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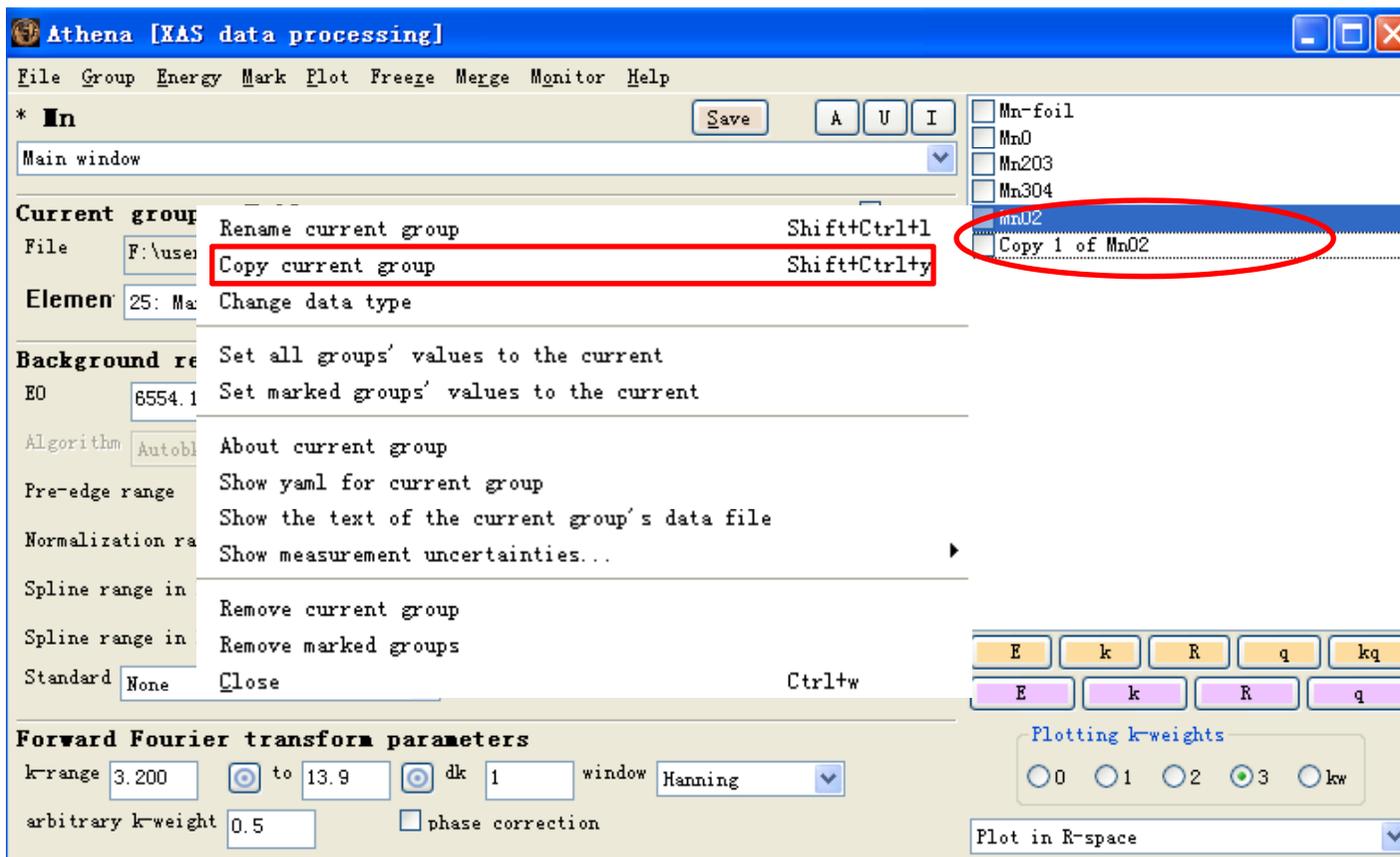
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# ATHENA功能介绍

## 复制数据

可以进行参数比较：例如Rbkg、归一化范围、k-range等



# 主要内容



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- XAFS数据处理的一般步骤
- Athena软件功能介绍
- 应用举例
- 实例分析与总结
- 上机练习



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# ATHENA软件应用举例

## XANES应用-铂纳米颗粒的电子结构和电荷转移研究

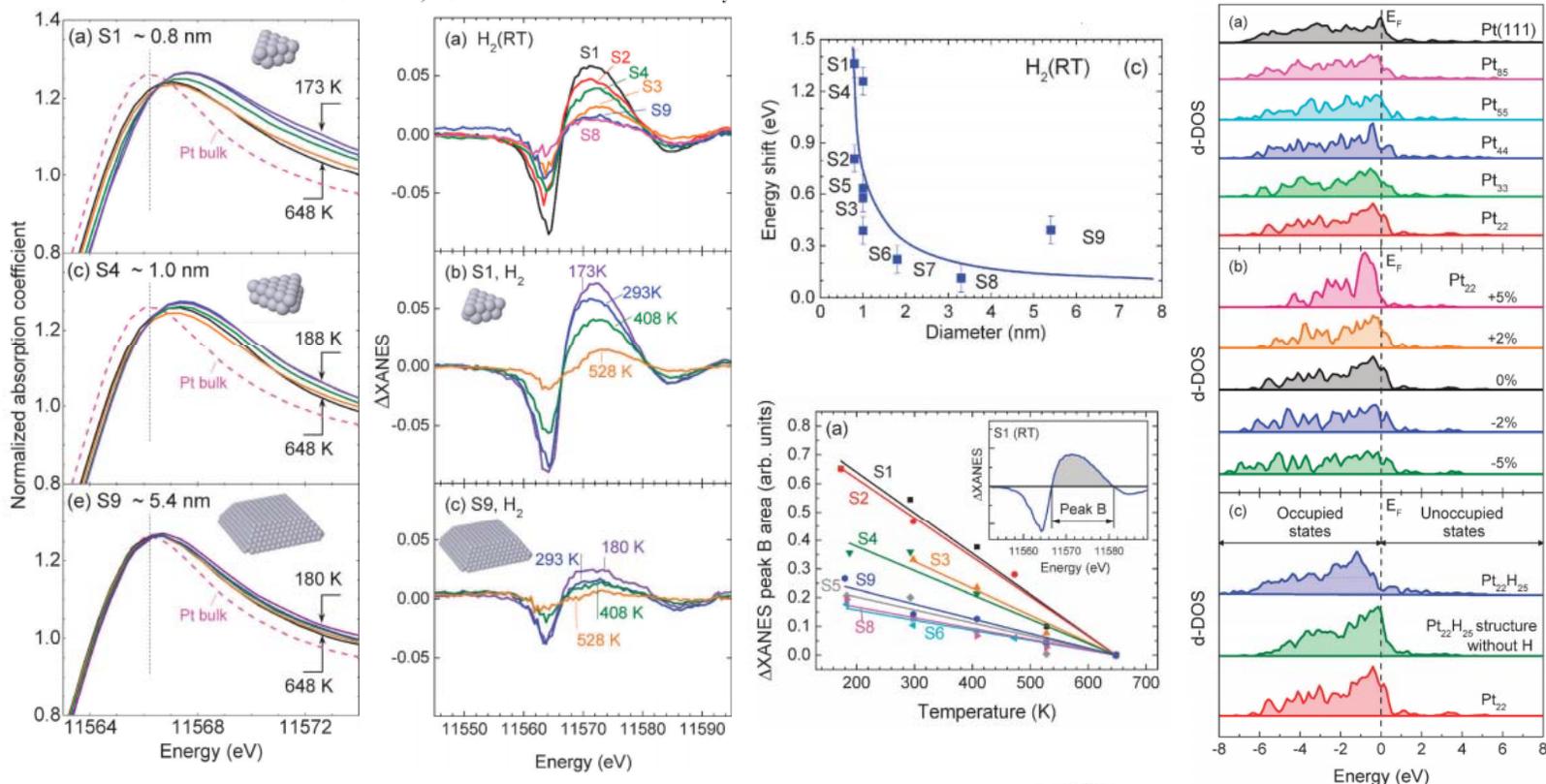
Cite this: *Phys. Chem. Chem. Phys.*, 2012, **14**, 11766–11779

[www.rsc.org/pccp](http://www.rsc.org/pccp)

PAPER

Electronic properties and charge transfer phenomena in Pt nanoparticles on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>: size, shape, support, and adsorbate effects†

F. Beharid,<sup>a</sup> L. K. Ono,<sup>a</sup> S. Mostafa,<sup>a</sup> J. R. Croy,<sup>a</sup> G. Shafai,<sup>a</sup> S. Hong,<sup>a</sup> T. S. Rahman,<sup>a\*</sup> Simon R. Bare<sup>b</sup> and B. Roldan Cuenya<sup>a\*</sup>





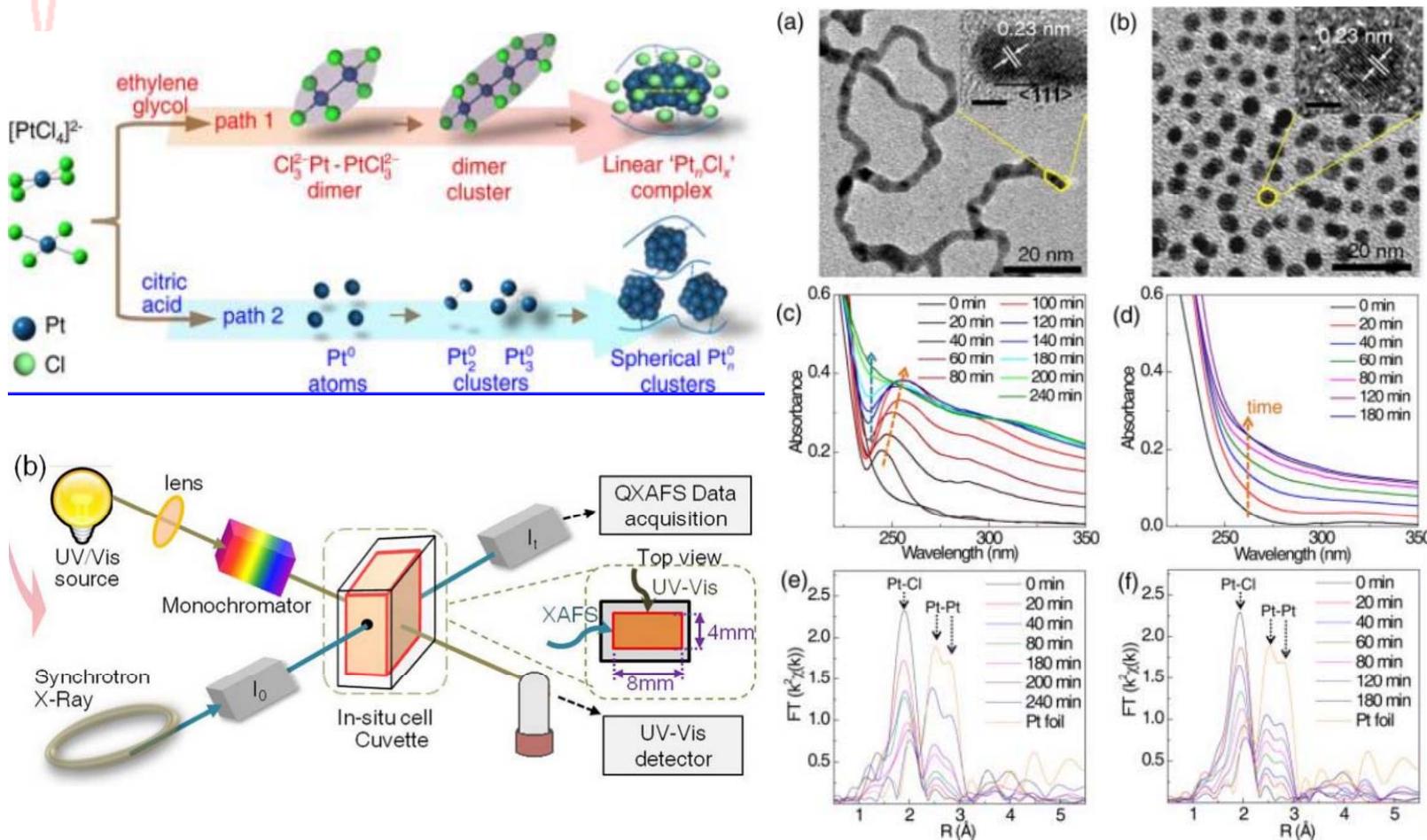
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# ATHENA软件应用举例

