







▶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
 >注意点及小技巧
 >上机练习



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振荡函数,得到这些数据的配位数,配 位键长,无序度因子等结构参数;

注: Demeter 正在研发中,因此会存在很多小bug,请大家发现后,上 传至程序下载的网站



和数据分析

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ARTEMIS软件简介





ARTEMIS软件简介

File: 文件打开、保存等 Monitor: 监控(所有的命令、操作) Fit: 拟合相关前置条件判定设置 Plot: 绘图设置 Help:帮助文档

GDS	Add	Feff calcula	Add	Name Fit 1 Fit description	Fit space: 🔿 k 📀 R	C q Save	
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拟合参数设定窗口: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)





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Artemis [Plot]	Artemis [Plot]	Artemis [Plot]	
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Freeze C1		Freeze Clear	
Save next plot to a fil	Save next plot to a	Save next plot to a file.	国科学院高能物理研究所

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绘图窗口: 数据、拟合结果等的图形化显示;



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Fit 1				
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拟合历史窗口: 多次拟合 结果、多次拟合的统计量、 拟合量的比较、添加至绘 图窗口等;

Restore fitting model from "Fit 3" Save log file for "Fit 3" Export "Fit 3" Discard "Fit 3"

Discard marked fits

Show YAML for "Fit 3"

Enter a regular expression	×
Mark fits matching this regular expression:	
OK Cancel	:

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🌉 Artemis [History]	
Fit history	Log file Reports Plot tool
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🔽 Fit 3	Report on a parameter
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	Show v=0
	# Report on statistical parameters
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	S.64
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All None Reger	P
About	
Close	fit Demekr 0.9.20 @ Bruce Ravel 2006-2014

Reports选项:可以选择多次拟合中的统计信息、键长、配位数等进行比较;



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🌉 Artemis [History]		📑 Artemis [Plot]	📓 Artemis [Plot] 📃 🗖 🔀
Fit history Fit 1 Fit 1 Fit 3 Hark fits All None Regexp About	Log file Reports Plot tool Click on a button Fit 1 cu010k Fit 3 cu010k	k R k-weight 0 1 2 3 kwith limits stack indic VPaths Plot × (R) Magnitude Real Imag. Plot × (q) Magnitude Real Imag. Plot fit Plot fit Plot vindow Plot running R-factor kmin kmax 15 rmin qmin qmax 15 Plotting list Plotting list Freeze Clear	k R q 0 1 2 3 kw limits stack indic VPaths Plot × (R) Magnitude Real Imag. Plot × (R) Magnitude Real Imag. Plot × (q) Magnitude Real Imag. Plot fit Plot bkg Plot window Plot residual Plot fit Plot bkg Plot running R-factor kmin 0 kmax 15 rmin 0 gmax 15 Plotting list V Data: cu010k row Fit 1 V Fit to cu010k from Fit 1 V Fit to cu010k from Fit 3
"Rit to av010k from Rit 3" was a	dded to the plotting list.	Save next plot to a file.	Save next plot to a file.

可以讲多次拟合结果添加至绘图操作窗口进行比较; Plot tool选项:



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数据操作窗口:对导入数据进行各种处理,导入模型,导入路径、设定拟 合参数等操作;



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晶体学计算窗口:模型的建立、feff计算、路径导出等;相当于原ifeffit的 theory选项





📲 Artemis [Log] Fit 3

Name : Fit 3 (tpyrc) Description : fit to cu010k Figure of merit : 3 Time of fit : 2014-11-19T22:31:30 Environment : Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2. Enterface : Artemis (Wx 0.9923) Prepared by : Contact :				^	
Description : fit to cu010k Figure of merit : 3 Time of fit : 2014-11-19T22:31:30 Environment : Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2. Enterface : Artemis (Wx 0.9923) Prepared by : Contact :	ane	ŝ	Fit 3 (tpyzc)		Ĩ
Figure of merit : 3 Time of fit : 2014-11-19T22:31:30 Environment : Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2. Enterface : Artemis (Wx 0.9923) Prepared by : Contact :	Description	2	fit to cu010k		
Time of fit : 2014-11-19T22:31:30 Environment : Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2. Enterface : Artemis (Wx 0.9923) Prepared by : Contact :	figure of merit	2	3		
Environment : Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2. Enterface : Artemis (Wx 0.9923) Prepared by : Contact :	lime of fit	2	2014-11-19T22:31:30		
Interface : Artemis (Wx 0.9923) Prepared by : Contact :	Environment	2	Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2.		
Prepared by : Contact :	Interface	2	Artemis (Tx 0.9923)		
Contact :	frepared by	2			
	Contact	2			

