



Athena 软件应用

储胜启

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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



- ◆ Athena简介
- ◆ EXAFS数据处理一般步骤
- ◆ Athena功能应用
- ◆ 应用举例
- ◆ 参考文献



Athena简介



- Athena是IFEFFIT软件中的一个独立的程序包，专门用来处理XAFS数据。

ATHENA User's Guide

Bruce Ravel
bravel@bnl.gov
<http://cars9.uchicago.edu/~ravel/software/exafs/>



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Athena简介



IFEFFIT下载链接:

<http://cars9.uchicago.edu/ifeffit/Downloads>

The screenshot shows the IFEFFIT website's download page. The page has a green header with the IFEFFIT logo and a search bar. A left sidebar contains navigation links: Ifeffit, Downloads, Documentation, Mailing_List, FAQ, XAFS, Help, 只读网页, 信息, and 附件. The main content area is titled "IFEFFIT: Download Page" and includes a social media sharing bar. Below this, it states: "The current version of IFEFFIT is: **Ifeffit 1.2.11**, released 11-Aug-2008, last updated 17-Nov-2008". A table lists download links for different systems and versions.

System	Version	From Sourceforge.net	From cars.uchicago.edu
Windows Installer			
Win32	1.2.11	ifeffit-1.2.11.exe	ifeffit-1.2.11.exe
Win32	1.2.10	ifeffit-1.2.10.exe	ifeffit-1.2.10.exe
Win32	1.2.9	ifeffit-1.2.9.exe	ifeffit-1.2.9.exe



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Athena软件安装



- **注意：安装时不能选择中文路径，同样在输入数据和保存数据时也不能使用中文文件名以及放在中文文件夹里！**



双击即可打开Athena程序！

Athena程序界面



主程序窗口

The screenshot shows the Athena software interface with several key components highlighted by red boxes and arrows:

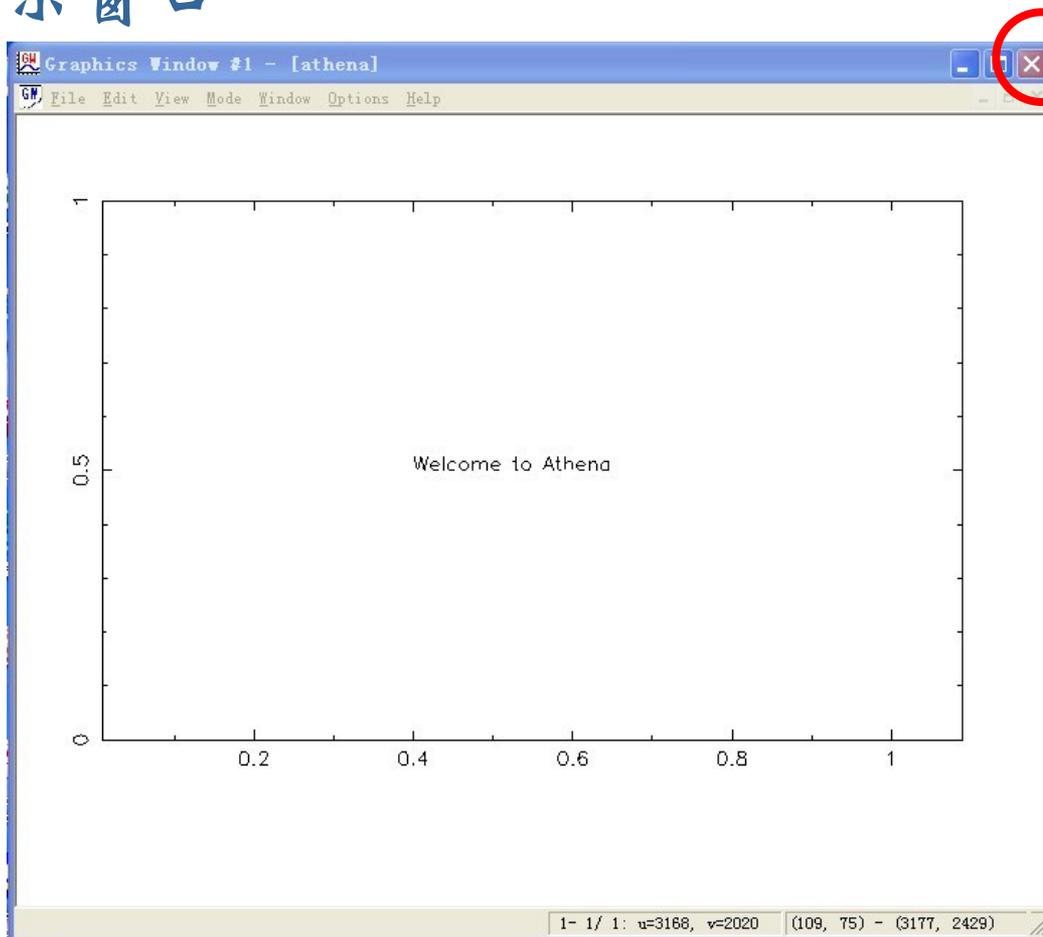
- 主窗口** (Main Window): Points to the central control panel containing sections for Project, Background removal, Forward Fourier transform, Backward Fourier transform, and Plotting parameters.
- 文件名列表** (File Name List): Points to the 'A U I' panel on the right side of the interface.
- 绘图按钮** (Plotting Buttons): Points to the row of buttons labeled E, k, R, q, and kq.
- k weight**: Points to the row of buttons labeled 0, 1, 2, 3, and kw.
- 绘图选项** (Plotting Options): Points to the 'Plotting options' panel on the right, which includes checkboxes for mu(E), background, pre-edge line, post-edge line, Normalized, and Derivative, along with Emin and Emax input fields.
- 提示信息** (Hint Message): Points to the bottom status bar which contains the text: "HINT: Athena allows configured key bindings -- see the Settings menu."



