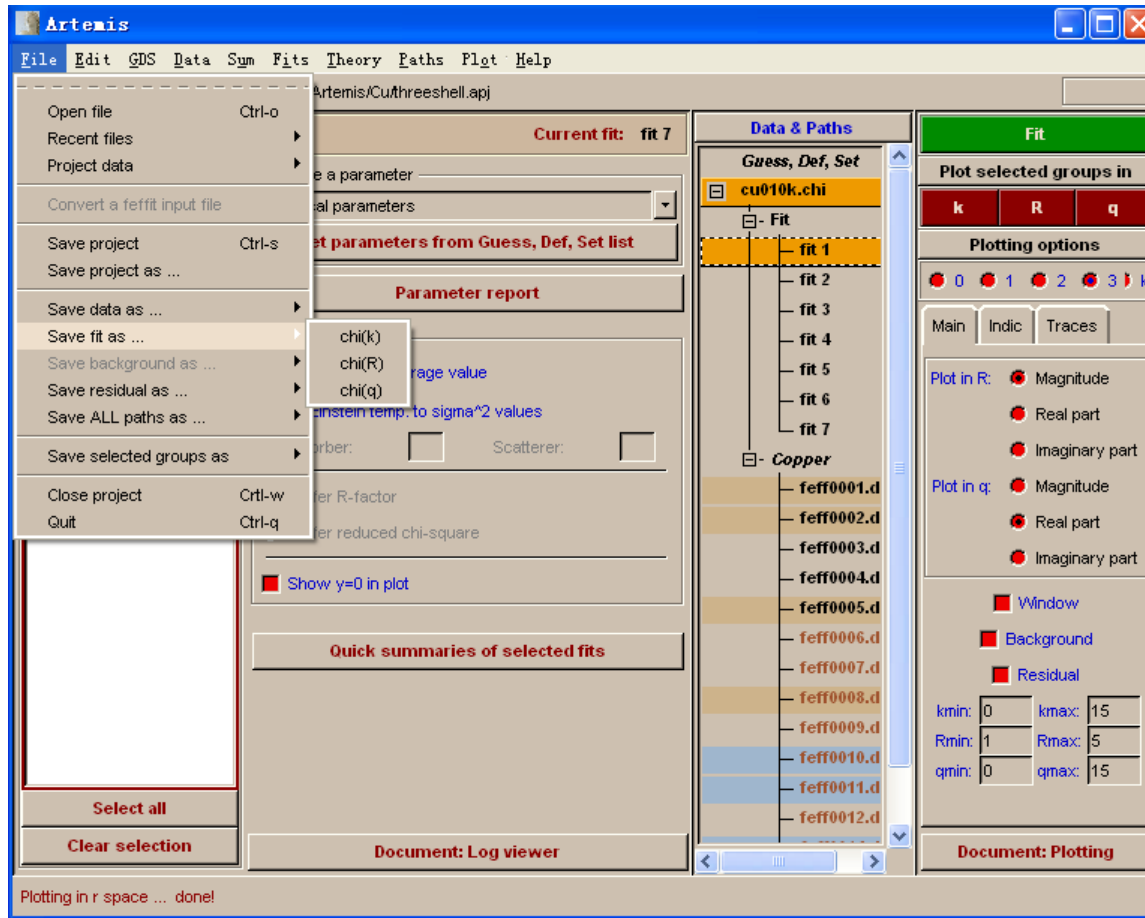
R-factor 
$$\mathcal{R} = \frac{\sum_{i=min}^{max} \left[ \text{Re} (\chi_d(r_i) - \chi_t(r_i))^2 + \text{Im} (\chi_d(r_i) - \chi_t(r_i))^2 \right]}{\sum_{i=min}^{max} \left[ \text{Re} (\chi_d(r_i))^2 + \text{Im} (\chi_d(r_i))^2 \right]}$$

Reduced Chi-square : 单一无法判定拟合结果的好坏;  
在拟合过程中如果变小, 说明拟合结果更优;

R-factor : <0.02 good; 0.02-0.05 模型稍有差异或数据质量欠佳; 0.05-0.1  
模型偏差大或数据质量很差; >0.1 模型错;



# 拟合结果输出



## ■ File/save fit as

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# 多壳层拟合



Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project: F:\feffit/examples\Artemis\Cu\oneshell.apj

Atoms feff.inp Interpretation

Interpretation of the FEFF Calculation

# TITLE Cu 222  
# Central atom: Copper (29) K edge energy = 8979 eV  
# The central atom is denoted by this token: [+]  
# Cluster size = 7.0 Angstroms, containing 135 atoms.  
# Curved wave criteria = 2.5.

#	Deg.	Reff	amp.	fs	Scattering Path
1	12	2.553	100.00		[+] Cu_1 [+]
2	6	3.610	22.98		[+] Cu_2 [+]
3	48	3.829	10.59		[+] Cu_1 Cu_1 [+]
4	48	4.358	8.65		[+] Cu_2 Cu_1 [+]
5	24	4.421	55.40		[+] Cu_3 [+]
6	48	4.763	10.62		[+] Cu_1 Cu_1 [+]
7	96	4.763	21.84		[+]
8	12	5.105	18.93		[+]
9	12	5.105	8.46		[+]
10	24	5.105	43.72	1	[+] Cu_4 Cu_1 [+]
11	12	5.105	8.20	1	[+] Cu_1 [+]
12	12	5.105	3.56		[+] Cu_1 [+]
14	12	5.105	32.79	2	[+] Cu_1 Cu_4 Cu_1 [+]
15	48	5.105	3.26		[+] Cu_1 Cu_1 Cu_1 [+]

Document: Feff interpretation

Showing header for "FEFF0: feff0006.dat"