Independent points		:	33.0371094
Number of variables		:	10
Chi-square		:	129.2209711
Reduced chi-square		1	5.6092528
R-factor		:	0.0026584
Measurement uncertainty	(k)	:	0.0002411
Measurement uncertainty	(R)	:	0.4706954
Number of data sets		:	1

Happiness = 98.00/100 color = #DDE895 Penalty of 2 : sigma2 for "Cu1.1 Cu1.1 " is negative. ****** Note: happiness is a semantic parameter and should ***** ****** NEVER be reported in a publication -- NEVER! *****

guess parameters:						_
delrcul	=	-0.00468980	# +/-	0.00107003	[0]	
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delrcucu11	=	0.33935481	# +/-	0.01100604	[0]	
eOcucu	=	-7.17075145	# +/-	1.76606094	[0]	~
<						>
Save			Abou	ıt	Close	



拟合结果窗口: 拟合得到 的结果、报错等信息;

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a 单壳层拟合
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单壳层拟合-Cu



Import an A	Artemis project or data	?×
查找范围(I):	🖻 example 🏼 🕑 🤌 📂 🛄 🗸	
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	文件类型(T): chi(k) column data (*. chi;*. dat) 🔽	取消

数据导入

方式1: 主窗口/File/open prject or data (适用于多种数据格式)







单壳层拟合-Cu



🌉 Artemis [EXAFS	data a	na	lysis] - Kunt	titled>	
File Monitor Fit Pl	ot Help				
Open project or data	Ctrl+o			Feff calculations	s ———
Recent files		►		Ad	d
Save project	Ctrl+s				
Save project as					
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Import		•	× (k) data		
Export		▶	Demeter fit se	rialization	
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Close	Ctrl+w	-	a morecure		
Exit	Ctrl+q		an old-style A	rtemis project	
			a feffit.inp f	ile	

方式2: 主窗口/File/import/x(k) data



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数据处理

Import cryst	al data				Artemis [Feff] Atoms and Feff	
査状范围(II): 査状范围(II): 我最近的文档	al Uata example multielectro Cu. inp	nexcitation effect		≫	Rename Discard Seff in Demeter Formula: Cu Rename Discard Seff in Demeter Formula: Cu	
 一 我的文档 一 我的电脑 一 教育 - 教育					Name Cu Space Group f m 3 m Space Group f m 3 m A 3.61 B 3.61 C 3.61 Edge K Style Feff6 - elem S Self-consistency Rscf 5.0 Aggregate degeneracy margins Radial distances Margin: 0.03 Beta: 3 Cluster size 6.00 Longest path 5.0 Add a site 0 0 0]]
	文件名 (87): 文件类型 (T):	Cu.inp input and CIF files (*.inp;*.cif)	•	Core El. x y z Tag 1 ✓ Cu 0.00000 0.00000 Cui 2	

方式1:单击数据操作窗口/Import cystal data or a Feff calculation 导入Cu.inp 弹出右侧 Atoms and Feff窗口 (inp文件在老版ifeffit软件安装目录下share/atomdb中有部分;也可 以导入*.cif 文件) 方式2:开始/所有程序/Demeter with strawberry perl/stand-alone Atoms 打开一个空白

的页面;





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单壳层拟合-Cu

模型建立

构建模型:开始/所 有程序/Demeter with strawberry perl/standalone Atoms

输入所需参数(空间 群、晶体学参数、原 子占位);

选定所需计算的团簇 尺寸,最长路径长度 等

shift victor (部分空 间群需要,如fd-3m)