Athena程序界面



图形显示窗口



提醒：程序运行过程中不能关闭图形显示窗口



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Athena主要功能



◆ 读取、显示和保存各类XAFS数据文件

- 读取和显示透射或荧光模式的XAFS数据
- 读取多元探测器的测量数据
- 合并多次扫描的数据
- 保存 $\mu(E)$, $\text{norm}(E)$, $\chi(k)$, $\chi(q)$, $\chi(R)$ 等
- 保存工程文件

◆ 处理XAFS数据

- 扣除边前和归一化
- E_0 校准和E-k转换
- 自动扣除背底(AUTOBK)
- Fourier变换和反Fourier变换
- 提取 $\chi(k)$



Athena主要功能



- ◆ 批量处理多组数据
- ◆ 其他
 - 去除glitch
 - 截断数据
 - 平滑数据
 - PCA和LCA分析
 - 对边前峰进行分峰拟合
 -



读取实验数据



原始的XAFS实验数据

- 透射模式
- 荧光模式
- 多元固体探测器
- 多次扫描



读取实验数据



数据文件格式

不同实验站数据格式会有所不同

透射模式: $\mu = \ln(I_0/I_1)$

荧光模式: $\mu = I_f/I_0$



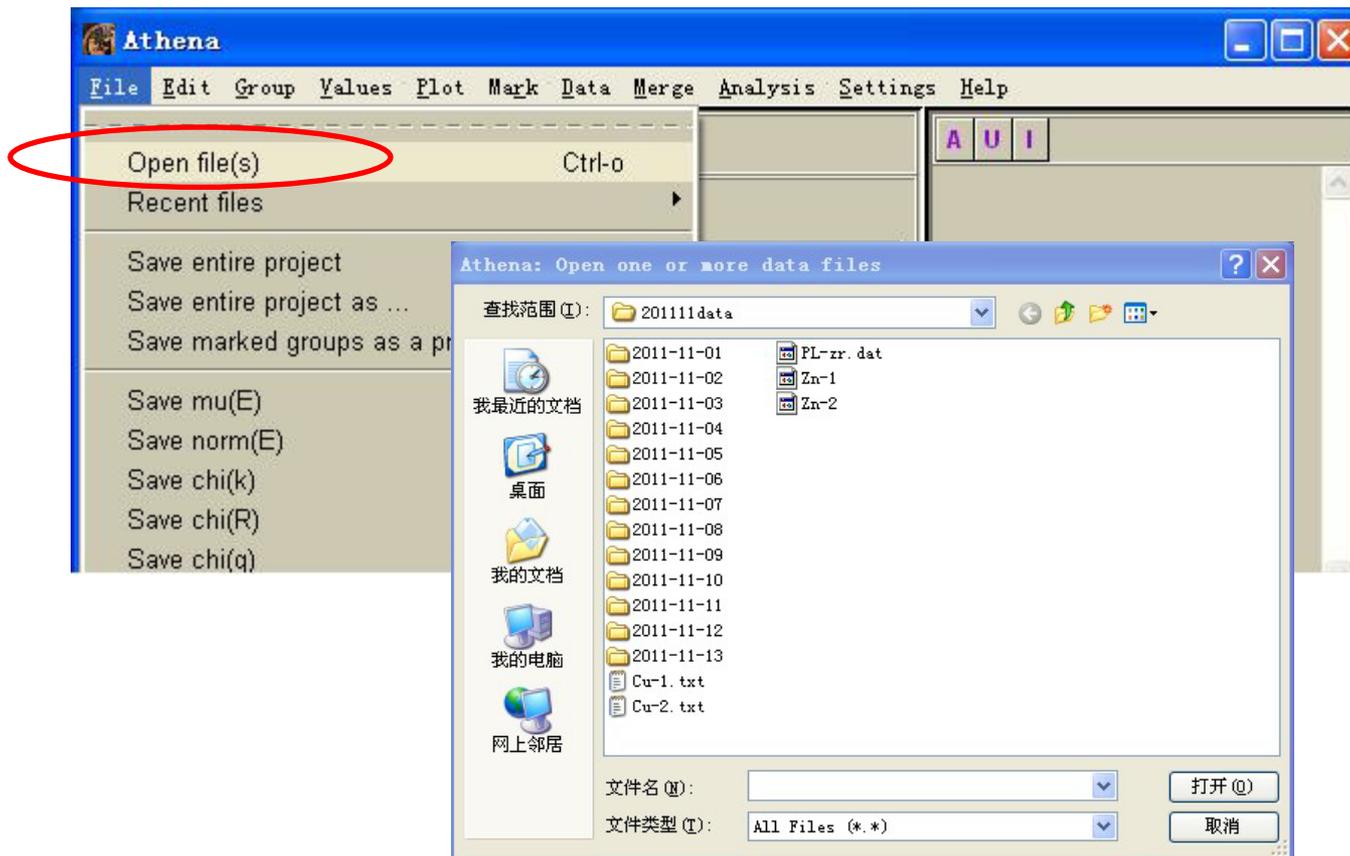
data.txt - 记事本

文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

#文件头

#Energy	I0	I1	If	mu
8807.136	444085	657695	0	-0.3927253
8810.622	449231	667007	0	-0.3952633
8814.334	449918	668594	0	-0.3961117
8818.123	450135	669270	0	-0.3966400
8822.065	450503	670238	0	-0.3972681
8825.935	450942	671399	0	-0.3980249
8829.809	450590	671141	0	-0.3984214
8833.687	451075	672298	0	-0.3990681
8837.531	451202	672861	0	-0.3996236
8841.453	451753	674097	0	-0.4002384
8845.303	452277	675370	0	-0.4009659
8849.195	452094	675365	0	-0.4013632
8853.165	452138	675677	0	-0.4017277
8857.064	452382	676463	0	-0.4023508

读取实验数据



可以同时导入一个或多个格式相同的数据



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读取实验数据



透射模式

第一列为能量

I_0 作为分子

I_1 作为分母

同时取对数

$$\mu = \ln(I_0/I_1)$$

The screenshot shows the Athena software interface for configuring data columns. The main window is titled "Athena: data columns". It features a table with 5 columns and 3 rows: Energy, Numerator, and Denominator. The first column is selected for all three rows. The "Natural log" checkbox is checked. The "mu(E)" field contains the formula $\ln(\text{abs}(\text{ywww.2}) / (\text{ywww.3}))$. The "Energy units" are set to "ev". The "Reference channel" section is also visible, with "Natural log" and "Same element" checked. A "Graphics Window #1" is open, displaying a plot of the calculated μ versus energy, showing a sharp peak around 9000 eV.