## EXAFS应用-不同形态铂纳米晶的生长过程原位研究



Tao Yao et al., Probing Nucleation Pathways for Morphological Manipulation of Platinum Nanocrystals, *J. Am. Chem. Soc.* 2012, 134, 9410-9416

# 主要内容



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# 实例分析与总结

- ◆ 打开数据文件时遇到的问题
- ◆ 数据信噪比判断
- ◆ 关于能量坐标

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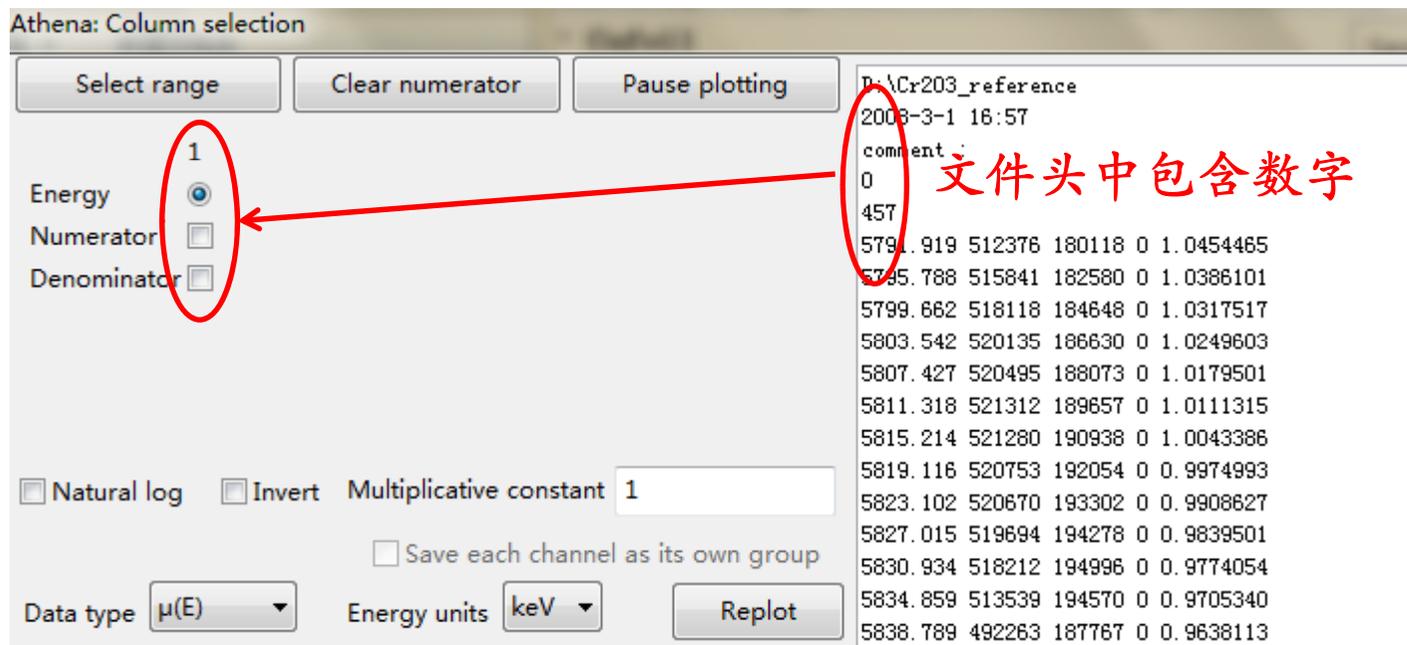


# 实例分析与总结

## Athena打开文件时

### 文件打不开?

- ◆ 文件名或者路径包含中文
- ◆ 文件格式：文件头和数据列
- ◆ 文件中存在异常数据点





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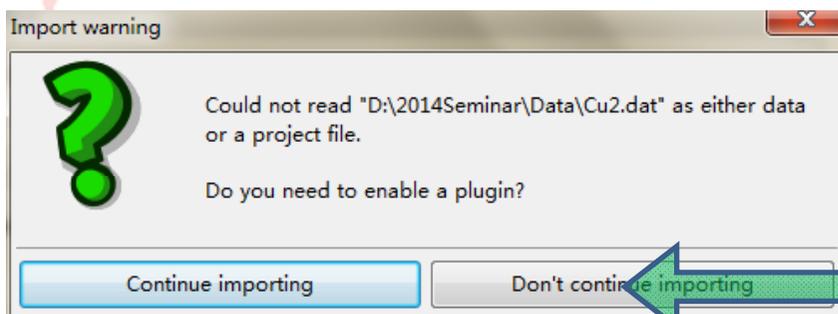
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# 实例分析与总结

## Athena打开文件时

文件中存在异常数据点



Cu2.dat - 记事本

文件(F)	编辑(E)	格式(O)	查看(V)	帮助(H)
9127.863	131284	13875	761294	2.2472781
9128.860	130992	13654	749266	2.2611076
9129.858	130462	13464	738868	2.2710254
9130.856	130302	13373	733897	2.2766132
9132.053	129512	13266	728070	2.2785692
9133.052	130509	13386	734784	2.2772328
INF	0	0	0	0
9135.049	130340	13483	740360	2.2687206
9136.048	130129	13546	743943	2.2623981
9137.047	129726	13600	746994	2.2553954
9138.047	129838	13722	753856	2.2472871
9139.046	129704	13832	760119	2.2382740
9140.046	129593	13964	767490	2.2279162
9141.046	128983	14064	773126	2.2160623

LD2Y-3.dat - 记事本

文件(F)	编辑(E)	格式(O)	查看(V)	帮助(H)			
2.450000E+0	2.230009E+1	2.980753E+5	3.000000E+0	2.959629E+0	2011-11-28	11:56:59	1.474924E+10
2.451000E+0	2.771271E+1	2.978887E+5	3.000000E+0	2.958931E+0	2011-11-28	11:57:09	1.475017E+10
2.452000E+0	3.212971E+1	2.977123E+5	3.000000E+0	2.956764E+0	2011-11-28	11:57:15	1.475167E+10
2.453000E+0	3.484134E+1	2.974723E+5	3.000000E+0	2.956259E+0	2011-11-28	11:57:20	1.474964E+10
2.454000E+0	3.576607E+1	2.972013E+5	3.000000E+0	2.963703E+0	2011-11-28	11:57:26	1.474589E+10
2.455000E+0	3.783664E+1	2.976313E+5	3.000000E+0	2.960094E+0	2011-11-28	11:57:31	1.478083E+10
2.456000E+0	4.496189E+1	2.970440E+5	3.000000E+0	2.958060E+0	2011-11-28	11:57:36	1.475999E+10
2.457000E+0	3.756085E+1	2.969000E+5	3.000000E+0	2.955205E+0	2011-11-28	11:57:42	1.476282E+10
2.458000E+0	5.244810E+1	2.967947E+5	3.000000E+0	2.955302E+0	2011-11-28	11:57:47	1.476818E+10
2.459000E+0	4.471975E+1	2.964020E+5	3.000000E+0	2.951716E+0	2011-11-28	11:57:53	1.475763E+10
2.460000E+0	5.271718E+1	2.964190E+5	5.000000E+0	4.931978E+0	2011-11-28	11:57:58	1.476975E+10
2.460500E+0	5.167106E+1	2.962646E+5	5.000000E+0	4.935065E+0	2011-11-28	11:58:05	1.476678E+10
2.461000E+0	5.881941E+1	2.961014E+5	5.000000E+0	4.930346E+0	2011-11-28	11:58:12	1.476332E+10
2.461500E+0	6.386001E+1	2.962560E+5	5.000000E+0	4.932665E+0	2011-11-28	11:58:19	1.477749E+10
2.462000E+0	6.786453E+1	2.961550E+5	5.000000E+0	4.936305E+0	2011-11-28	11:58:25	1.477747E+10
2.462500E+0	6.809414E+1	2.960330E+5	5.000000E+0	4.934345E+0	2011-11-28	11:58:32	1.477629E+10

非数据列



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# 实例分析与总结

## Athena打开文件时

文件打开方式不对?

- ◆ 透射数据没有取对数
- ◆ 数据列选择不对

Athena: Column selection

Select range    Clear numerator    Pause plotting

1 2 3 4 5

Energy

Numerator

Denominator

```
# F:\201111\Cu.dat
# 2011-11-8
# comment : N2 -30%
# 0
# 467
8839 334 169003 118578 1269768 0 3543455
```

Natural log     Invert    Multiplicative constant 1

Save each channel as

Data type  $\mu(E)$     Energy units eV

Energy hgxxa.1

$\mu(E)$  (hgxxa.2) / (hgxxa.3)

Athena[Plot.1]