全部输入后,建议将 模型保存,便于后续 再次调用; save data



Artemis [Feff] Atoms and Feff 🄒 Feff doc Rename Discard 💓 Feff in Demeter 🐗 Atoms Taths 🌇 Path-like 🥦 Feff Console N Open file Save data Export Clear all Run Atoms Aggregate Titles name: copper formula: Cui > Lattice Constants Name Cu в С Å 3.61 3.61 3.61 Space Group fm 3 m Style Feff6 - elem α β 90 ¥ 90 90 Edge K Self-consistency Reaf Radial distances Aggregate degeneracy margins Cluster size 6.00 Longest path 5.0 Beta: Margin: Shift vector Add a site 0 0 0 insert Core E1. Tag x y z 1 ~ Cu. 0.00000 0.00000 0.00000 Cm12 3 4 5 6

http://www.springermaterials.com/docs/vsp.html http://chem5.nchc.org.tw/icsd/index.php



数据处理



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模型建立



Artemis [Feff] Atoms and Feff	
📼 Rename 🍟 Discard 🞯 Feff in Demeter 💡 Feff doc	
Atoms 🐝 Feff 🔯 Paths 🗞 Path-like 👹 Console	
Open file Save file Clear all Template Run Feff	
Name: Cu Margin: 0.03 Beta: 3	
(Feff input file-	
* This feff6 file was generated by Demeter 0.9.20 * Demeter written by and convright (c) Bruce Ravel, 2006-2014	^

* total mu*x=1: 4.057 microns, unit edge step: 4.726 microns	=
* specific gravity. 0.911 *************	
* normalization correction: U.UUU46 ang 2 *************	
TITLE name: copper TITLE formula: Cu TITLE sites: Cu1 TITLE refer1: Kittel, ISSP TITLE refer2: TITLE schoen: TITLE schoen: TITLE notes1: metal, fcc	
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单击Rum Atoms 可以弹出以上界面;



\Rightarrow	单壳层拟合-	Cu 模型建立	数据处理
Reiting Sundanting Padiation	Feff文件信息 →	Artemis [Feff] Atoms and Feff Rename Discard Feff in Demeter Feff Atoms Feff Zeff Zeff Open file Save file Clear all Template Run Feff Name: Cu Margin: 0.1 Feff input file * This feffő file was generated by Demeter 0.9.20 * Demeter written by and copyright (c) Bruce Ravel, 2006-20 * -**-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*	Console 03 Beta: 3 04 04 05 05 05 05 05 05 05 05 05 05 05 05 05
····································		<pre>*************</pre>	<pre><**** <*** </pre>