	1	2	3	4	5
Energy	<input checked="" type="checkbox"/>				
Numerator	<input checked="" type="checkbox"/>				
Denominator	<input checked="" type="checkbox"/>				

Energy: ywww.1
mu(E): $\ln(\text{abs}(\text{ywww.2}) / (\text{ywww.3}))$
Data type: mu(E) Energy units: ev

Reference channel:
The reference uses the same energy array as the data.
Numerator:
Denominator:
Natural log: Same element:

Plot reference
Clear reference channels

OK Cancel

Graphics Window #1 - [athena]
current column selection
y: -0.5 to 1.5
x: 8800 to 10000

读取实验数据



荧光模式

第一列为能量

I_f 作为分子

I_0 作为分母

$$\mu = I_f / I_0$$

The screenshot shows the Athena software interface for data column selection. The main window is titled "Athena: data columns" and contains a table of data columns with checkboxes for selection. The "Energy" column is selected in the first row. The "Numerator" column is selected in the second row, and the "Denominator" column is selected in the third row. The "mu(E)" field is set to "(rdls.4) / (rdls.2)". The "Energy units" are set to "ev". The "Reference channel" section is also visible, with the "Numerator" and "Denominator" columns selected. The "OK" button is circled in red. A "Graphics Window #1" is open, showing a plot of the data with a sharp peak at approximately 9000 eV.

1	2	3	4	5	
Energy	<input checked="" type="checkbox"/>				
Numerator	<input checked="" type="checkbox"/>				
Denominator	<input checked="" type="checkbox"/>				

mu(E): (rdls.4) / (rdls.2)

Energy units: ev

Reference channel

1	2	3	4	5	
Numerator	<input checked="" type="checkbox"/>				
Denominator	<input checked="" type="checkbox"/>				

OK

Graphics Window #1 - [athena]

current column selection

Plot showing a sharp peak at approximately 9000 eV.