Cu.dat in energy

9137.06, 8.66966

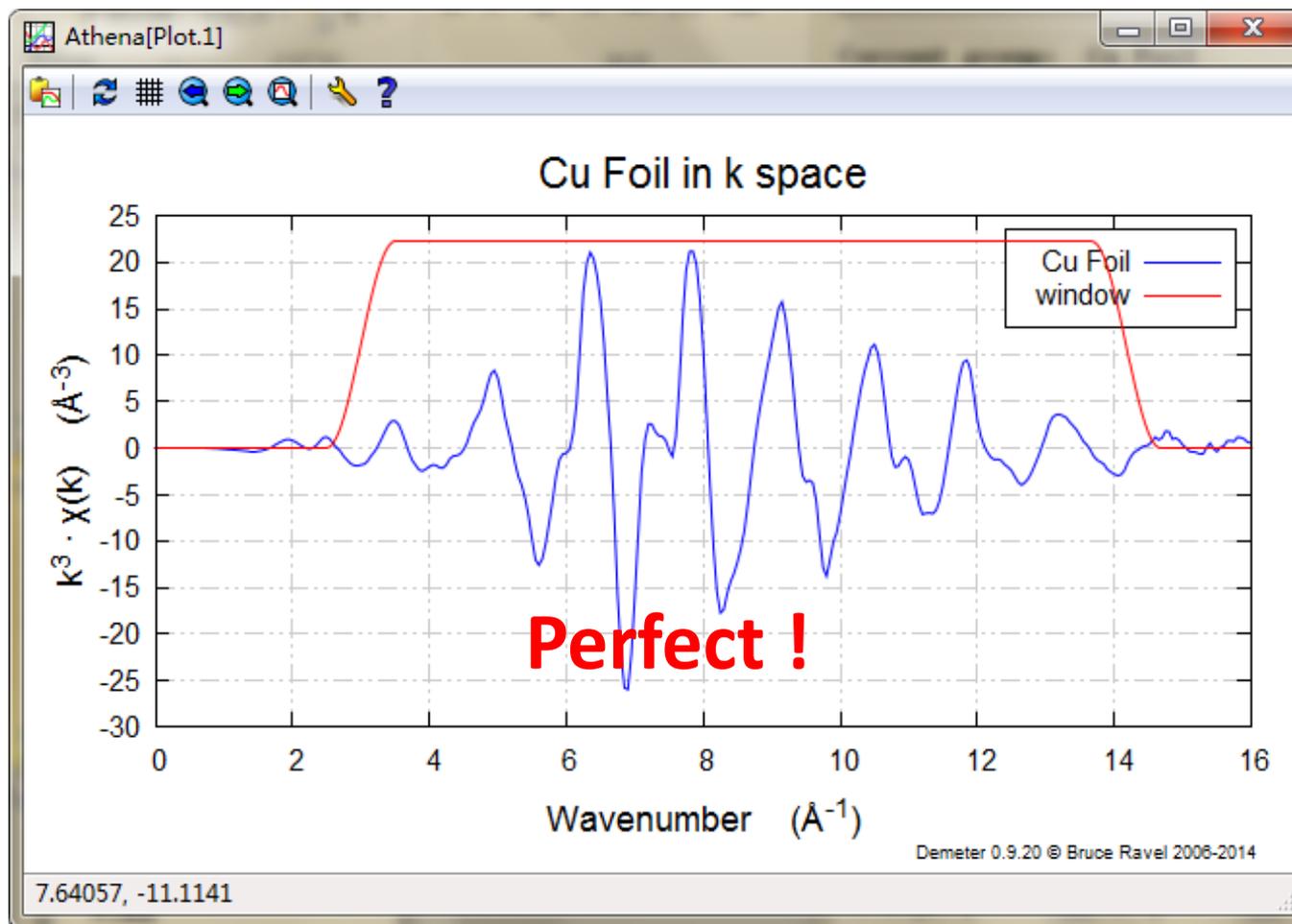
取对数!



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# 常见问题

数据信噪比 在K空间中进行判断



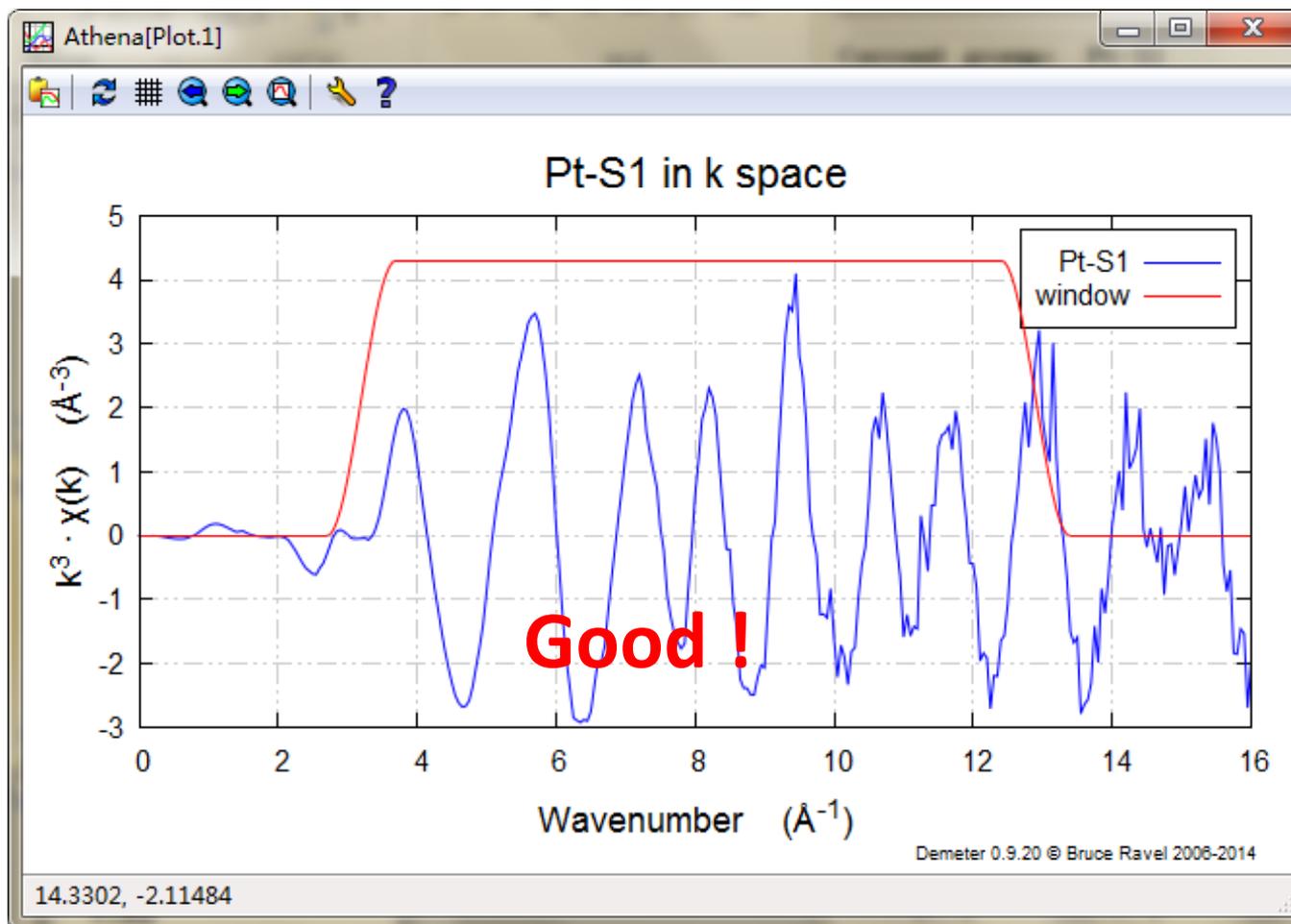
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# 常见问题

数据信噪比 在K空间中进行判断



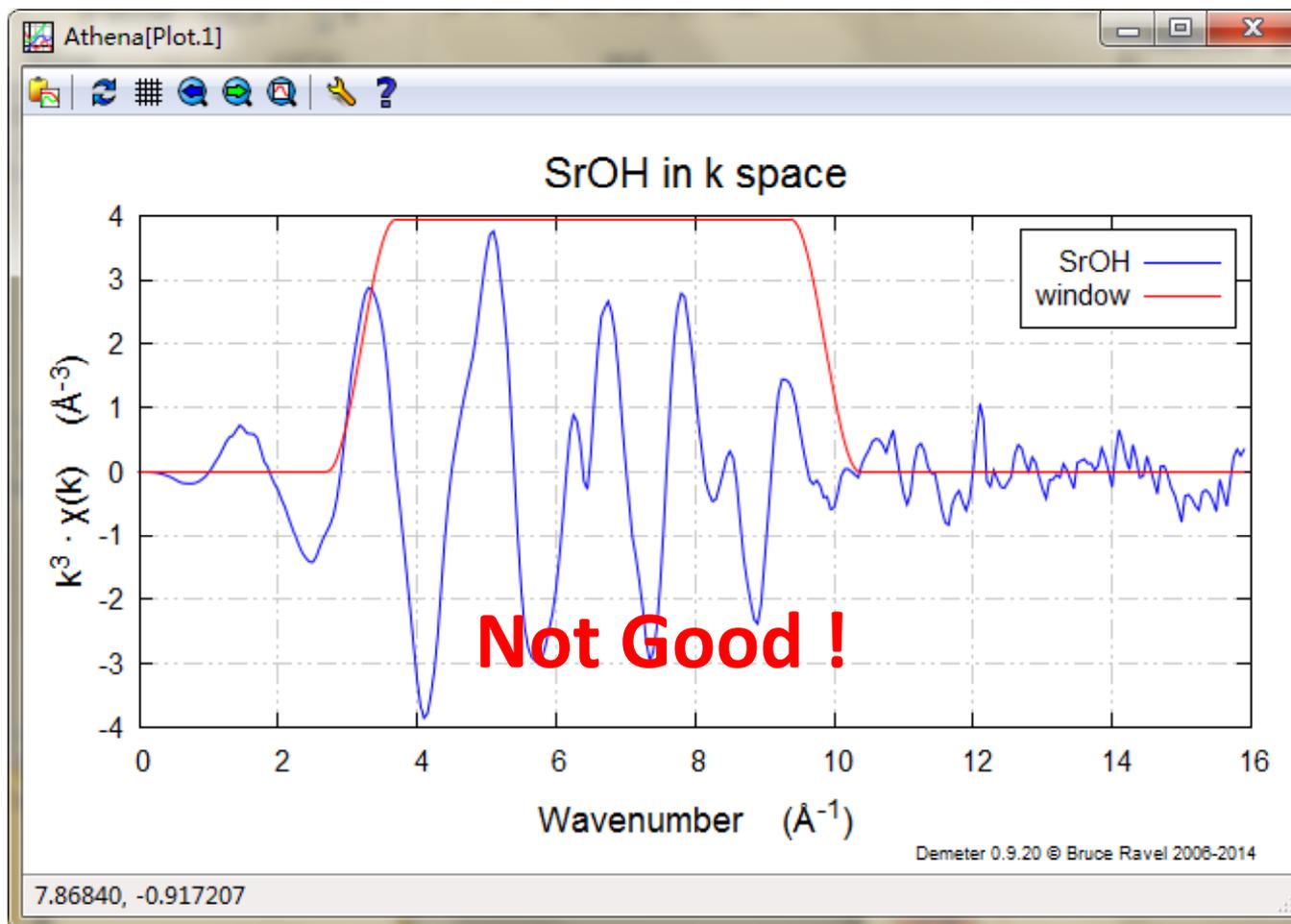
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# 常见问题