单击Rum Atoms 可以弹出以上界面;检查路径文件是否正确(原子间距是否合理),点击save file 保存feff.inp; 中國科學院為能物理研究所

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单壳层拟合-Cu



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# 8 pat # Forwa # TITLE Scatter 0000 0001 0002 0003 0004 0005 0006 0007	hs were for rd scatter sites: Cu ing Paths Degen 12.000 6.000 48.000 24.000 48.000 24.000 48.000 96.000	Reff 2.5527 3.6100 3.8290 4.3577 4.3577 4.4213 4.7633 4.7633	n 5.000 Å ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.3 @ Deff constanting math	Rank 100.00 22.98 10.59 3.39 8.58 55.41 10.63 21.75	Legs 2 3 3 3 2 3 3 3 3 3	Type single scattering acute triangle other double scatter other double scatter single scattering obtuse triangle	ing
# 8 pat # Forwa # TITLE Scatter 0000 0001 0002 0003 0004 0005 0006 0007	hs were for rd scatter sites: Cu Degen 12.000 6.000 48.000 24.000 48.000 24.000 48.000 96.000 Degen	Reff 2.5527 3.6100 3.8290 4.3577 4.3577 4.4213 4.7633 4.7633	n 5.000 A ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.3 @ Reff scattering path	Rank 100.00 22.98 10.59 3.39 8.58 55.41 10.63 21.75 Rank	Legs 2 3 3 3 2 3 3 3 3 3 3	Type single scattering acute triangle other double scatter other double scatter single scattering obtuse triangle obtuse triangle Legs t	ring
# 8 pat # Forwa # TITLE Scatter 0000 0001 0002 0004 0005 0006 0007	hs were for rd scatter sites: Cu ing Paths Degen 12.000 6.000 48.000 24.000 48.000 24.000 48.000 96.000 Degen I田公本前日	Number Numer Numer Numer <td>n 5.000 A ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.3 @ Reff scattering path 田公友理 上、共存自于现在交</td> <td>Rank 100.00 22.98 10.59 3.39 8.58 55.41 10.63 21.75 Rank 廿 束井 其田 公</td> <td>Legs 2 3 3 3 2 3 3 3</td> <td>Type single scattering acute triangle other double scatter other double scatter single scattering obtuse triangle obtuse triangle Legs t 类在目录反 次类在类和</td> <td>ring ring 文pe 白子米田</td>	n 5.000 A ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.3 @ Reff scattering path 田公友理 上、共存自于现在交	Rank 100.00 22.98 10.59 3.39 8.58 55.41 10.63 21.75 Rank 廿 束井 其田 公	Legs 2 3 3 3 2 3 3 3	Type single scattering acute triangle other double scatter other double scatter single scattering obtuse triangle obtuse triangle Legs t 类在目录反 次类在类和	ring ring 文 pe 白子米田
# 8 pat # Forwa # TITLE Scatter 0000 0001 0002 0003 0004 0005 0006 0007 序号	hs were for rd scatter sites: Cu Degen 12.000 6.000 48.000 24.000 48.000 24.000 48.000 96.000 Degen 理论配	bund withi ring cutof 11 Reff 2.5527 3.6100 3.8290 4.3577 4.4213 4.7633 4.7633 4.7633 F 位数理	n 5.000 A ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.3 @ Reff scattering path 世论键长 散射路径	Rank 100,00 22.98 10,59 3.39 8.58 55.41 10.63 21.75 Rank 相对理论	Legs 2 2 3 3 3 2 3 3 3 3 3 3	Type single scattering acute triangle other double scatter other double scattering obtuse triangle obtuse triangle Legs t 散射路径数 散出	^{ing} ype 射类型
# 8 pat # Forwa # TITLE Scatter 0000 0001 0002 0004 0005 0006 0007	hs were for rd scatter sites: Cu Degen 12.000 6.000 48.000 24.000 48.000 24.000 48.000 96.000 Degen 理论配	bund withi ring cutof al Reff 2.5527 3.6100 3.8290 4.3577 4.3577 4.4213 4.7633 4.7633 4.7633 F 位数理	n 5.000 A ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.2 @ @ Cul.1 Cul.3 @ Reff scattering path L论键长 散射路径 (分	Rank 100.00 22.98 10.59 3.39 8.58 55.41 10.63 21.75 Rank 相对理论 5.40	Legs 2 2 3 3 2 3 3 2 3 3 3 2 3 3 3 3 2 3	Type single scattering acute triangle other double scatter other double scatter single scattering obtuse triangle obtuse triangle Legs t 散射路径数散	ing ing ype 射类型
# 8 pat # Forwa # TITLE Scatter 0000 0002 0003 0004 0005 0005 0005	hs were for rd scatter sites: Cu Degen 12,000 6,000 48,000 24,000 24,000 24,000 24,000 24,000 96,000 Degen 理论配	bund withi ring cutof al Reff 2.5527 3.6100 3.8290 4.3577 4.4213 4.7633 4.7633 4.7633 F 位数理	n 5.000 A ff 20.00 Scattering path @ Cul.1 @ @ Cul.2 @ @ Cul.1 Cul.1 @ @ Cul.1 Cul.2 @ @ Cul.1 Cul.2 @ @ Cul.3 @ @ Cul.1 Cul.3 @ Reff scattering path 世论键长 散射路径 (算	Rank 100.00 22.98 10.59 3.39 8.58 55.41 10.63 21.75 Rank 相对理论 第一条为定	Legs 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 3 2 3 3 3 2 3 3 3 2 3 3 3 3 2 3	Type single scattering acute triangle other double scatter other double scatter single scattering obtuse triangle Legs t 散射路径数散 00,其他为相对伯	^{ring} ring 射类型 宜)