读取实验数据



简单的导入

mu直接作为分子

The screenshot shows the Athena software interface. The main window is titled "Athena: data columns" and displays a table of data columns. The columns are numbered 1 to 5. The "Energy" column is selected with a red dot. The "Numerator" and "Denominator" columns are also selected with red dots. The "Data type" is set to "mu(E)" and the "Energy units" are set to "ev". The "Reference channel" section is also visible, with "Natural log" and "Same element" checked. A "Graphics Window #1" is open, showing a plot of the data. The plot has a y-axis ranging from -0.5 to 1.5 and an x-axis ranging from 8600 to 10000. The plot shows a sharp peak at approximately 8900 eV, followed by a decay. The "OK" button at the bottom of the Athena window is circled in red.

#	Energy	I0	I1	If	mu
8807.136	444085	657695	0	-0.3927253	
8810.622	449231	667007	0	-0.3952633	
8814.334	449918	668594	0	-0.3961117	
8818.123	450135	669270	0	-0.3966400	
8822.065	450503	670238	0	-0.3972681	
8825.935	450942	671399	0	-0.3980249	
8829.809	450590	671141	0	-0.3984214	
8833.687	451075	672298	0	-0.3990681	
8837.531	451202	672861	0	-0.3996236	
8841.453	451753	674097	0	-0.4002384	
8845.303	452277	675370	0	-0.4009659	
8849.195	452094	675365	0	-0.4013632	



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读取实验数据



Athena

File Edit Group Values Plot Mark Data Merge Analysis Settings Help

Project

Current group cu_foil.dat

File: F:/2011/BSRFseminar/cu-foil.dat

Z: Cu Edge: K E shift: 0 Importance: 1

Background removal Show additional parameters

E0: 8975.8 Rbkg: 1.0

k-weight: 2 Edge step: 1.87311 fix step

Pre-edge range: -150 to -30

Normalization range: 150 to 843.4510

Spline range: k: 0.0 to 15.736

E: 0.000 to 943.435

Forward Fourier transform

k-range: 2 to 13.736

dk: 1 window type: hanning

Phase correction: no arbitrary k-weight: 0.5

Backward Fourier transform

R-range: 1 to 3

dr: 0.0 window type: hanning

Plotting parameters

plot multiplier: 1 y-axis offset: 0

plotting in energy from group `cu_foil.dat' ... done!

A U I modified

cu_foil.dat

E k R q kq

E k R q

0 1 2 3 kw

v Plotting options

E k R q Stack Ind PF

mu(E)