数据信噪比 在K空间中进行判断



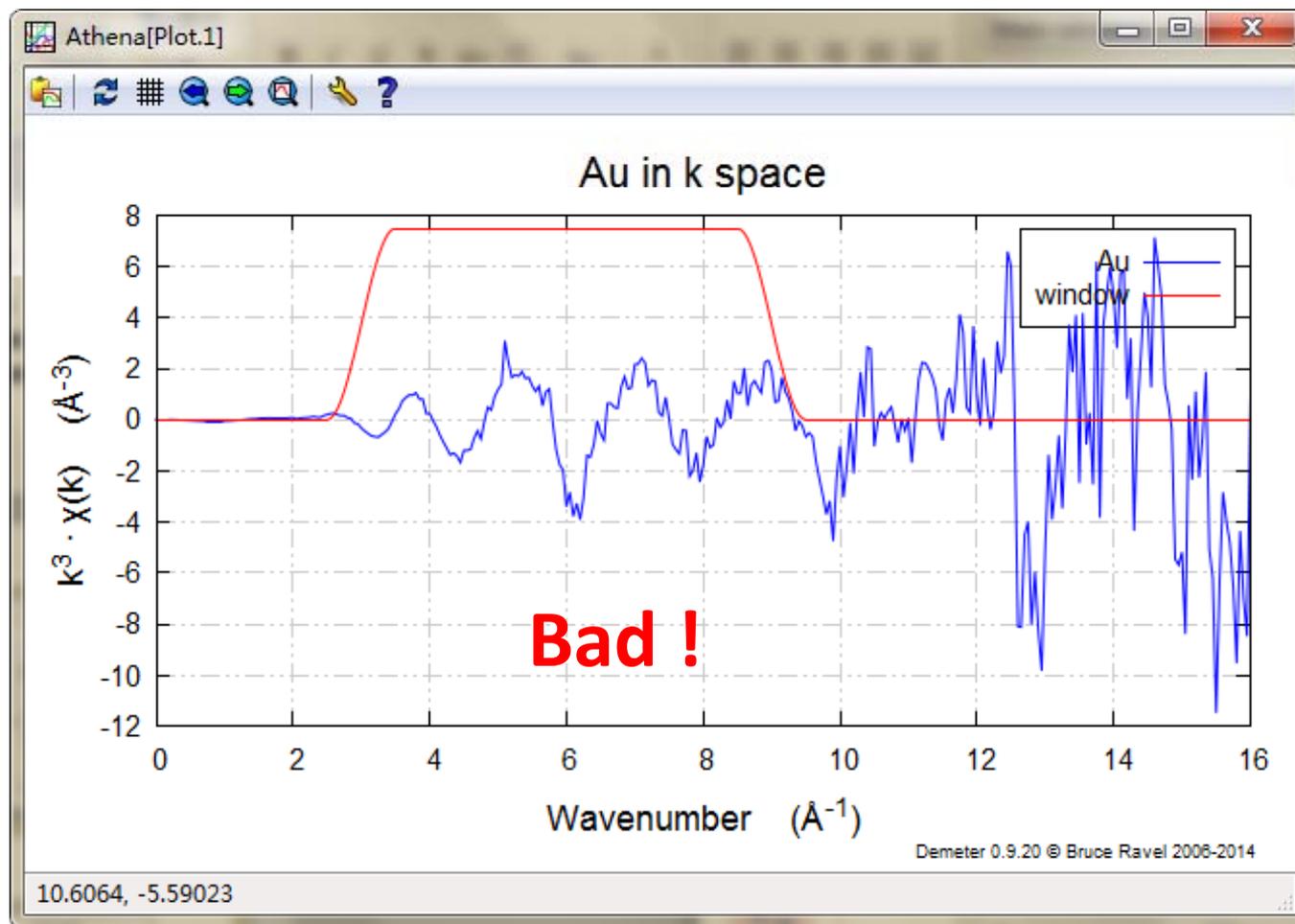
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# 常见问题

数据信噪比 在K空间中进行判断



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# 常见问题



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## 关于能量坐标

- ◆ 能量坐标的确定
- ◆ 能量坐标的调整 (Align Data)
- ◆ 价态比较

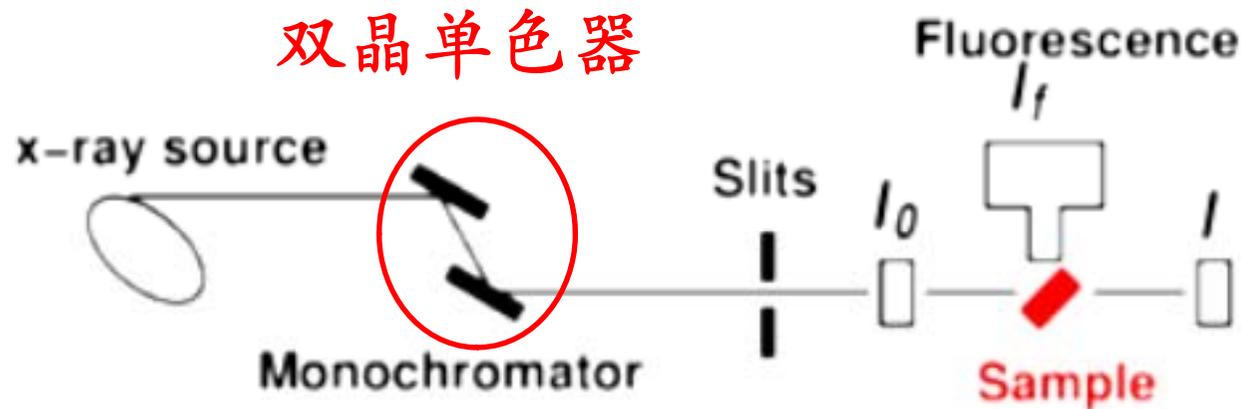
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# 常见问题

## 关于能量坐标

- ▶ 实验上对能量坐标的确定



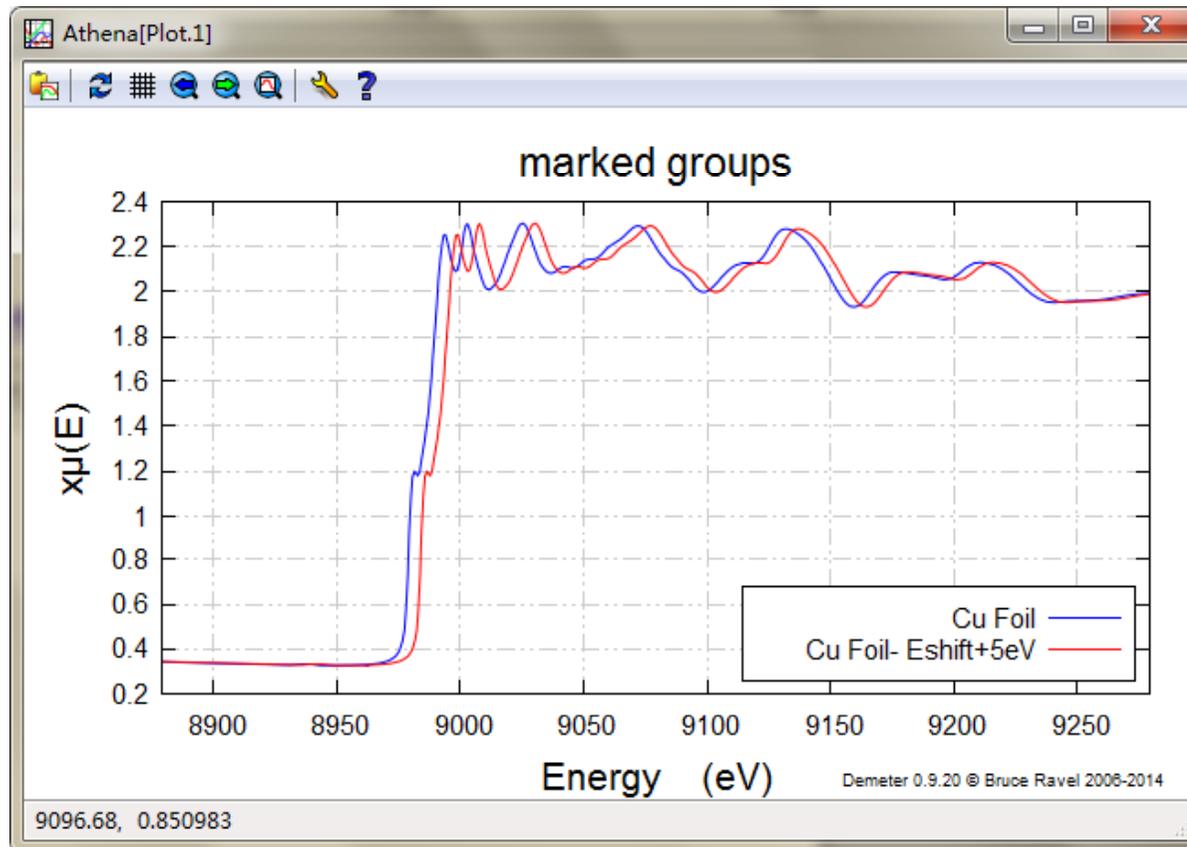
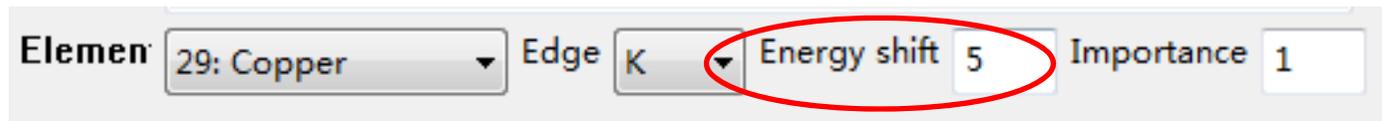
$$\text{布拉格公式：} 2d\sin\theta = n\lambda$$

实验前利用标准金属foil进行能量标定，消除机械误差，但是每次标定可能会存在1-2eV的人为误差。

# 常见问题

## 关于能量坐标

### ➤ Athena软件对能量坐标的调整



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# 常见问题

## 关于能量坐标

- Athena软件Align Data功能：调节E-shift

Align data

Aligning Cu Foil- Eshift+5eV

Standard Cu Foil

Plot as smoothed deriv(E)

Fit as smoothed deriv(E)

Shift by 5 eV Uncertainty 0

Replot

Auto align Align marked groups

-5	+5
-1	+1
-0.5	+0.5
-0.1	+0.1



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# 常见问题



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## 关于能量坐标

### ➤ 关于价态分析

- ◆ 由于能量标定误差的存在，进行价态比较时，建议使用同一批次的样品；
- ◆ 对于不同批次的样品，需要有1-2个标样或者样品在每个批次都进行采集，可以利用Athena软件的Align Data功能对能量坐标进行调整；
- ◆ 最好的方式是采用“三电离室模式”

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# 常见问题



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## 关于能量坐标

- 关于能量坐标的调整(Align Data)
  - ◆ 合并多次扫描的数据
  - ◆ 不同批次的样品进行价态比较
- 关于能量坐标的校准(Calibrate Data)
  - ◆ 当绝对能量坐标与实际能量差别很大的时候
- 关于 $E_0$ 的确定
  - ◆ 在能量坐标上选取相对应的电离阈值位置

# 主要内容



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- 上机练习

# 上机练习



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## 以 $\text{Co}_3\text{O}_4$ 为例

1. 打开数据文件
2. 预处理
3. 扣除边前本底及归一化
4. 确定 $E_0$ 及E-k转换
5. 扣除原子吸收本底background
6. Fourier变换
7. 反Fourier变换
8. 保存文件