模型建立

单击Rum Feff 可以弹出以上界面, 左键Cu的第一路径, 将其拖数据操作窗口的pathlist



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单壳层拟合-Cu

拟合参数设定



👰 Artemis [Data] cu010k	
Data Path Marks Actions Debug Help	
cu010k CV 3	[Cu] Cu1.1 [Cu] Cu1.1
Data source E:\data process\2014\example\cu010k. chi Plot this data set as k123 R123 Rmr Rk kq	 ✓ Include path □ Plot after fit □ Use this path for phase corrected plotting. @ Cul. 1 @ (0000) single scattering, high (100.00) x y z ipot label 1.805000 1.805000 0.000000 1 'Cul. 1'
Title lines	0.000000 0.000000 0.000000 0 abs 路径信息描述 <u>Reff=2.553, nleg=2, degen=12</u> <u>12</u>
Fourier transform parameters kmin 3.000 Image: state stat	$\frac{SO^2}{\Delta E}$ σ^2
Fitting k weights ♥1 ♥2 ♥3 ○ other 0.5 Other parameters ♥ Include in fit ○ Plot after fit ○ Fit background ε (k) ○ ○ Plot with phase correction	Ni 初合参数设定 3rd 11
Check here to make plots using phase corrected Fourier transform	s. Note that the fit is NOT made using phase corrected transfo

左键Cu的第一路径,将其拖入pathlist, 即可出现以上界面





单壳层拟合-Cu

🚺 Artemis [Data] cu010k



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Data Path Marks Actions Debug Help		
CV 3	Cufeff] Cul.1	1
Data source E:\data process\2014\example\cu010k.chi	✓ Include path Use this path for phase c	Plot after fit orrected plotting.
Plot this data set as	(0000) single scatter	ing, high (100.00)
Title lines	1. 805000 0. 000000 0. 000000	0.000000 1 'Cul.1 ' 0.000000 0 'abs '
	Label Reff=2.553, nleg	;=2, degen=12
Fourier transform parameters	<u>SO</u> ² ampculst	
kmin 3.000 o kmax 22.950 o dk 1	△E0 eOculst △R rculst	
	$\frac{\sigma^2}{ssculst}$	
✓ 1 ✓ 2 ✓ 3 other 0.5	<u>Ei</u> <u>3rd</u>	
Cother parameters ✓ Include in fit □ Plot after fit □ Fit background	4th	
Created "scoulet" as mass		
oreace start as Eacos		

拟合参数设定

单击路径,在右侧红色框内输入需要拟合的变量(以字母与数字组成,其他符号可能出错);并在变量处右键,选择guess变量,将其添加至GDS窗口 (注:artemis具有内部参量如E0等,注意添加相应后缀,减少程序警告)





单壳层拟合-Cu 拟合参数设定

	Type	Name	∎ath expression	Evaluated	🧡 Vse best fi
1	guess	ampculst	1.00000		🙆 Reset all
2	guess	eOculst	0		
3	guess	rculst	0		🁋 Highlight
4	guess	ssculst	0.00300		🗑 Evaluate
5	guess				9
6	guess				Tennert GDS
7	guess				Import obb
8	guess				📑 Export GDS .
9	guess				(N
10	guess				🔊 Discard all
11	guess				
12	guess				SUE) 664 👁
				~	
				>	

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



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ARTEMIS软件简介

Beijing Synchrotron Radiation Facility guess enot=0 辎 set S02=0.85 裝 当有多条路径 s factor=100: g enot=0 s scale=2000;

Guess: 设定初始值,不做限制; Def: 设定参数间的数学关系式; def delr 1=alfa*reff guess alfa=0.01 Set: 设定成固定值,不做改变; lguess: 多数据定义 lguess ss=0.003 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 r enot_res=scale*penality(enot,-5,5) 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)

其中Guess Def Set Skip Restrain 较为常用;





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单壳层拟合-Cu





g(R):原子对分布函数



晶体等有序体系或弱无序体系(高斯分布)



**中等无序体系:累积量展开





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单壳层拟合-Cu 拟合结果解读



	Artemis [Log	Fit 1
	Hame Description Figure of merit Time of fit Environment Interface Prepared by Contact	: Fit 1 : fit to cu : 1 : 2014-11-2 : Demeter (: Artemis) : :
本次拟合的统计信息	=*=*=*=*=*=*=*=*=*=* Independent points Number of variables Chi-square Reduced chi-square R-factor	:=*=*=*=*=*=* : 24 : 4 : 85 : 40 : 0
	Measurement uncerta Measurement uncerta Number of data sets Happiness = 100.00/1 ***** Note: happines ***** NEVER be re	nty (k) : 0.1 nty (k) : 0.1 : 1 :00 ss is a seman :ported in a ;
	<u>guess parameters:</u> ampculst	= 0.90751
	eOcu	= 5.46149
拟合参数最优值与不确定度	delrcuist	= -0.00466
		- 0.00245