Data & Paths

Guess, Def, Set

cu010k.chi

Fit

fit 1

FEFF0

feff0001.d

feff0002.d

feff0003.d

feff0004.d

feff0005.d

Fit

Plot selected groups in

k R q

Plotting options

0 1 2 3 k

Main Indic Traces

Plot in R: Magnitude  
Real part  
Imaginary part

Plot in q: Magnitude  
Real part  
Imaginary part

Window  
Background  
Residual

kmin: 0 kmax: 15  
Rmin: 0 Rmax: 6  
qmin: 0 qmax: 15

Document: Plotting

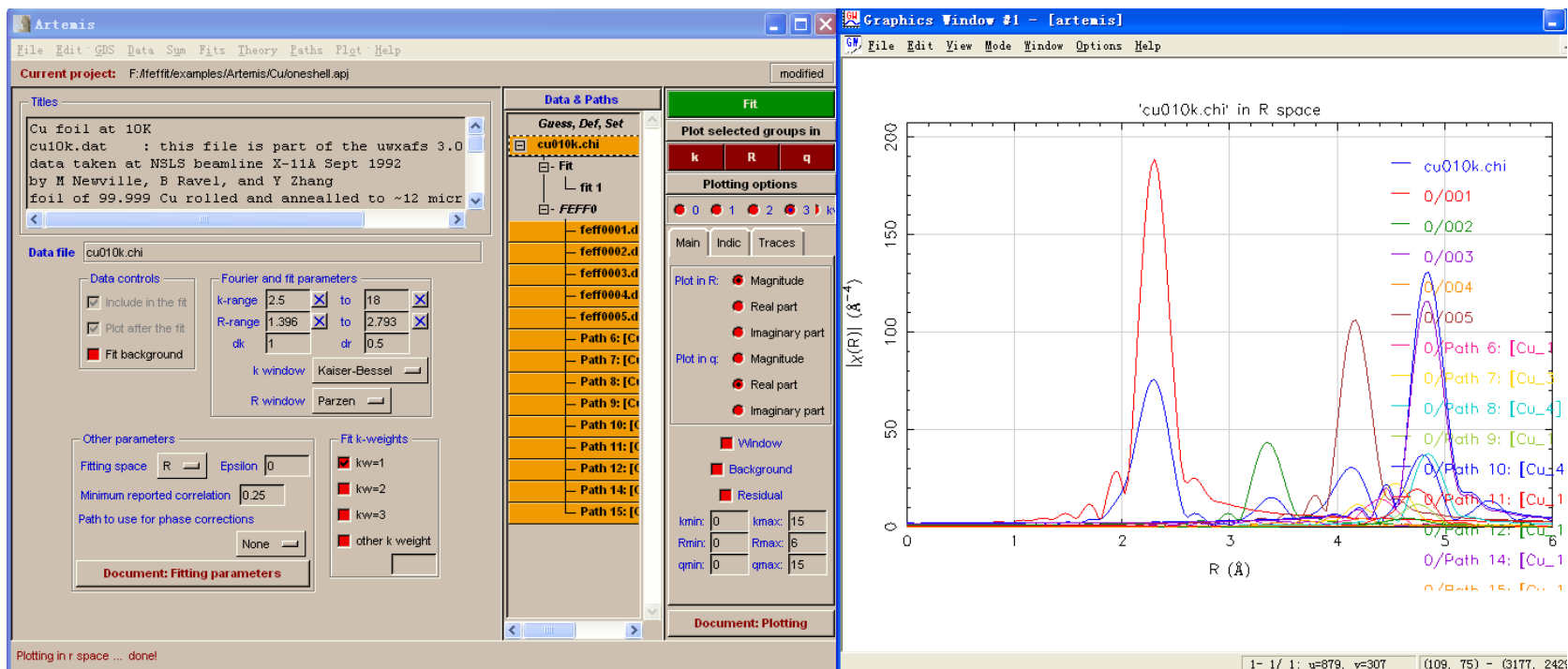
## ■ 增加路径



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# 多壳层拟合



确认增加的路径在范围内



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# 多壳层拟合



The screenshot shows the Artemis software interface with several windows open. The main window displays the fit configuration for 'FEFF0: feff0001.dat'. It shows two legs with parameters:  $r_{leg}=2.5527$ ,  $\beta=180.000$ , and  $\text{amp}=100.000$ . The fit parameters are listed as  $2 \text{ legs}$ ,  $R_{eff}=2.5527$ ,  $\text{amp}=100.000$ , and  $\text{degen}=12$ . The path parameter math expressions are shown with a table:

label:	
N:	12 X S02: amp
delE0:	enot
delR:	delr
sigma^2:	sigsq + signor
Ei:	
3rd:	
4th:	

The 'Fit' dialog box is open, showing 'Plot selected groups in' with 'k', 'R', and 'q' selected. The 'Plotting options' section has radio buttons for '0', '1', '2', '3', and 'k'. The 'Artemis: read math expression' dialog is also open, showing the math expression 'amp' and options to add it to the calculation. The 'Document: edit math expression' window is also visible.