background

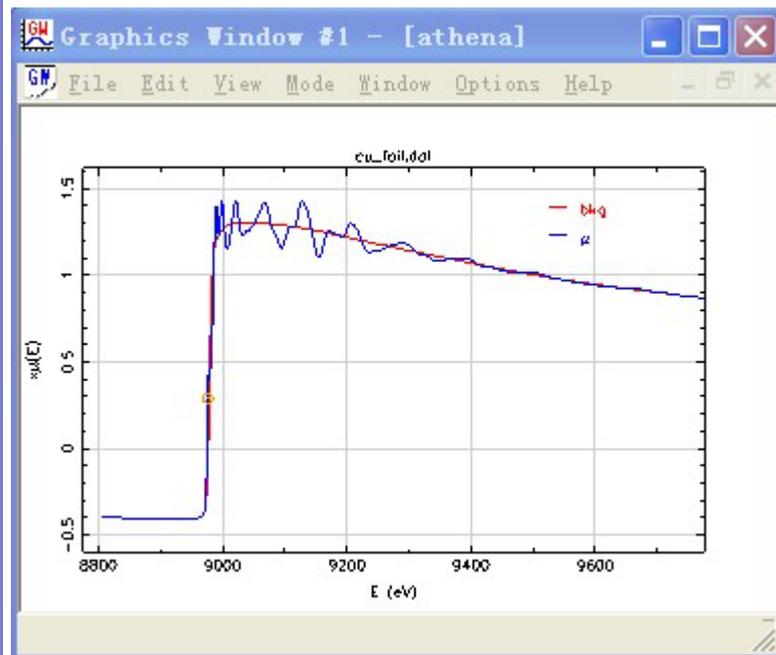
pre-edge line

post-edge line

Normalized

Derivative

Emin: -200 Emax: 800



$\mu(E)$ 曲线



读取实验数据



多元固体探测器测量的数据

- ◆ 19元固体探测器数据：第一列为能量E，第二列为入射X光光强 I_0 ，第5,8,11, ...列为每个探测器阵列元的 I_f 数据。

pilao-zr.dat - 记事本

文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

#E	I1	I2	I3	ux	SCA00	ICR0	OCR0	SCA10	ICR1	OCR1	SCA20	ICR2	I				
17867.299	342770	15793	50			1121	11252	0	1007	11334	0	931	10318	0	1172	11834	0
17871.190	343509	15830	50			1168	11175	0	1076	11260	0	1002	10384	0	1187	11800	0
17875.083	342401	15773	50			1133	11200	0	1070	11254	0	974	10289	0	1185	11745	0
17878.977	341866	15733	50			1089	11146	0	1075	11286	0	945	10210	0	1178	11705	0
17882.873	341723	15729	50			1186	11071	0	1109	11233	0	879	10249	0	1209	11887	0
17886.771	340898	15676	50			1133	11179	0	1069	11275	0	975	10270	0	1190	11811	0
17890.670	340825	15684	50			1164	11139	0	1064	11240	0	925	10245	0	1219	11861	0
17894.571	338793	15582	50			1205	11143	0	1069	11245	0	905	10146	0	1145	11704	0
17898.474	339345	15619	50			1152	11151	0	1094	11243	0	930	10203	0	1180	11781	0
17902.379	338533	15603	50			1159	11082	0	1071	11264	0	1013	10257	0	1209	11671	0
17906.285	337986	15594	50			1141	11063	0	1040	11182	0	996	10186	0	1107	11681	0
17910.193	338375	15618	50			1197	11113	0	1107	11227	0	918	10293	0	1273	11728	0
17914.103	336998	15522	50			1136	11099	0	1138	11315	0	1027	10174	0	1211	11676	0
17918.014	337503	15572	50			1131	11081	0	1085	11223	0	985	10186	0	1211	11770	0
17921.928	336708	15587	50			1123	11011	0	1049	11168	0	982	10122	0	1246	11650	0
17925.843	337138	15592	50			1223	11130	0	1114	11221	0	1033	10155	0	1212	11702	0
17929.759	336624	15680	50			1154	11082	0	1094	11130	0	966	10167	0	1243	11680	0
17933.678	336093	15687	50			1130	11073	0	1086	11151	0	953	10114	0	1205	11667	0
17937.598	335954	15712	50			1194	11073	0	1113	11168	0	981	10125	0	1231	11668	0
17941.519	335724	15714	50			1205	10941	0	1113	11114	0	987	10140	0	1310	11635	0
17945.443	335448	15691	50			1240	11024	0	1109	11195	0	996	10121	0	1272	11569	0
17949.368	334845	15728	50			1178	11018	0	1199	11143	0	997	10104	0	1189	11589	0
17953.295	334006	15696	50			1237	10977	0	1146	11172	0	1089	10178	0	1246	11550	0
17957.224	334128	15699	50			1223	11003	0	1127	11050	0	1067	10191	0	1298	11607	0
17961.154	333873	15694	50			1265	11013	0	1153	11122	0	1099	10096	0	1242	11613	0



读取实验数据



多元固体探测器测量的数据

选择是否将每一元的数据保存为单独的一个 group

The screenshot displays the Athena software interface. The main window, titled "Athena: data columns", shows a table of data columns with columns labeled #E, I1, I2, I3, ux, SCA00, ICRO, Ocro, and SCA1. The table contains numerical data for each column. Below the table, there are several control panels. The "Natural log" panel has a checkbox labeled "Save each channel as a group" which is checked and circled in red. The "Reference channel" panel shows a formula for mu(E): $(ilqm.11 + ilqm.14 + ilqm.17 + ilqm.20 + ilqm.23)$, which is also circled in red. The "Graphics Window #1 - [athena]" window shows a plot titled "current column selection" with a y-axis from 0 to 1.5 and an x-axis from 17800 to 18800. The plot shows a sharp peak at approximately 18000.



读取实验数据



多元固体探测器测量的数据

The screenshot shows the Athena software interface. The main window is titled "Athena" and has a menu bar with "File", "Edit", "Group", "Values", "Plot", "Mark", "Data", "Merge", "Analysis", "Settings", and "Help".

Project

Current group PL_zr.dat_5
File: F:/2011/201111data/PL-zr.dat
Z: Zr Edge: K E shift: 0 Importance: 1

Background removal Show additional parameters
E0: 18003.71 Rbkg: 1.0
k-weight: 2 Edge step: 0.04790 fix step
Pre-edge range: -128.631 to -30
Normalization range: 150 to 665.3100
Spline range: k: 0.0 to 14.173
E: 0.000 to 765.326

Forward Fourier transform
k-range: 2 to 12.173
dk: 1 window type: hanning
Phase correction: no arbitrary k-weight: 0.5

Backward Fourier transform
R-range: 1 to 3
dr: 0.0 window type: hanning

Plotting parameters
plot multiplier: 1 y-axis offset: 0

File List (right panel):

- PL_zr.dat_5 (highlighted in red)
- PL_zr.dat_8
- PL_zr.dat_11
- PL_zr.dat_14
- PL_zr.dat_17
- PL_zr.dat_20
- PL_zr.dat_23
- PL_zr.dat_26

Buttons (right panel):

- E k R q kq
- E k R q
- 0 1 2 3 kw
- Plotting options
- E k R q Stack Ind PF
- mu(E) background pre-edge line post-edge line Normalized Derivative
- Emin: -200 Emax: 800