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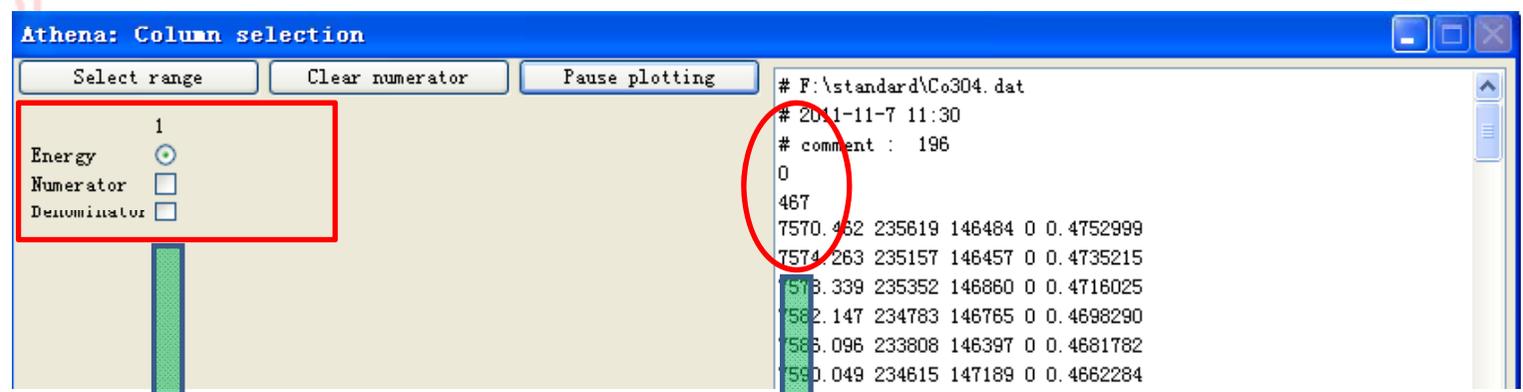
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# 上机练习

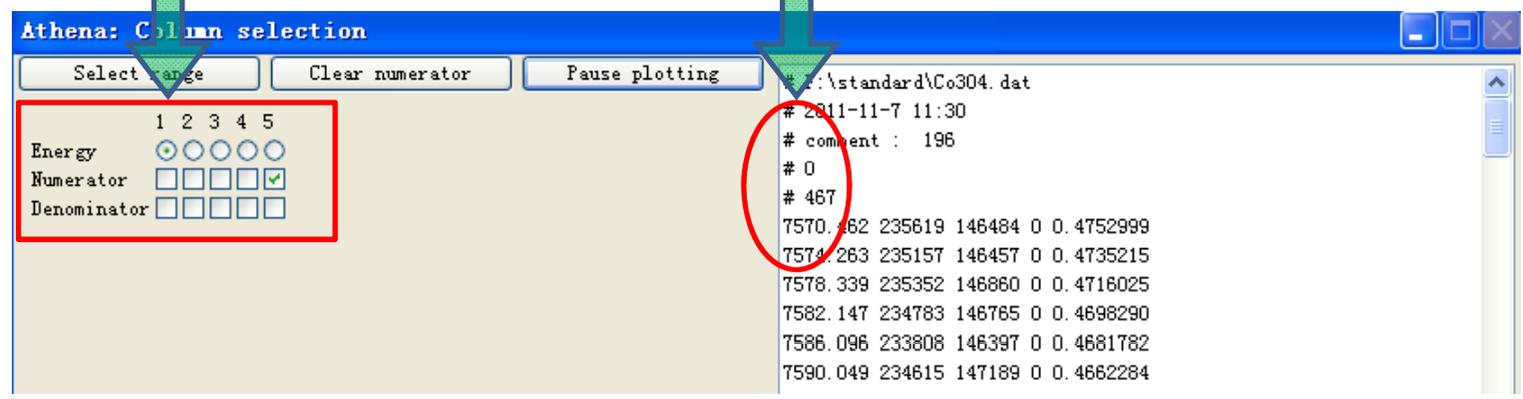


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## 1、打开数据文件



数据文件头中包含纯数字行，可以在其前面加“#”注释，或者把文件头部分直接删除。



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# 上机练习

## 2、预处理 - deglitch



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Athena [XAS data processing]

File Group Energy Mark Plot Freeze Merge Monitor Help

\* <untitled> Save A U I

Deglitch and truncate data

Deglitch a single point

Plot as

$\mu$  (E)   $\times$  (E)

Choose a point Remove point Replot

Deglitch many points

Athena [Plot. 1]

Co3O4.dat in E space

Co3O4.dat

$k^2 \cdot X(k)$  ( $\text{\AA}^{-2}$ )

Energy (eV) Demeter 0.9.20 © Bruce Ravel 2006-2

8553.66, 0.716726

Document section: deglitching and truncating

Emin 0 Emax 800

Plot the marked groups in q — Right click: biquad plot

Plotting k-weights

0  1  2  3  kw

Plot in energy

$\mu$  (E)   $\mu$  (E)

Background  pre-edge line

post-edge line  Normalized

Normalized  Derivative

Derivative  2nd derivative

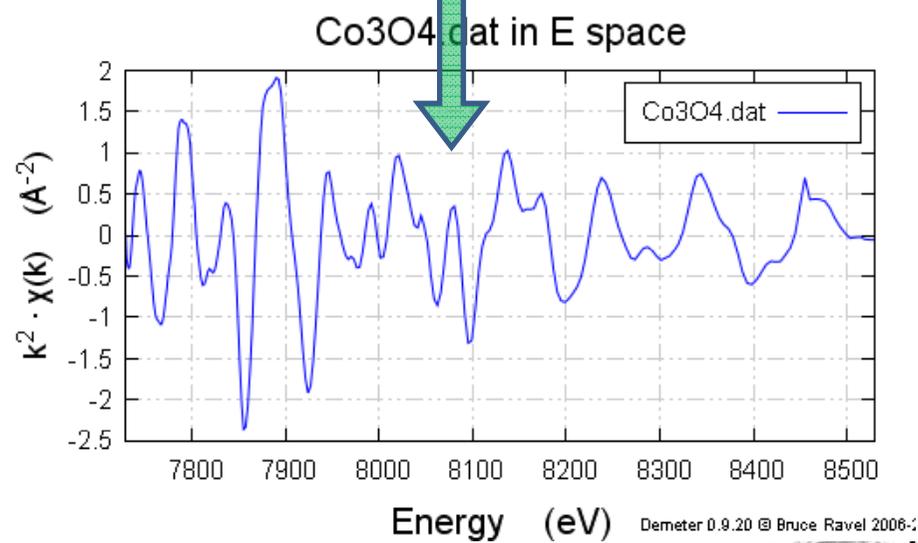
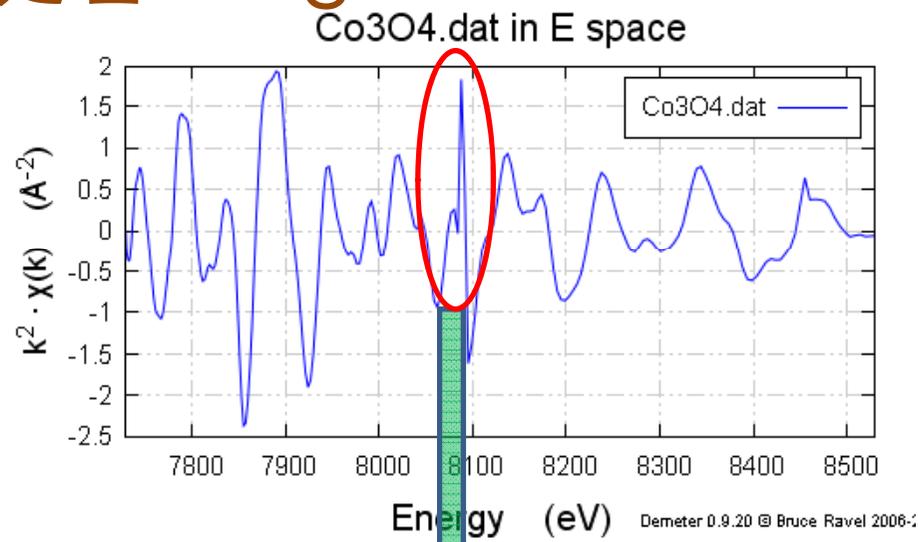
2nd derivative