## ■ 为新添路径设置参数

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# 多壳层拟合



$N_{\text{idp}} \approx 2\Delta k \Delta R / \pi$  最大对立拟合参数个数

例：k-range 2.5-18； R-range 1.7-5.1

$N_{\text{idp}} \approx 33.5$

每一条路径需要至少4个独立拟合参数；因此最多可以选取8条路径；

如果  $N_{\text{var}} > N_{\text{idp}}$  独立拟合参数多于可用独立节点数，此时拟合的结果是一个多解的结果

## ■ 独立节点概念！！！！



# 多壳层拟合



## ■ 拟合策略:

所有路径  $S02$  可设成统一

相同原子所有路径  $\sigma^2$  可设成统一

相同原子  $\Delta E0$  可设成统一

配位数可以通过模型限定或合理限定

$\Delta R$  可以用热膨胀或与结构关联起来

对于金属体系,  $\sigma^2$  可以用 Debye 模型  
或关联 Einstein 模型进行关联

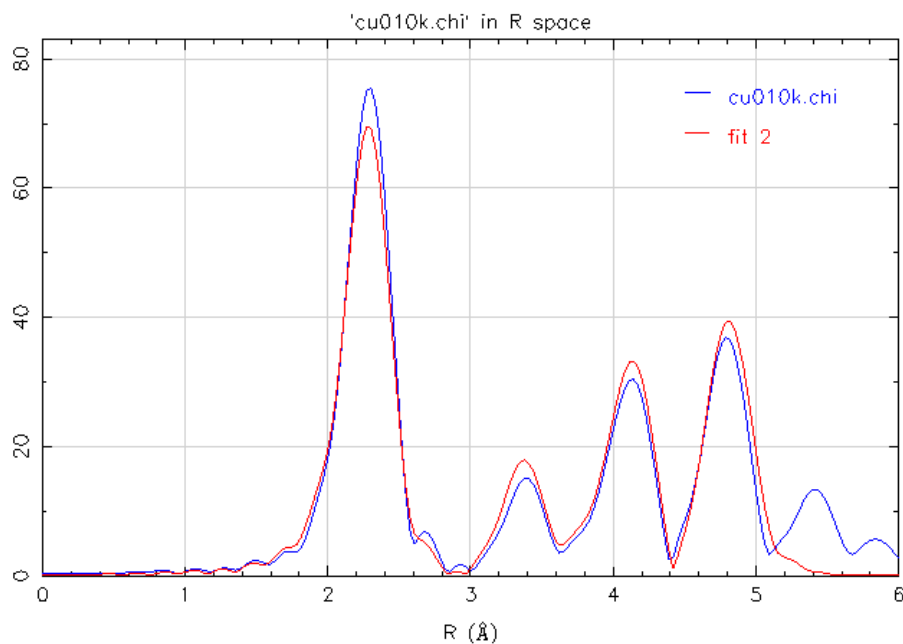


# 多壳层拟合



```
Independent points      =      33.495117188
Number of variables     =      4.000000000
Chi-square              =     2849.187637658
Reduced Chi-square      =     96.598620699
R-factor                =      0.023635132
Measurement uncertainty (k) =      0.001130698
Measurement uncertainty (R) =      0.004441269
Number of data sets    =      1.000000000

Guess parameters +/- uncertainties (initial guess):
amp      =      0.9572390 +/-      0.0578760 (0.9000)
enot     =      4.5524130 +/-      0.4672840 (0.0000)
delr     =     -0.0065590 +/-      0.0034980 (0.0000)
ss       =      0.0040400 +/-      0.0004380 (0.0030)
```



参数设置：统一S02、 $\Delta E0$ 、 $\sigma^2$ ，  
 $\Delta R = \alpha \cdot \text{reff}$

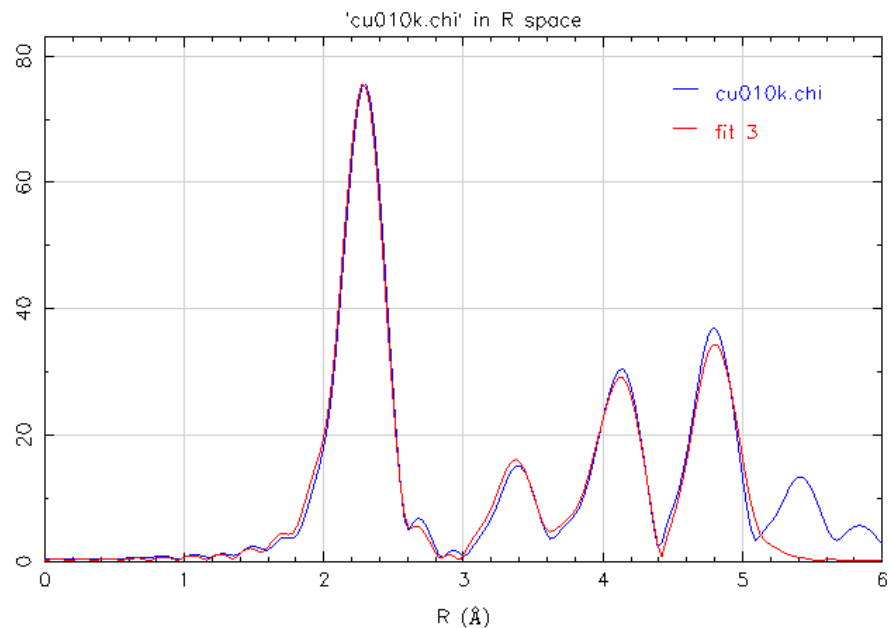


# 多壳层拟合



```
Independent points      =      33.495117188
Number of variables     =      5.000000000
Chi-square              =     437.769495322
Reduced Chi-square      =     15.362965256
R-factor                =      0.007740291
Measurement uncertainty (k) = 0.000529236
Measurement uncertainty (R) = 0.441518688
Number of data sets    =      1.000000000

Guess parameters +/- uncertainties (initial guess):
amp      = 0.9176620 +/- 0.0337030 (0.9000)
enot     = 3.9682010 +/- 0.3536980 (0.0000)
delr     = -0.0083760 +/- 0.0015520 (0.0000)
ss       = 0.0044180 +/- 0.0001940 (0.0030)
ss_1     = 0.0034830 +/- 0.0001660 (0.0030)
```