🌲 Artemis [Lo	og] Fit 1				
Name Description Figure of meri Time of fit Environment Interface Prepared by Contact	: Fit 1 : fit to it : 1 : 2014-1 : Demete : Artemi : :	(ntgtd) cu010k 1-20T01:21:32 r 0.9.20 with s (Tx 0.9923)	perl 5.0180	D2 and using Ife	£fit 1.2 .
=*=*=*=*=*=*=*=*=	*=*=*=*=*=	*=*=*=*=*=*=*=*	=*=*=*=*=*=*=*=	*=*=*=*=*=*=*=*=	
Independent point Number of variabl Chi-square Reduced chi-squar B-factor	s : es : e :	24. 8750000 4 852. 5924664 40. 8427529 0. 0029767			
Measurement uncer Measurement uncer Number of data se 	tainty (k) : tainty (R) : ts :	0.0007215 0.0040810 1			
Happiness = 100.0 ***** Note: happi ***** NEVER be	0/100 ness is a se reported in	color = #) mantic parameter . a publication ·	D8E796 r and should ** NEVER! **	okokok okokok	
<u>guess parameters:</u>					_
ampculst eOcu delrculst	= 0.90 = 5.46 = -0.00	751600 # +/- 149455 # +/- 466465 # +/-	0.02148118 0.29447058 0.00141034	[1.00000] [0] [0]	
ssculst	= 0.00	345442 # +/-	0.00013616	[0.00300]	
<u>Correlations betw</u>	een variable	5:			~
<					>
Save		Abo	out	Close	





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数据处理

拟合参数相关性

各壳层的拟合结果

Artemis [Log]	Fit 1				
delrcu1st = sscu1st =	-0.00466465 0.00345442	# +/- # +/-	0.00141034 0.00013616	[0] [0.00300]	<u> </u>
orrelations between v delrcu1st & sscu1st & ll other correlations	variables: t eOcu t ampculst s below 0.4	> >	0. 8498 0. 8475		-
==== Data set >> o	2u010k << =====	=======			
file name k-range dk k-window k-weight	<pre>= I:\example\cu = cu010k = 3.000 - 22.950 = 1 = hanning = 1, 2, 3</pre>	010k. chi 0			
R-range dR R-window fitting space background function phase correction R-factor by k-weight name N	= 1 - 3 = 0.0 = hanning = r = no = : = 1 -> 0.00411, S02 sigma ²	2 -> 0 e0	.00222, 3-> delr Re:	0.00260 ff R	
Cul.1 12.000 O. name ei	908 0.00345 ! third four	======= 5.461 -0 th	. 00466 2. 552'	70 2.54804	
Cul.1 0.00000 C	0.00000 0.00000	====		L-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1-1	-4-
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单壳层拟合-Cu 统计信息定义

Chi-square Reduced Chi-square

$$\chi^{2} = \frac{N_{idp}}{\epsilon N_{data}} \sum_{i=min}^{max} \left[\operatorname{Re} \left(\chi_{d}(r_{i}) - \chi_{t}(r_{i}) \right)^{2} + \operatorname{Im} \left(\chi_{d}(r_{i}) - \chi_{t}(r_{i}) \right)^{2} \right]$$
$$\chi^{2}_{\nu} = \frac{\chi^{2}}{\nu}$$
$$\nu = N_{idp} - N_{var}$$
$$\epsilon = \text{measurement uncertainty}$$

不确定度

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

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;



数据处理



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N: 配位数 S02: 振幅衰减因子 (0.7,1) Sigma ² : 无序度因子 (Debye-Waller factor) C_4 : 4阶累积量	(0.003, 0.02)
$ \begin{cases} R: 原子间距; (delR < 0.5A) \\ C_3: 3 \cap R \oplus R \oplus E_i \\ E_i: 能移展宽 \\ \triangle E_0: 能量零点偏移 (+-10eV以内) \end{cases} $	
N: +-20% R: 0.01A 原子种类: +-4	
注1: 实际拟合中,S02可以小于0.7; 注2: 重金属原子(Pb),ΔE0可能大于10ev	