# 上机练习



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## 2、预处理 - deglitch



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# 上机练习

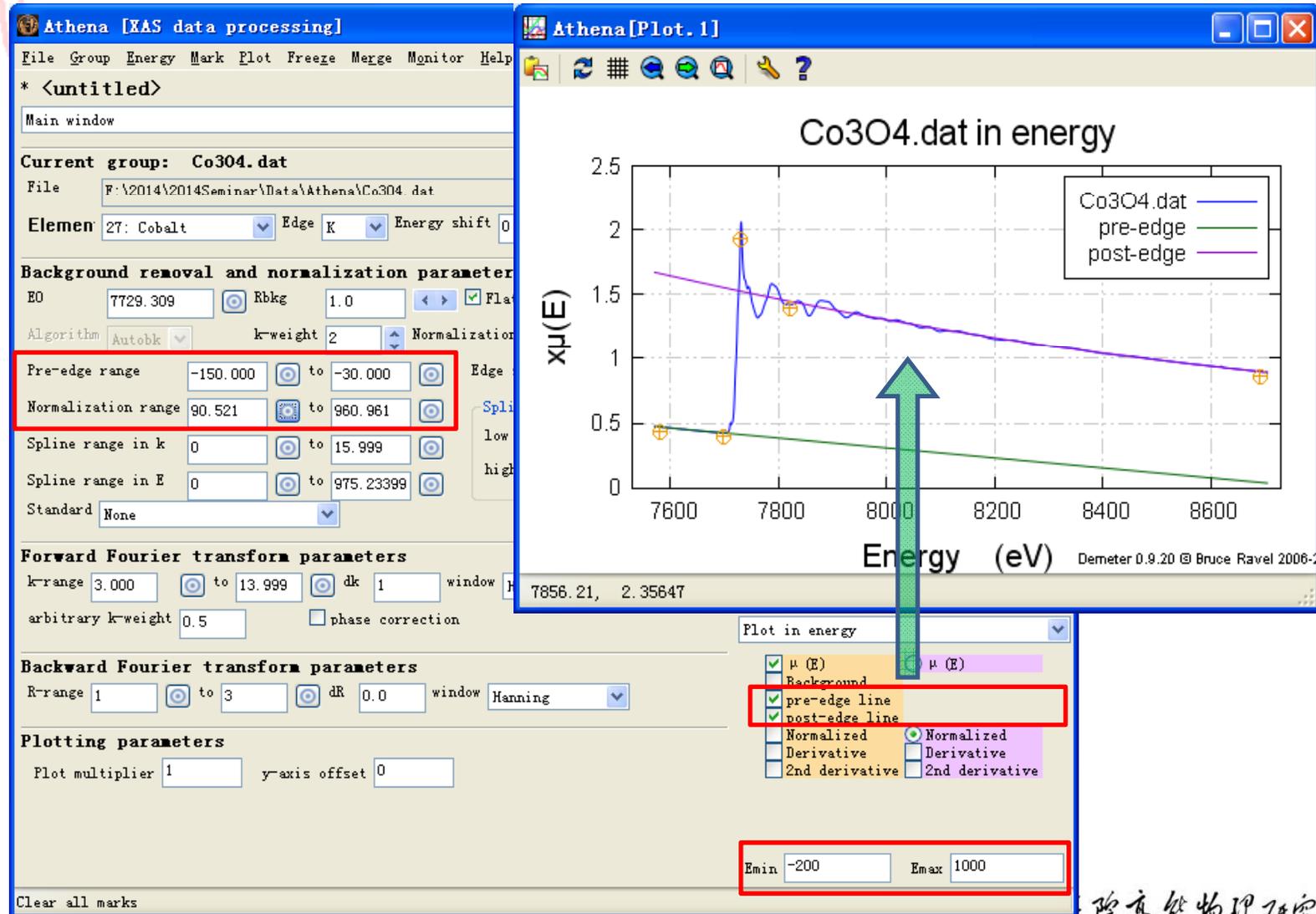
## 3、扣除边前本底及归一化



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# 上机练习

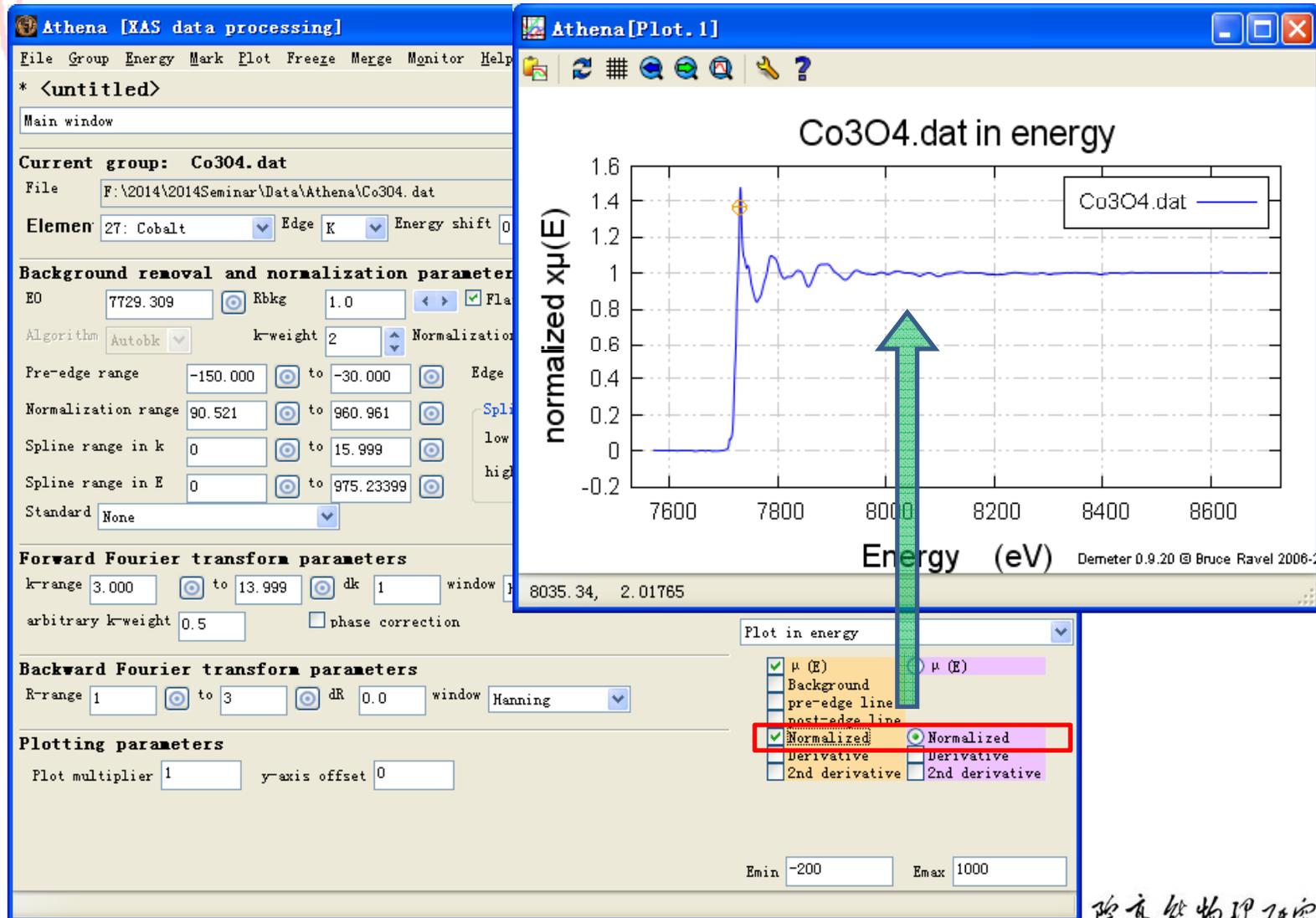
## 3、扣除边前本底及归一化



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# 上机练习

## 4、确定 $E_0$ 及E-k转换



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The screenshot shows the Athena software interface for XAS data processing. The main window displays the current group 'Co304.dat' and the element 'Cobalt'. The 'Background removal and normalization parameters' section is highlighted, showing the  $E_0$  value set to 7729.309 eV. A green arrow points from this value to the plot window, which shows a peak at approximately 7730 eV. A red text box in the plot window states: '在此例中程序默认选择的 $E_0$ 位置有点偏大, 需要调整' (In this example, the default  $E_0$  position chosen by the program is a bit too large, it needs adjustment). The plot window also shows the 'Plot in energy' options, with 'Normalized' selected. The 'Emin' and 'Emax' values are set to -50 and 100, respectively.

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# 上机练习

## 4、确定 $E_0$ 及E-k转换



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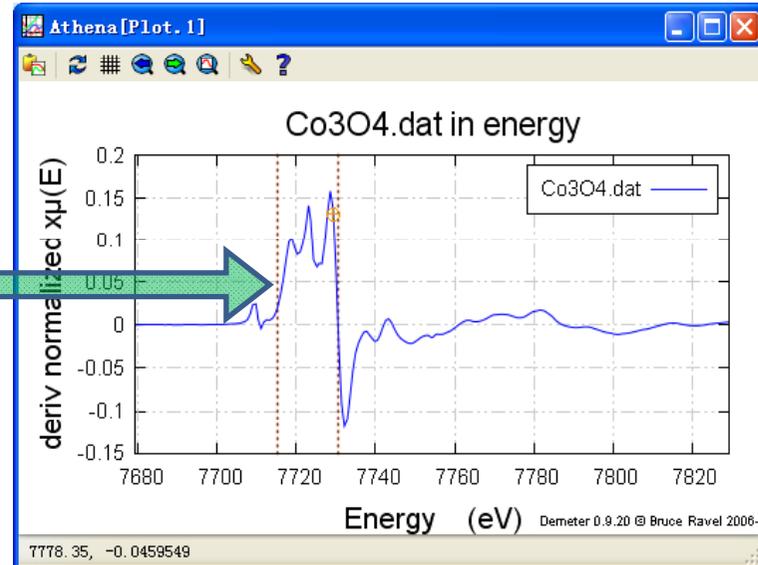
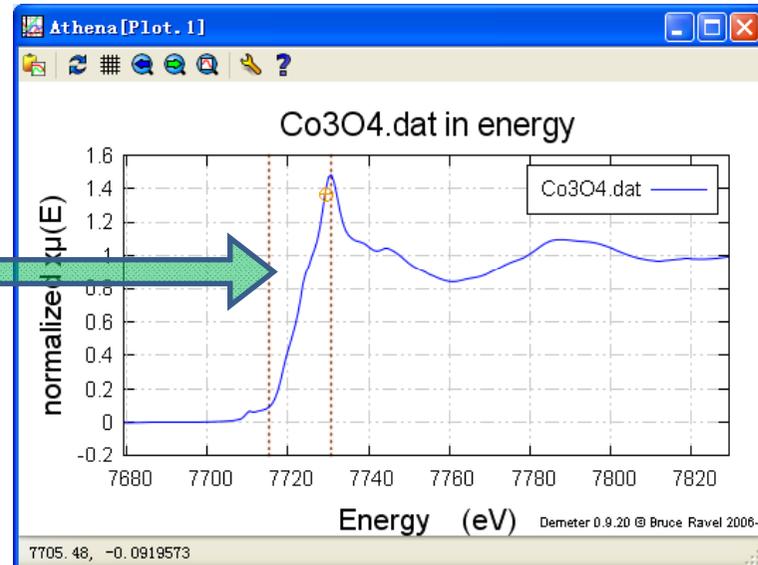
Indicators

Indicator	Type	Value	Target
1	E	-14.03%	Target
2	E	1.361	Target
3			Target
4			Target

Plot all Plot none

Plot in energy

<input checked="" type="checkbox"/> $\mu(E)$	<input type="checkbox"/> $\mu(E)$
<input type="checkbox"/> Background	
<input type="checkbox"/> pre-edge line	
<input type="checkbox"/> post-edge line	
<input checked="" type="checkbox"/> Normalized	<input checked="" type="checkbox"/> Normalized
<input checked="" type="checkbox"/> Derivative	<input type="checkbox"/> Derivative
<input type="checkbox"/> 2nd derivative	<input type="checkbox"/> 2nd derivative



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# 上机练习

## 4、确定 $E_0$ 及E-k转换



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The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group as 'Co304.dat' and the element as 'Cobalt'. The 'Background removal and normalization parameters' section is highlighted, with the  $E_0$  value set to 7729.309 eV. The 'Forward Fourier transform parameters' section shows a k-range from 3.000 to 13.999. The 'Plotting parameters' section shows the plot multiplier set to 1 and the y-axis offset set to 0. The 'Athena[Plot. 1]' window shows a plot of the derivative of normalized absorption,  $\mu'(E)$ , versus Energy (eV) for 'Co3O4.dat'. The plot shows a peak at approximately 7728 eV, which is marked with a red arrow and text indicating it is the first maximum of the derivative in the absorption edge region. The plot also shows the original data,  $\mu(E)$ , and the background line. The 'Plot in energy' dropdown menu is set to 'Normalized', and the 'Derivative' checkbox is checked. The 'Emin' and 'Emax' values are set to -50 and 100, respectively.