将最近邻的 $\sigma^2$ 设成独立项，其他不变



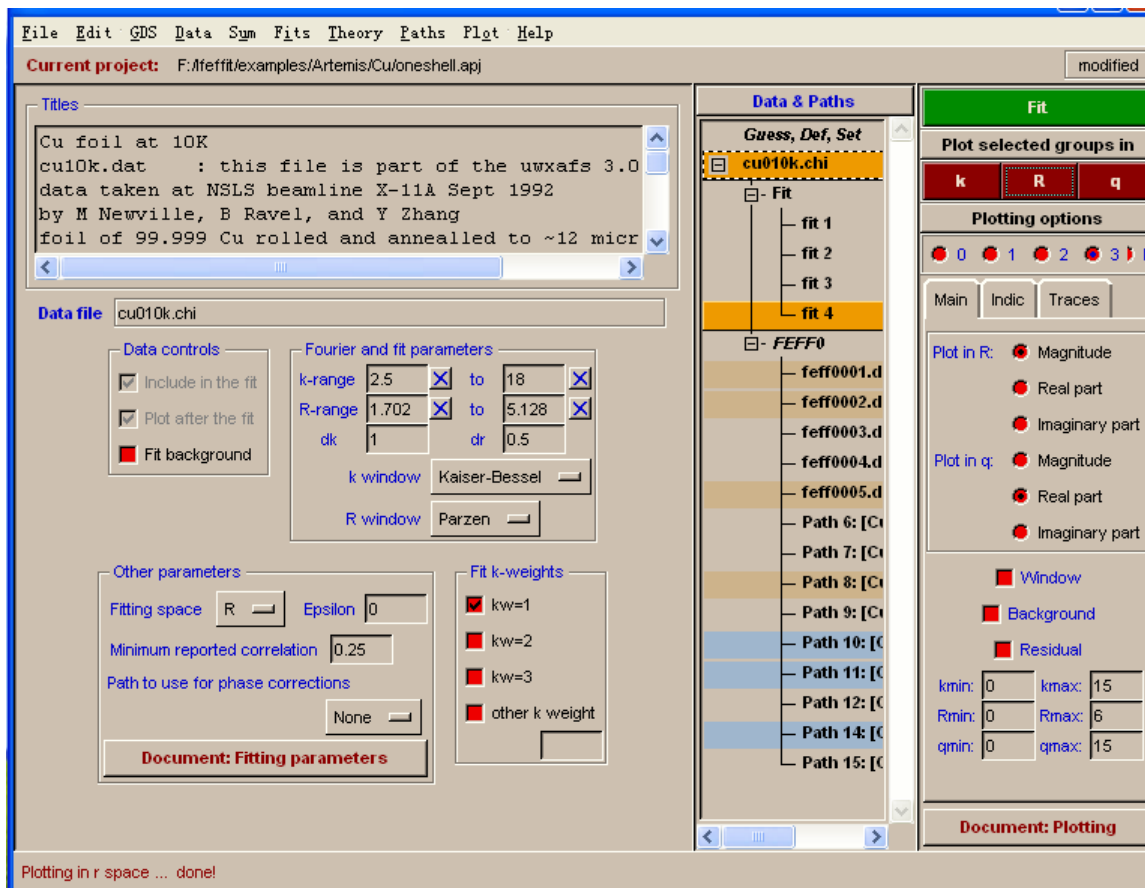
# 主要内容



- ◆ 软件简介
- ◆ 数据处理
  - a 单壳层拟合
  - b 多壳层拟合
  - c 多权重拟合
  - d 多Feff拟合
  - e 多数据拟合



# 多权重拟合



## ■ 将拟合权重同时选中

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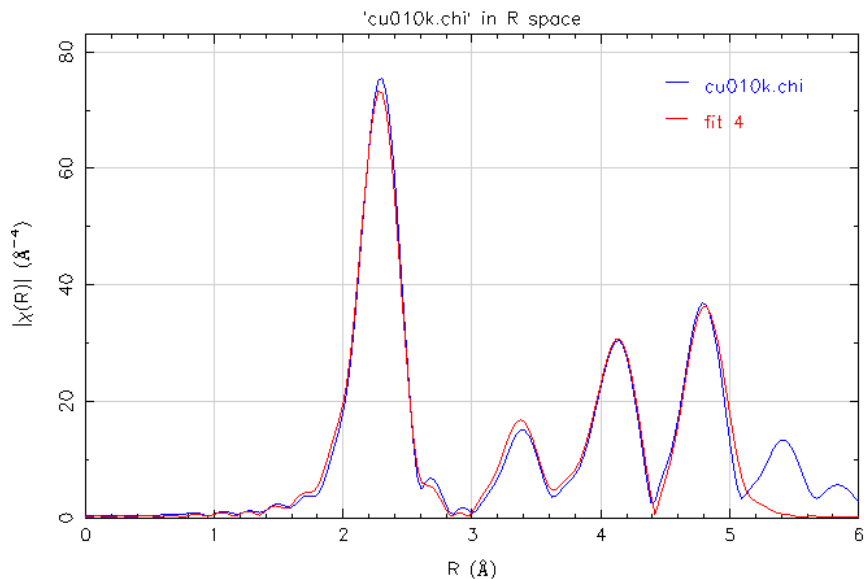


# 多权重拟合



```
Independent points      = 33.495117188
Number of variables     = 5.000000000
Chi-square              = 2680.660982650
Reduced Chi-square     = 94.074397554
R-factor                = 0.022237137
Measurement uncertainty (k) = 0.001130698
Measurement uncertainty (R) = 0.004441269
Number of data sets    = 1.000000000

Guess parameters +/- uncertainties (initial guess):
amp      = 0.9466660 +/- 0.0565830 (0.9000)
enot     = 4.5458370 +/- 0.4634740 (0.0000)
delr     = -0.0068020 +/- 0.0034040 (0.0000)
ss       = 0.0043280 +/- 0.0005090 (0.0030)
ss_1     = 0.0037540 +/- 0.0004610 (0.0030)
```



- 选取fit k-weight为1时的拟合结果

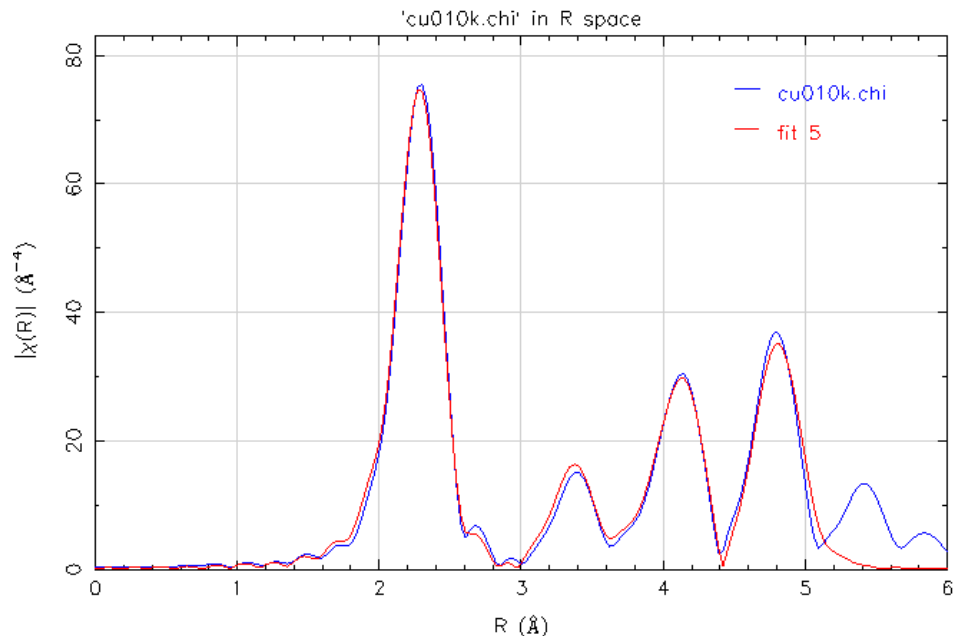


# 多权重拟合



```
Independent points      =      33.495117188
Number of variables    =      5.000000000
Chi-square             =     4219.035038864
Reduced Chi-square     =     148.061684081
R-factor              =      0.014197641
Measurement uncertainty (k) = 0.001130698
Measurement uncertainty (R) = 0.004441269
Number of data sets    =      1.000000000

Guess parameters +/- uncertainties (initial guess):
amp      = 0.9400230 +/- 0.0451410 (0.9000)
enot     = 4.3813570 +/- 0.4145220 (0.0000)
delr     = -0.0072330 +/- 0.0024860 (0.0000)
ss       = 0.0044320 +/- 0.0003360 (0.0030)
ss_1     = 0.0036380 +/- 0.0002910 (0.0030)
```