PL_zr.dat_5 is at the top of the list

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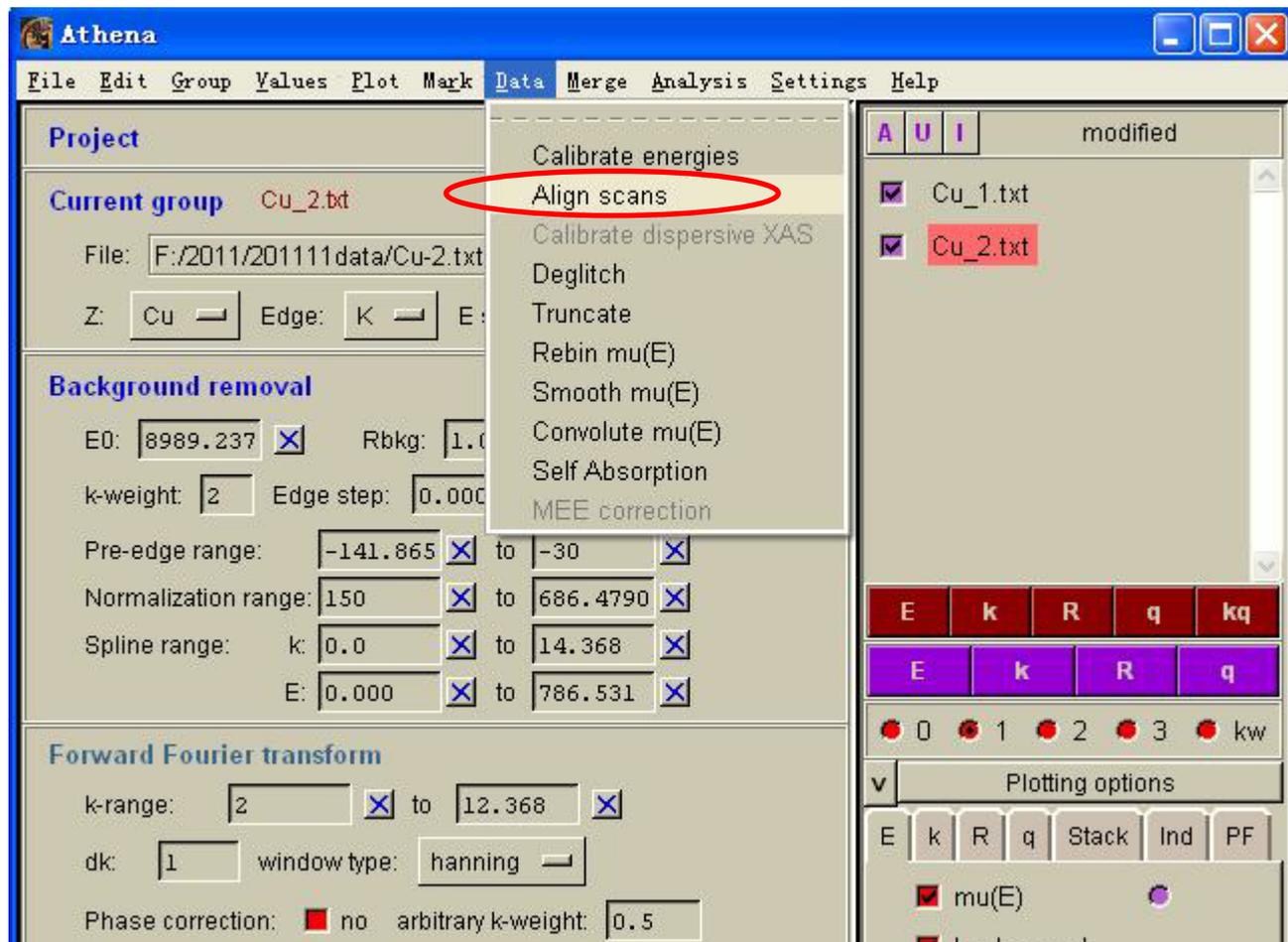
读取实验数据



多次扫描数据

分两步进行:

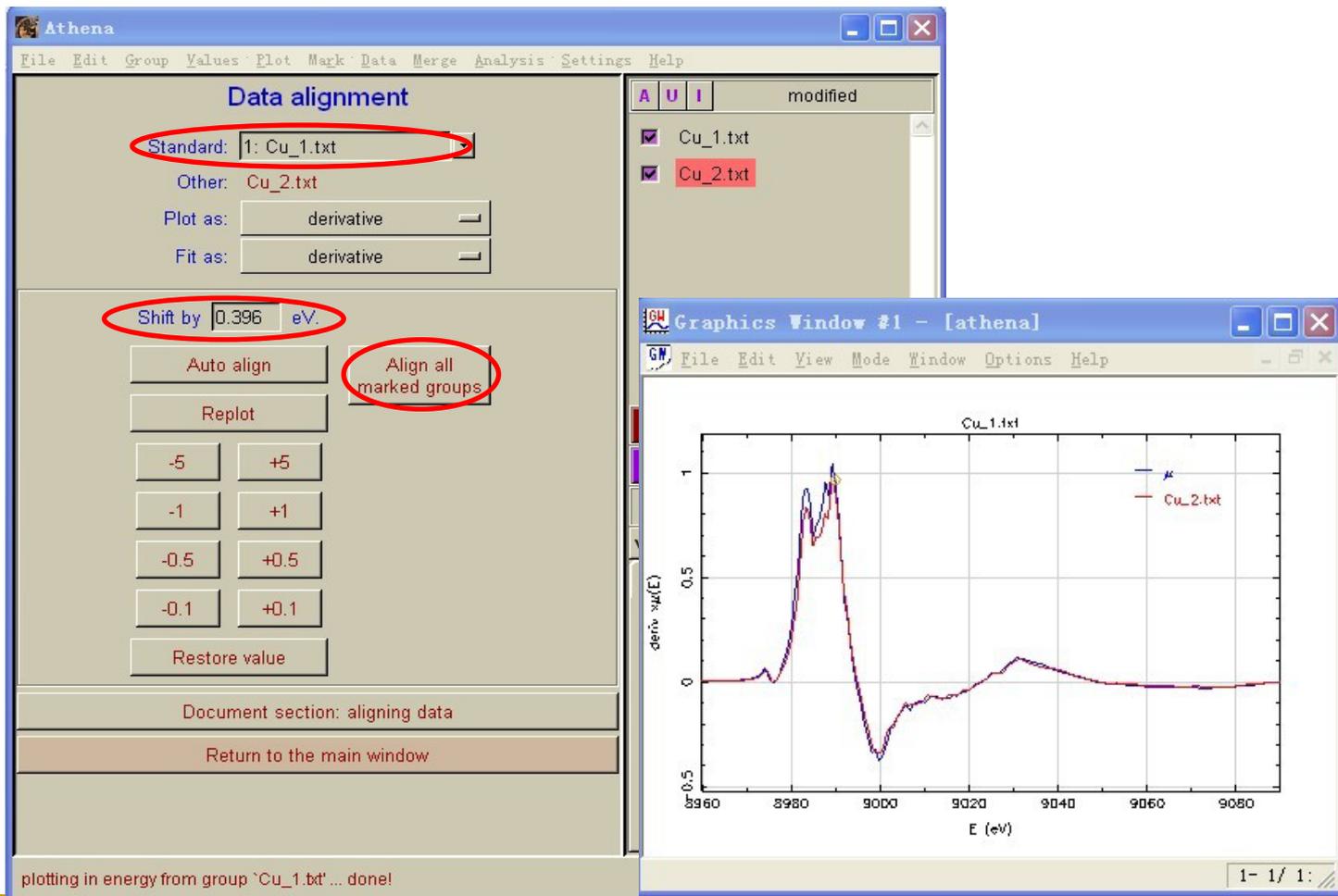
1. 校准能量
2. 合并数据



读取实验数据



校准能量坐标



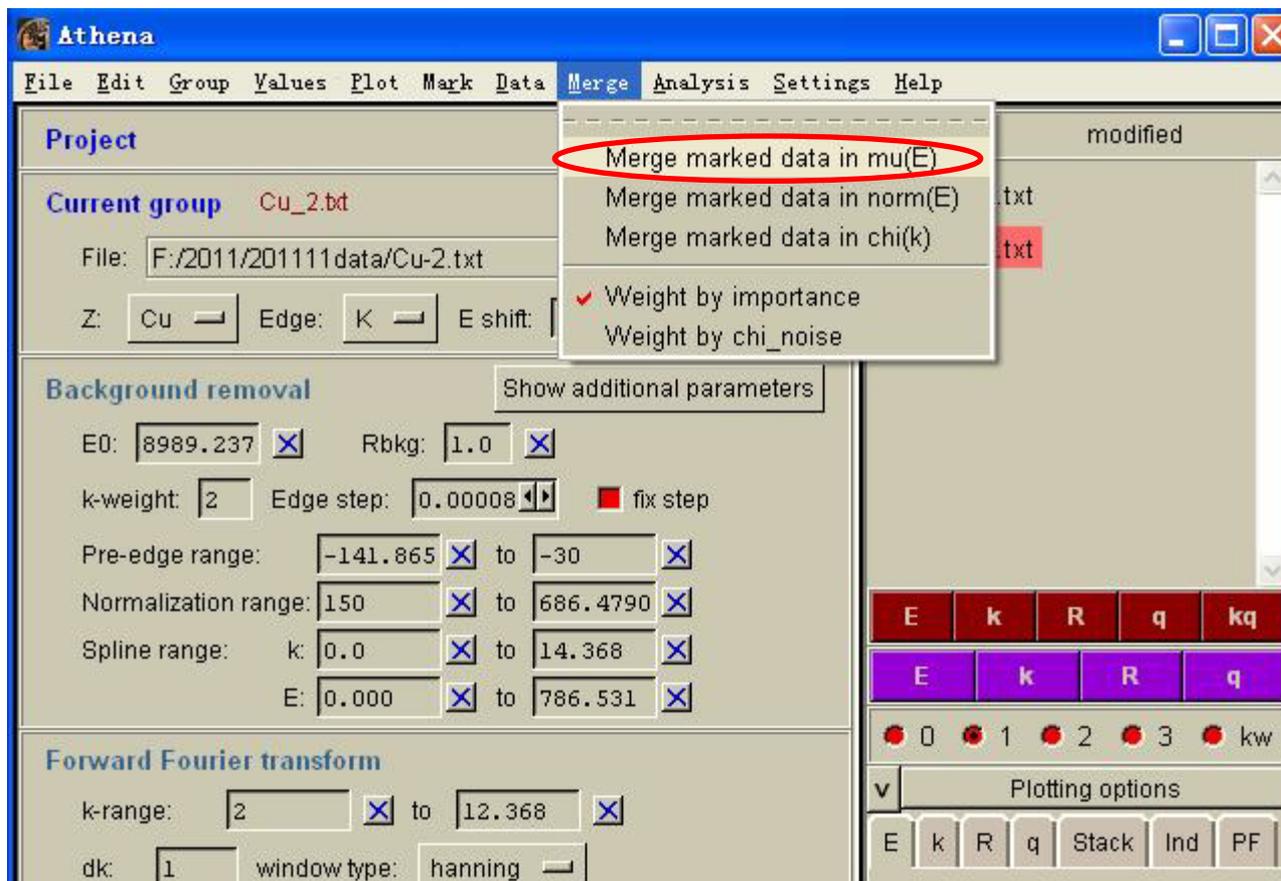
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读取实验数据