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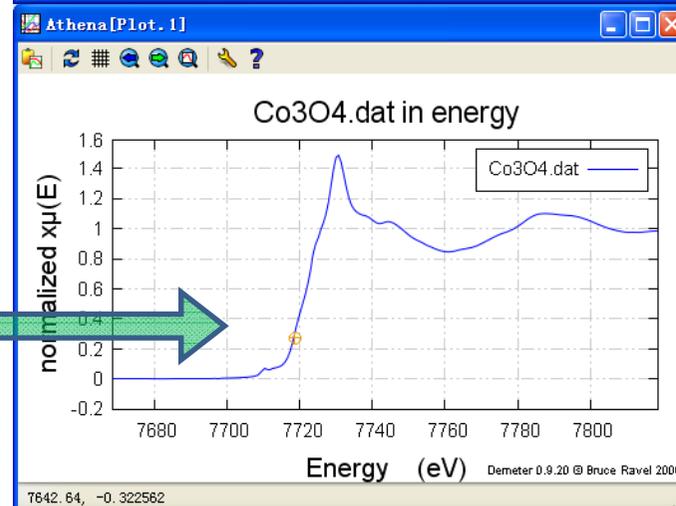
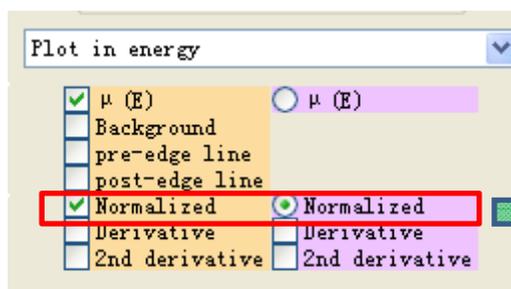
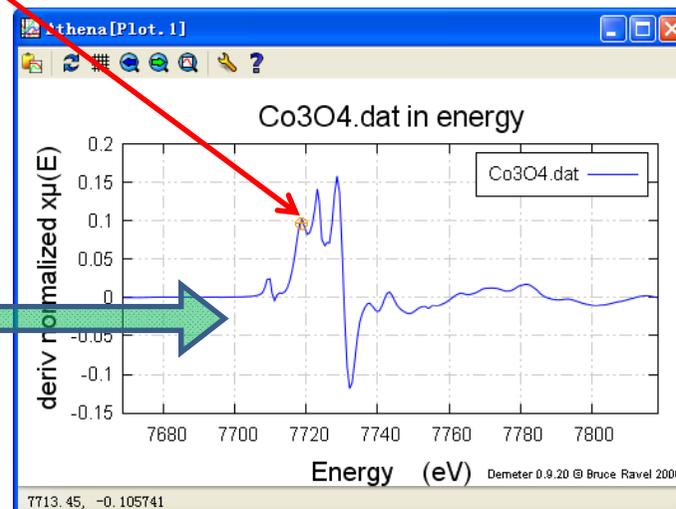
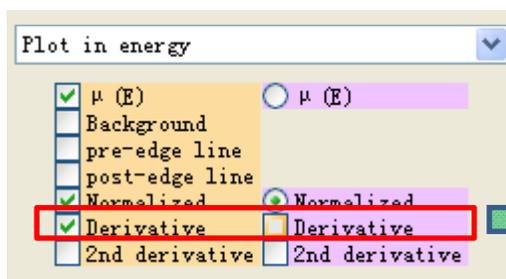
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## 4、确定 $E_0$ 及E-k转换

调整后的 $E_0$ 位置  $E_0$  7718.600



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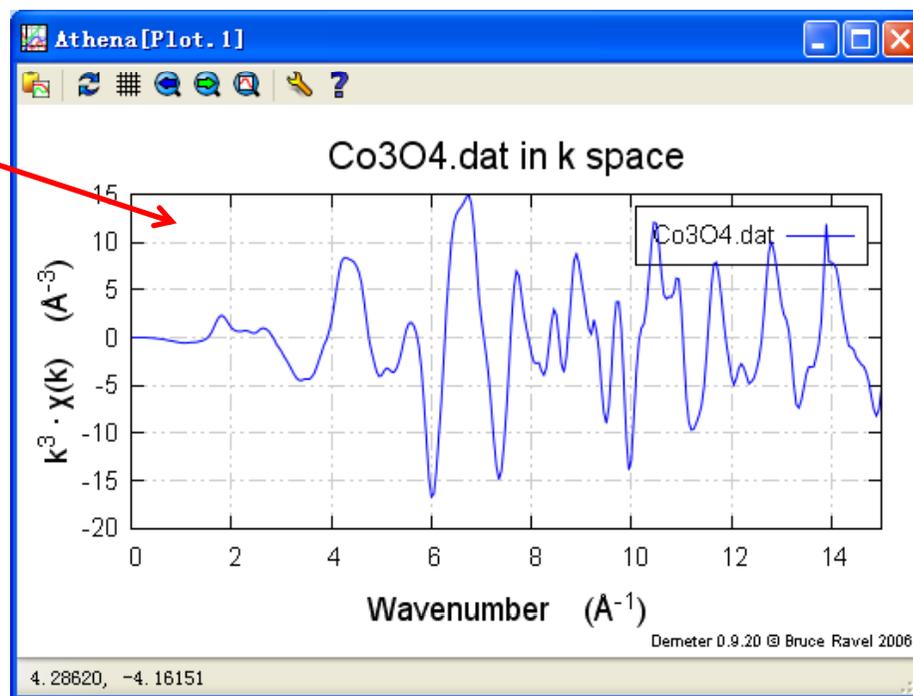
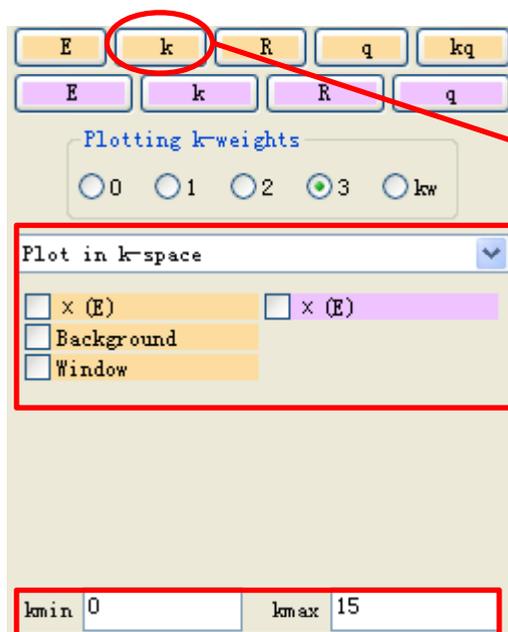
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## 4、确定 $E_0$ 及E-k转换

由E空间变换到k空间



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## 5、扣除原子吸收本底background



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The screenshot shows the Athena software interface for XAS data processing. The main window displays parameters for the current group 'Co304.dat', including the file path, element (Cobalt), and edge (K). The 'Background removal and normalization parameters' section is highlighted with a red box, showing 'Rbkg' set to 0.8, 'Spline range in k' from 0 to 15.999, and 'Spline range in E' from 0 to 975.23399. The 'Forward Fourier transform parameters' section shows 'krange' from 3.000 to 13.999. The 'Backward Fourier transform parameters' section shows 'Rrange' from 1 to 3. The 'Plotting parameters' section shows 'Plot multiplier' set to 1. The plot window, titled 'Athena[Plot. 1]', displays the XAS data for 'Co3O4.dat in R space'. The y-axis is labeled  $|X(R)| (A^{-4})$  and the x-axis is labeled 'Radial distance (A)'. A red arrow points to the first peak in the plot, with a red text annotation: 'Rbkg大致设置为第一配位距离的一半'. The plot shows several peaks, with the first peak at approximately 1.5 Å. The plot window also shows a 'Plot in R-space' dropdown menu with 'Magnitude' selected, and 'Rmin' set to 0 and 'Rmax' set to 6.

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## 6、Fourier变换



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The screenshot displays the Athena software interface for XAS data processing. The main window is titled "Athena [XAS data processing]" and shows the current group as "Co3O4.dat". The file path is "F:\2014\2014Seminar\Data\Athena\Co3O4.dat". The element is set to "Cobalt" and the edge is "K". The background removal and normalization parameters are configured with E0 at 7718.600, Rbkg at 0.8, and k-weight at 2. The forward Fourier transform parameters are set with a k-range from 3.22 to 13.3, a window of "Hanning", and a k-weight of 0.5. The backward Fourier transform parameters are set with an R-range from 1 to 3 and a window of "Hanning". The plotting parameters show a plot multiplier of 1 and a y-axis offset of 0. The plot window, titled "Athena[Plot. 1]", shows the data "Co3O4.dat in k space" with the y-axis labeled  $k^3 \cdot X(k) \text{ (}\text{\AA}^{-3}\text{)}$  and the x-axis labeled "Wavenumber ( $\text{\AA}^{-1}\text{)}$ ". The plot shows a blue line representing the data and a red line representing the window. The plot is displayed in k-space with the following options:   $\times$  (E),  Background, and  Window. The plot range is from kmin 0 to kmax 15.

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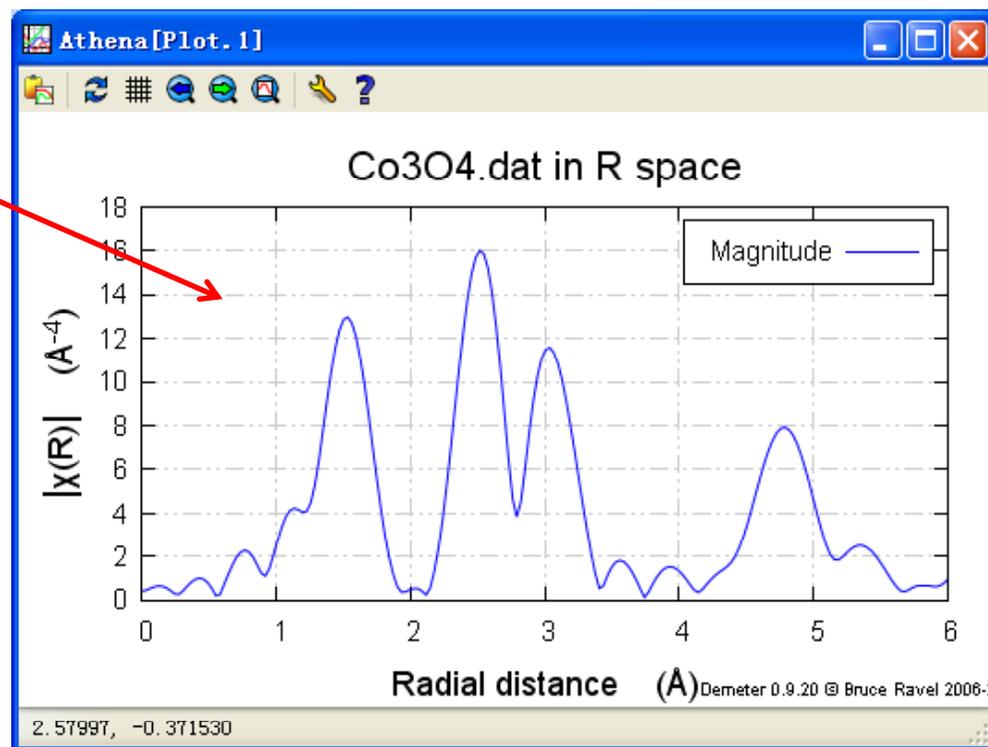
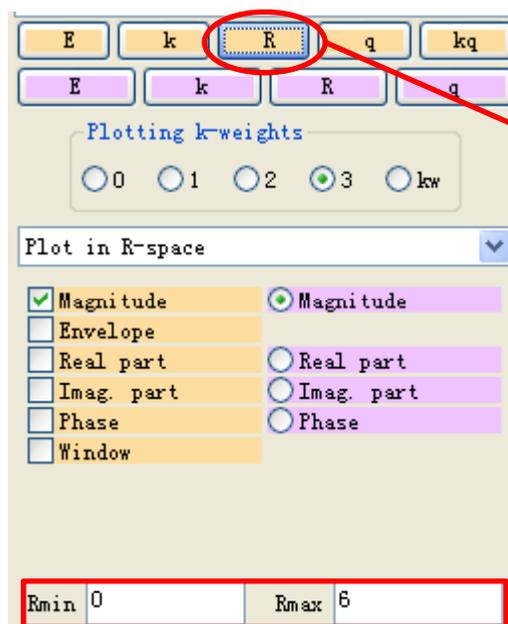
## 6、Fourier变换



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# 上机练习

## 7、反Fourier变换



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The screenshot displays the Athena software interface for XAS data processing. The main window shows the current group 'Co304.dat' and various parameters for background removal and normalization. The 'Backward Fourier transform parameters' section is highlighted with a red box, showing an R-range from 0.95 to 3.41 and a dR of 0.0. The 'Plotting parameters' section is also highlighted, showing 'Window' checked. A plot window titled 'Athena [Plot. 1]' shows the magnitude of the data in R space, with a red window overlaid on the plot. The plot shows a blue line representing the magnitude and a red line representing the window. The y-axis is labeled  $|X(R)| \text{ (}\text{\AA}^{-4}\text{)}$  and the x-axis is labeled 'Radial distance (A)'. The plot title is 'Co3O4.dat in R space'. The plot shows several peaks, with the most prominent one around 2.5 A. The window is centered around this peak, extending from approximately 0.95 to 3.41 A. The plot also shows a legend for 'Magnitude' (blue line) and 'window' (red line). The plot is titled 'Co3O4.dat in R space' and the axes are labeled 'Radial distance (A)' and  $|X(R)| \text{ (}\text{\AA}^{-4}\text{)}$ . The plot shows a blue line representing the magnitude and a red line representing the window. The plot title is 'Co3O4.dat in R space' and the axes are labeled 'Radial distance (A)' and  $|X(R)| \text{ (}\text{\AA}^{-4}\text{)}$ . The plot shows several peaks, with the most prominent one around 2.5 A. The window is centered around this peak, extending from approximately 0.95 to 3.41 A. The plot also shows a legend for 'Magnitude' (blue line) and 'window' (red line).