chi-square 与reduced chi-square 就计算为所有k权重的和；  
从拟合结果看，有一定的改善；  
依据：不同原子对于k的响应不同；  
 $\sigma^2$ 、 $\Delta R$ 、 $\Delta E_0$ 对k的响应为非线性；



# 主要内容



- ◆ 软件简介
- ◆ 数据处理
  - a 单壳层拟合
  - b 多壳层拟合
  - c 多权重拟合
  - d 多Feff拟合
  - e 多数据拟合



# 多Feff拟合



例  $\text{YBa}_2\text{Cu}_3\text{O}_7$  : Cu有两种占位

```
title YBCO: Y Ba2 Cu3 O7
space = P M M M
rmax = 7.2  a=3.817 b=3.882 c=11.671
core = cu1
atoms
! At.type  x      y      z      tag
  Y        0.5    0.5    0.5
  Ba        0.5    0.5    0.1839
  Cu        0      0      0      cu1
  Cu        0      0      0.3546  cu2
  O         0      0.5    0      O1
  O         0      0      0.1589  O2
  O         0      0.5    0.3780  O3
  O         0.5    0      0.3783  O4
```



# 多Feff拟合



The screenshot shows the Artemis software interface. A context menu is open over the 'Data' section, listing options such as 'Fit', 'Sym', 'Fits', 'Theory', 'Paths', and 'Plgt'. The 'Paths' option is highlighted, and a sub-menu is visible with options like 'Clone a FEFF calculation ...', 'Rename these data', 'View this data file', 'Restore default parameter values', 'Discard this data set', and 'What is epsilon\_k?'. The main window displays the 'Current project' 'YBCO: Y Ba2 Cu3 O7' and a table of atoms with their coordinates and core levels.

Space group	P	M	M	M	Core	EI	X	Y	Z
A	3.82300				1	Y	0.50000	0.50000	0.50000
B	3.88600				2	Ba	0.50000	0.50000	0.1840
C	11.68100				3	Cu	0.00000	0.00000	0.0000
Alpha					4	Cu	0.00000	0.00000	0.3560
Beta					5	O	0.00000	0.50000	0.0000
Gamma					6	O	0.00000	0.00000	0.1580
Cluster size	5.20000				7	O	0.00000	0.50000	0.3790
Edge	K				8	O	0.50000	0.00000	0.3770
Shift vector	0								

## ■ 增加Feff计算

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# 多Feff拟合



Artemis

File Edit GDS Data Sum Fits Theory Paths Plot Help

Current project: modified

Atoms feff.inp Interpretation

Titles  
YBCO: Y Ba2 Cu3 O7

Space group	P	M	M	M	Core	EI	X	Y	Z	
A	3	.82300			1	<input checked="" type="checkbox"/>	Y	0.50000	0.50000	0.5000
B	3	.88600			2	<input checked="" type="checkbox"/>	Ba	0.50000	0.50000	0.1840
C	11	.68100			3	<input checked="" type="checkbox"/>	Cu	0.00000	0.00000	0.0000
Alpha					4	<input checked="" type="checkbox"/>	Cu	0.00000	0.00000	0.3560
Beta					5	<input checked="" type="checkbox"/>	O	0.00000	0.50000	0.0000
Gamma					6	<input checked="" type="checkbox"/>	O	0.00000	0.00000	0.1580
Cluster size	5	.20000			7	<input checked="" type="checkbox"/>	O	0.00000	0.50000	0.3790
Edge	K				8	<input checked="" type="checkbox"/>	O	0.50000	0.00000	0.3770
Shift vector	0									

Edit selected site  
Element:  Tag:  Define  
X:  Y:  Z:  New

Run Atoms Document: Atoms

Excluded selected paths from fitting.

Data & Paths

- fit
  - 3
    - Path 1: [o2\_1]
    - Path 2: [o1\_1]
    - Path 3: [o1\_1 o2\_1]
    - Path 4: [Ba\_1]
    - Path 5: [o2\_1 o2\_1]
    - Path 6: [o2\_1 [+] o2\_1]
    - Path 7: [o2\_1 [+] o2\_1]
    - Path 8: [cu1\_1]
    - Path 9: [cu1\_2]
    - Path 10: [o1\_1 o1\_1]
  - 4
    - Path 1: [o4\_1]
    - Path 2: [o3\_1]
    - Path 3: [o2\_1]
    - Path 4: [Y\_1]
    - Path 5: [o3\_1 o4\_1]
    - Path 6: [cu2\_1]
    - Path 7: [Ba\_1]
    - Path 8: [o3\_2]
    - Path 9: [o4\_2]
    - Path 10: [o2\_1 o4\_1]