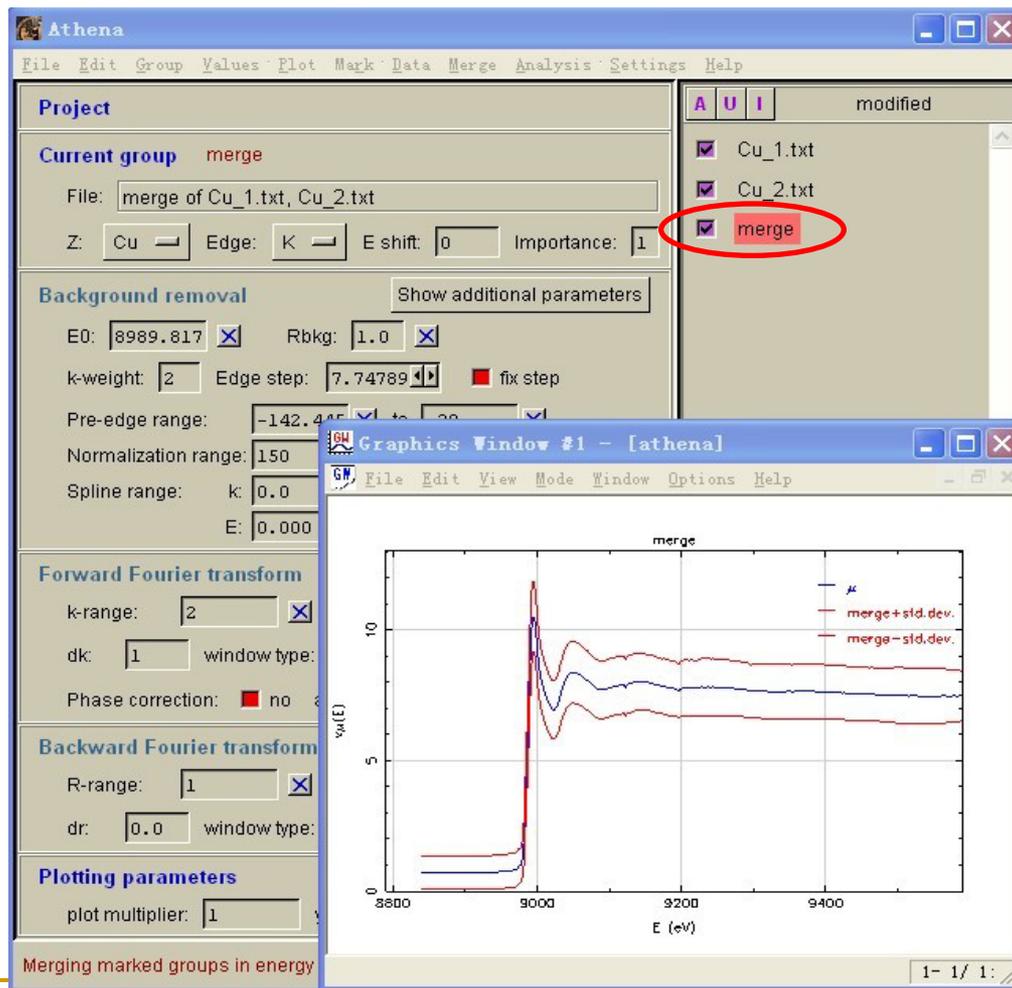
合并数据



读取实验数据



多次扫描数据



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