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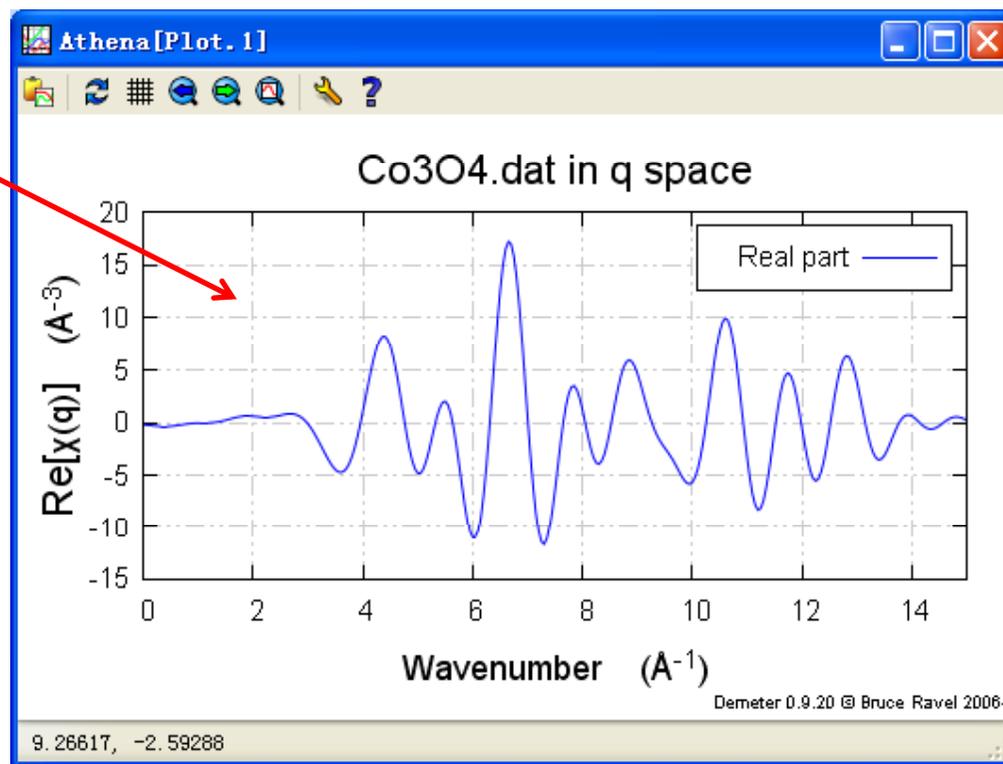
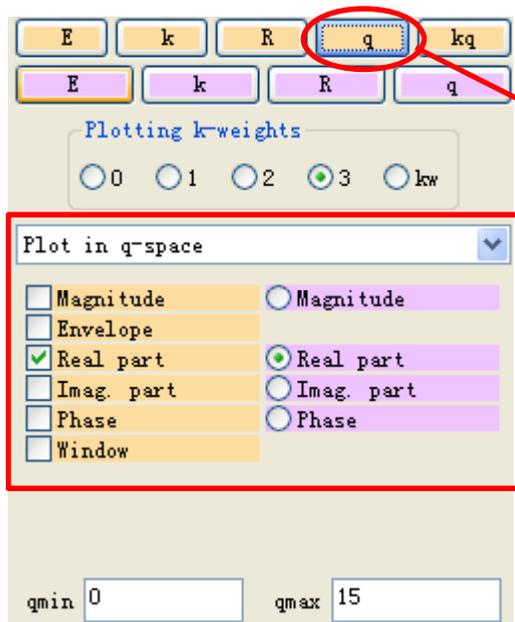
## 7、反Fourier变换



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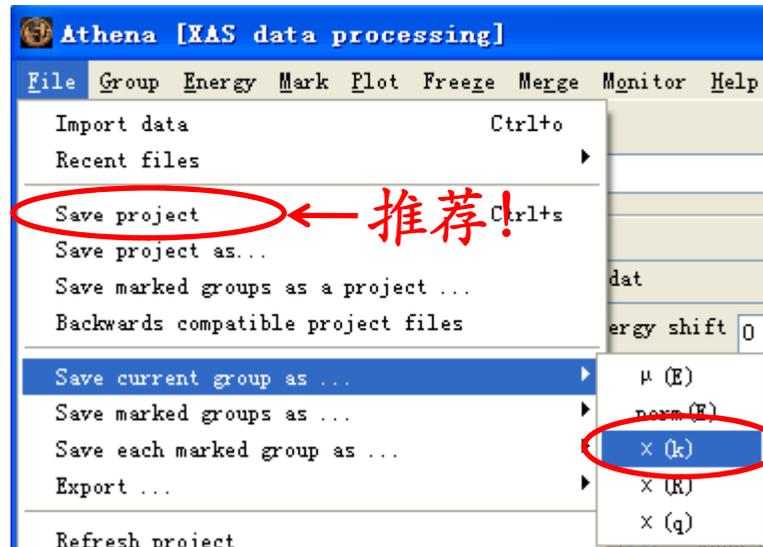
将某一或者某几个指定配位层所包含的XAFS信号提取出来，而后就可以将其导入Artemis程序中进行拟合。

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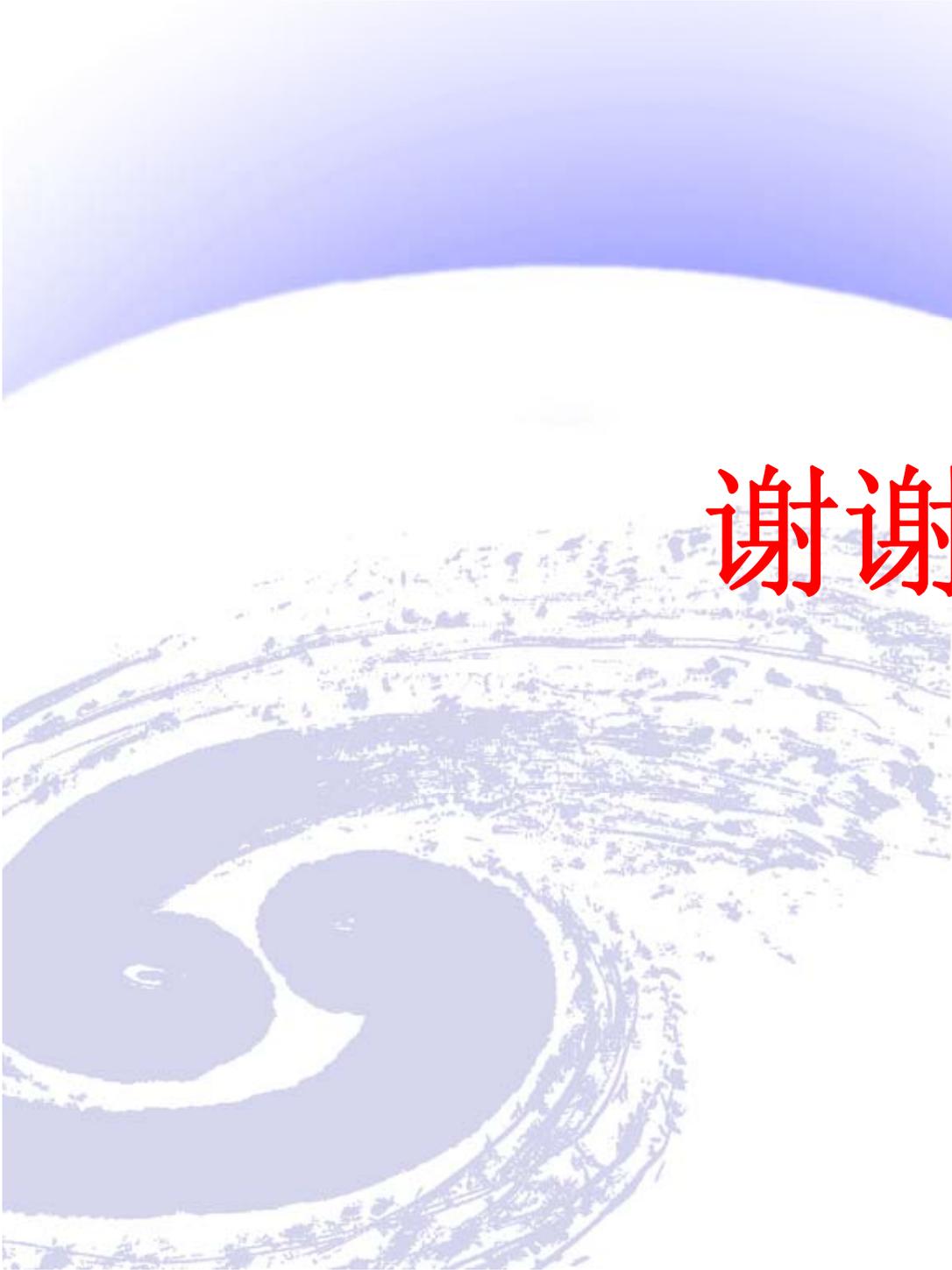
## 8、保存文件



Athena提供了多种文件保存格式，如果要提供给Artemis进行拟合，需要将数据保存成  $\chi(k)$ ，或者工程文件 (\*.prj)。推荐后者，将文件保存为Co3O4.prj，以备Artemis拟合使用。

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An aerial photograph of a terraced agricultural field. In the foreground, there is a large, circular pond with a dark, still surface. The terraces are arranged in concentric, roughly circular patterns, creating a spiral-like effect. The fields are filled with green crops, and the overall scene is captured from a high angle, looking down on the landscape. The background shows a clear blue sky with a slight gradient.

谢谢