Fit

Plot selected groups in  
k R q

Plotting options  
 0  1  2  3 kw

Main Indic Traces

Plot in R:  Magnitude  
 Real part  
 Imaginary part

Plot in q:  Magnitude  
 Real part  
 Imaginary part

Window  
 Background  
 Residual

kmin: 0 kmax: 15  
Rmin: 0 Rmax: 6  
qmin: 0 qmax: 15

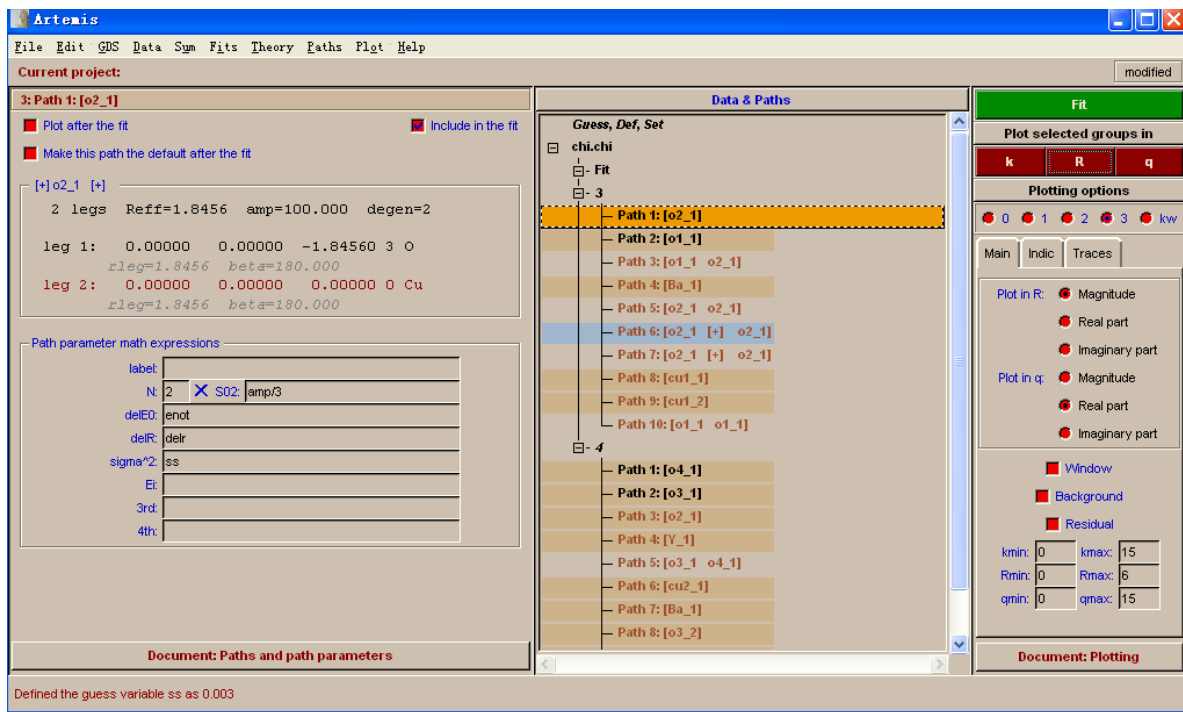
Document: Plotting

## 重新选择吸收原子位置

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# 多Feff拟合



- 修正拟合参数（占位1 配位数\*1/3，占位2 配位数\*2/3）



# 主要内容

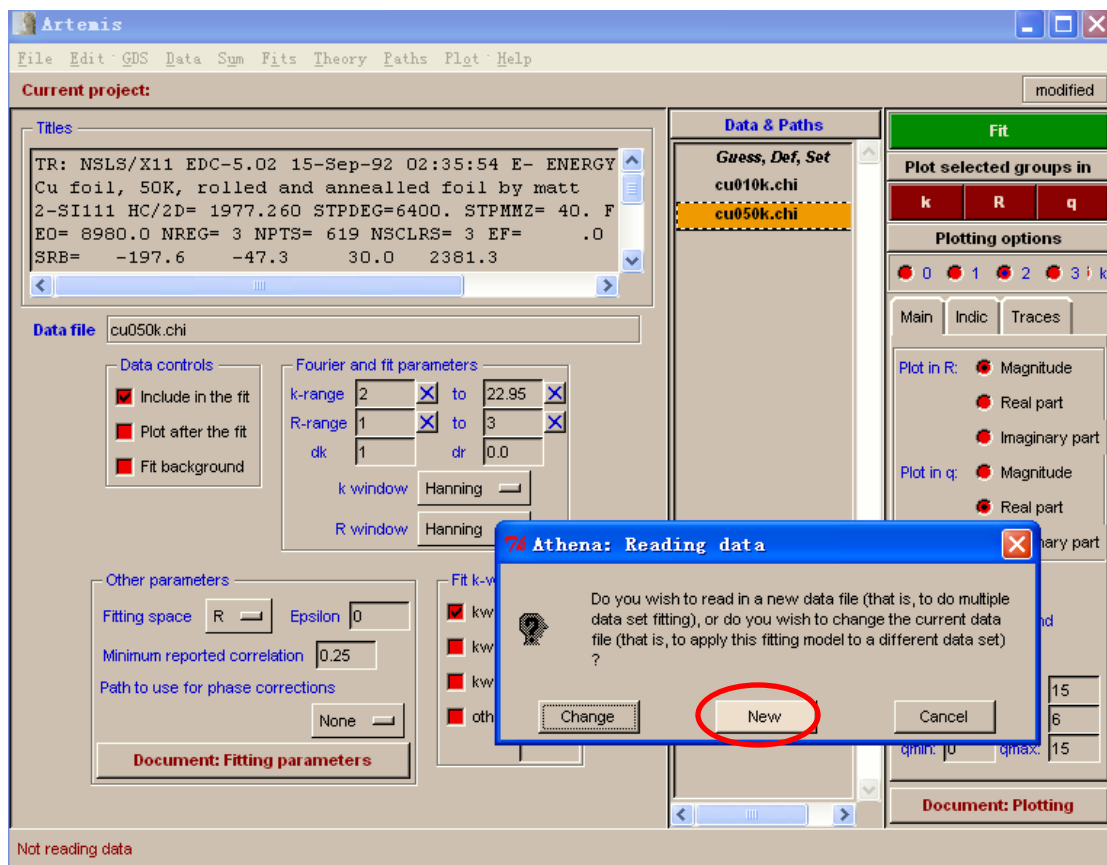


- ◆ 软件简介
- ◆ 数据处理
  - a 单壳层拟合
  - b 多壳层拟合
  - c 多权重拟合
  - d 多Feff拟合
  - e 多数据拟合





# 多数据拟合



- 导入多个数据



# 多数据拟合



The screenshot shows the Artemis software interface. The main window displays the current project information, including the data file 'cu150k.chi' and various fitting parameters. A context menu is open over the 'Data & Paths' panel, showing options like 'Fit', 'Save background subtracted as chi(k)', 'Make difference spectra using selected paths', 'Clone a FEFF calculation...', 'Rename these data', 'View this data file', 'Restore default parameter values', 'Discard this data set', 'What is epsilon\_k?', and 'How many independent points?'. The 'Fit' option is highlighted, and a 'link copy' button is visible next to it.

Artemis  
File Edit GDS Data Sym Fits Theory Paths Plgt Help  
Current project: modified

Titles  
TR: NSLS/X11 EDC-5.02 15-Sep-92 04:05:24 E- ENERGY  
Cu foil, 150K x11 standard foil  
2-SI111 HC/2D= 1977.260 STPDEG=6400. STPMZ= 40. F  
EO= 8980.0 NREG= 3 NPTS= 636 NSCLRS= 3 EF= .0  
SRB= -205.8 -55.6 30.0 2381.3

Data file cu150k.chi

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

Fourier and fit parameters  
k-range 2 to 22.95  
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

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

Document: Fitting parameters

78 independent points data points (Nyquist): (3 data sets) (4 variables)

详细信息  
多壳层拟合4. bmp  
多壳层拟合5. bmp  
多壳层拟合6. bmp  
多壳层拟合7. bmp  
多壳层拟合8. bmp  
多壳层拟合9. bmp  
多权重拟合. bmp  
多权重拟合2. bmp

Data & Paths  
Path 2: [C]  
Path 3: [C]  
Path 4: [C]  
Path 5: [C]  
Path 6: [C]  
Path 7: [C]  
Path 8: [C]  
Path 9: [C]  
Path 10: [C]  
cu050k.chi  
FEFF0  
Path 1: [C]  
Path 2: [C]  
Path 3: [C]  
Path 4: [C]  
Path 5: [C]  
Path 6: [C]

Fit  
Plot selected groups in  
k R q  
Plotting options  
0 1 2 3 k  
Main Indic Traces  
Plot in R: Magnitude  
Real part  
Imaginary part  
Plot in q: Magnitude  
Real part  
Imaginary part  
Window  
Background  
Residual  
kmin: 0 kmax: 15  
Rmin: 0 Rmax: 6  
qmin: 0 qmax: 15

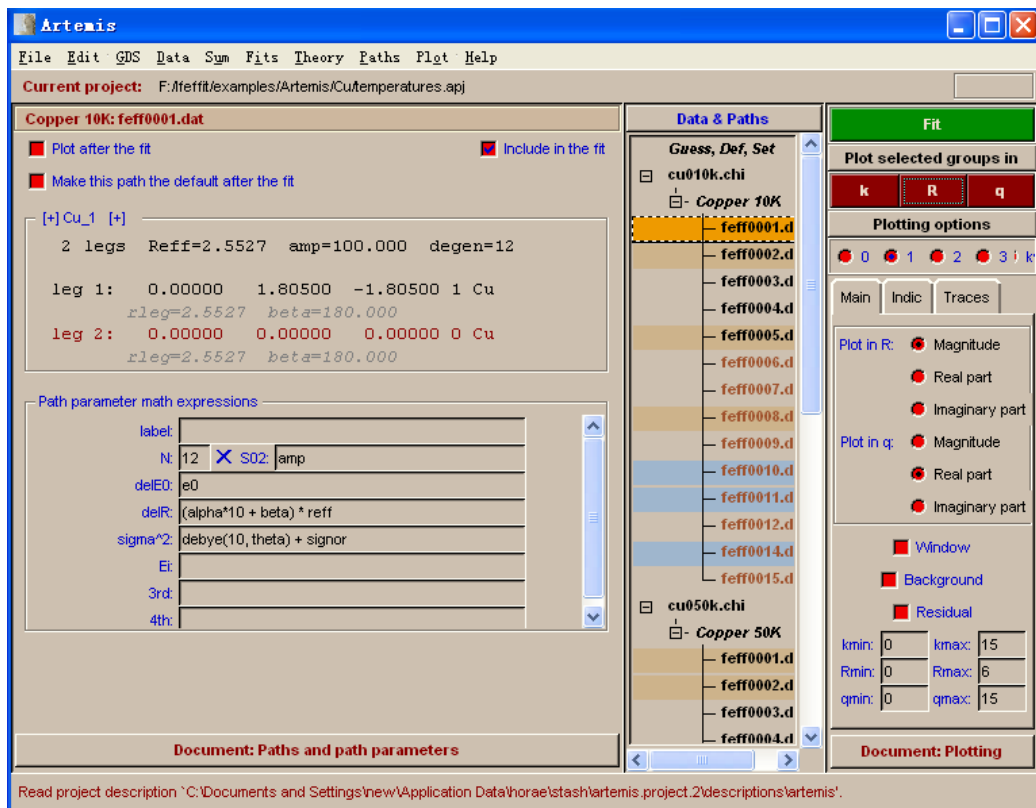
File  
Edit  
GDS  
Data  
Sym  
Fits  
Theory  
Paths  
Plgt  
Help  
Fit  
Save background subtracted as chi(k)  
Make difference spectra using selected paths  
Clone a FEFF calculation ...  
Rename these data Ctrl-n  
View this data file  
Restore default parameter values  
Discard this data set  
What is epsilon\_k?  
How many independent points?

link  
copy

每个数据都进行一次feff计算



# 多数据拟合



修改拟合参数:  $\text{delr} = (\text{alfa} * 10 + \text{beta}) * \text{reff}$  (键长设为部分与温度相关)  
 $\text{sigma}^2 = \text{debye}(\text{temp}, \text{thetad}) + \text{signor}$  (debye模型关联)

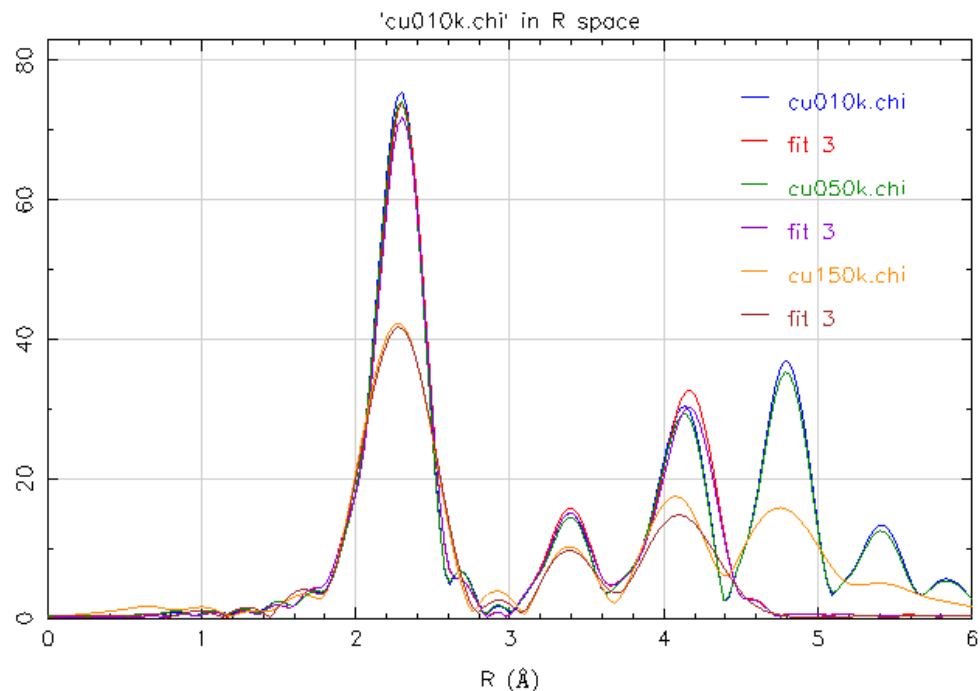


# 多数据拟合



```
Independent points      =      65.707031250
Number of variables     =      6.000000000
Chi-square              =     17631.101105636
Reduced Chi-square      =     295.293548122
R-factor                =      0.032624040
Measurement uncertainty (k) = 0.001094974
Measurement uncertainty (R) = 0.002335866
Number of data sets     =      3.000000000
```

```
Guess parameters +/- uncertainties (initial guess):
amp      = 0.9623560 +/- 0.0483510
alpha    = 0.0000070 +/- 0.0000090
beta     = 0.0011760 +/- 0.0009400
theta    = 320.3720870 +/- 26.3435590
signor   = 0.0008900 +/- 0.0004300
enot     = 6.0127540 +/- 0.3944250
```

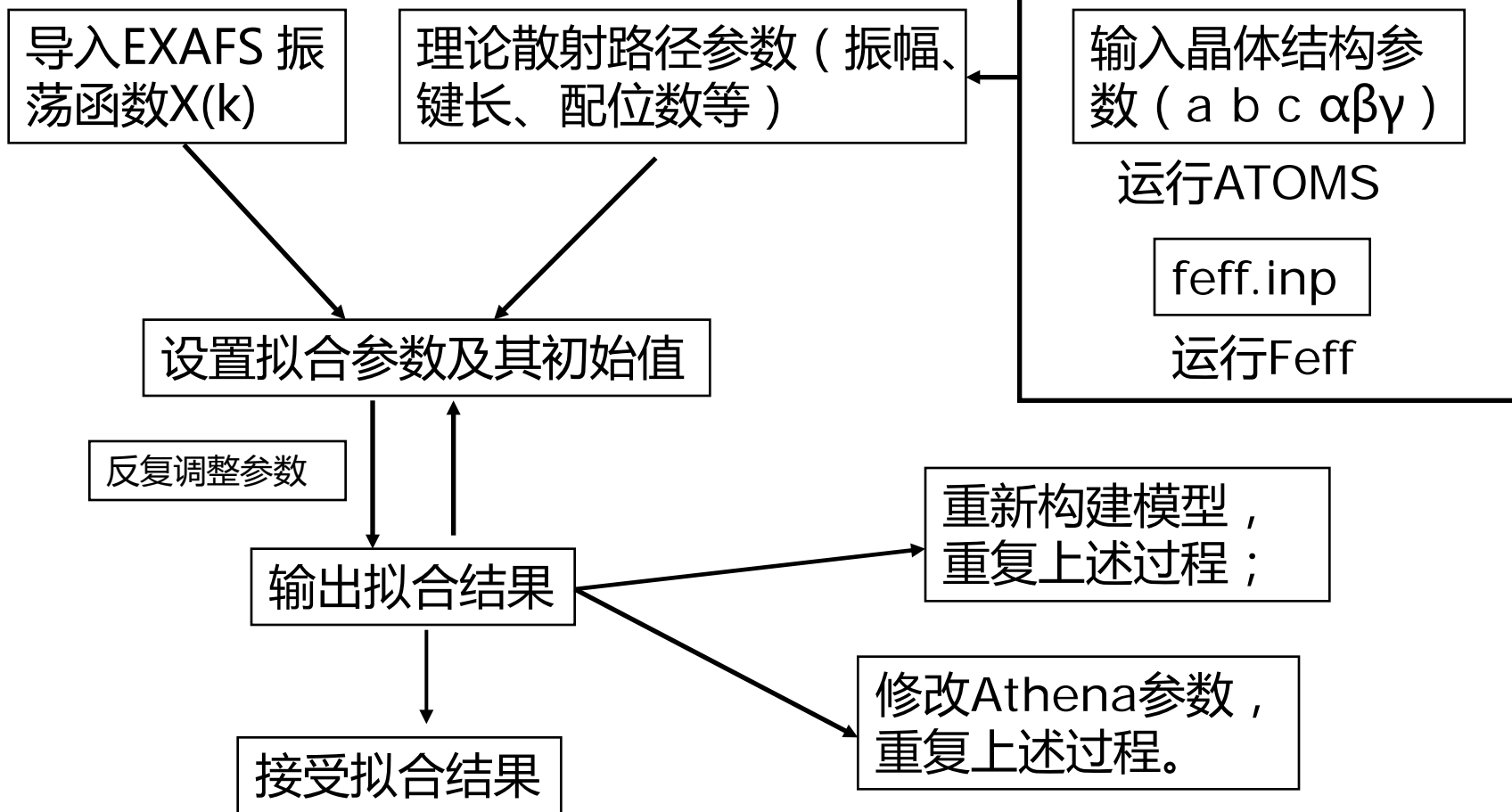


# 总结:



## 前期数据处理

## 构建模型





# 良好的数据 准确的模型



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谢谢!  
欢迎指正!



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