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单壳层拟合-Cu



Beiji H	h = 1	🌉 Artemis [Hi
京同步辐射	Artemis [EXAFS data analys File Monitor Fit Plot Help Image: GDS Add Image: Plot Add Image: Hist Jow	Fit history Fit 1 Fit 2
· Facility	Use this space to fully describe this	

单击操作界面左侧 History键,弹出历史 窗口,查看多次拟合 结果;

	🌉 Artemis [History]	
lys	Fit history	Log file Reports Plot tool
1 10101	Fit 1	Hame : Fit 2 (fcbzu) Description : fit to cu010k Figure of merit : 2 Time of fit : 2014-11-16T13:49:31 Environment : Demeter 0.9.20 with perl 5.018002 and using Ifeffit 1.2.1 Interface : Artemis (Tx 0.9923) Prepared by : Contact :
		=+
.hi s		Independent points : 24.8750000 Number of variables : 4 Chiraguare : 852 5924664
		Reduced chi-square : 40.8427529
		R-factor : 0.0029767
		Measurement uncertainty (k) : 0.0001215 Measurement uncertainty (R) : 0.0040810 Number of data sets : 1
		Nappiness = 100.00/100 color = #D8E796 ****** Note: happiness is a semantic parameter and should ***** ***** NEVER be reported in a publication NEVER! *****
		<u>guess parameters:</u> ampculst = 0.90751600 # +/- 0.02148118 [1.00000] obseitet = 5.48149455 # +/- 0.22447158 [0]
1	-Mark fits	reulst = $-0.00466465 \# +/- 0.00141034 [0]$
	All None Regexp	
	About	Save this log
	Close	




单壳层拟合-Cu 结果输出



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Save project	file					? 🔀
保存在(II):	🚞 example		*	G 🦻	ب 🔝 👏	
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[]] 桌面						
我的文档						
夏 夏 我的电脑						
マラン マー マー						
	文件名 (M):	cu010k-1path-v1.fp	pj		~	保存(S)
	保存类型 (T):	Artemis project (*. fpj)		~	取消

主窗口/file/save project as





单壳层拟合-Cu

数据处理

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Artemis [Data] cu010k			
Data Path Marks Actions Debug Help			
cu010k CV	3 [cufeff] Cui.1	💻 💽 [cufeff] C	u1.1
Data source E:\data process\2014\example\cu010k.chi		✓ Include path Use this path for ph @ Cul. 1 @ (@ Cul. 1 @	Plot after fit ase corrected plotting.
Flot this data set as k123 R123 Rmr Rk	kq	x y 1.805000 1.805 0.000000 0.000	z ipot label 000 0.000000 1 'Cu1.1 ' 000 0.000000 0 'abs '
		Label Reff=2.553,	nleg=2, degen=12
		<u>N</u> 12	
Fourier transform parameters		A TO	
kmin 3.000 0 kmax 22.950 0 dk 1		A P e0culst	
rmin 1 0 rmax 3 0 dr 0.0		a ² reulst	
Fitting k weights		ssculst	
♥1 ♥2 ♥3 other 0.5		2.4	
Other parameters		445	
✓ Include in fit ☐ Plot after fit ☐ Fit backgrown c (k) 0 ☐ Plot with phase correction	Ind	416	
Plot this data set as $ \times (R) $ and $Re[\times (R)]$.			

保存拟合结果

数据操作窗口/file/save project as









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>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

 >注意点及小技巧
 >上机练习









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1数据操作窗口:扩大rmax至5.1A; 2将R小于5.4A的单散路径(leg=2)添加到pathlist中; 利用绘图窗口,确认路径对需要拟合的区域有贡献;





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将4条单散路径的参数都设置后添加进GDS窗口, (4pathx4拟合参数)





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多壳层拟合-Cu



Nidp≈2 Δ k Δ R/π 最大对立拟合参数个数例:

k-range 2.3-20.3; R-range 1.7-5.1 Nidp≈38.9

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9条独立路径;

如果Nvar>Nidp独立拟合参数多于可用独立节点数,此时拟合的结果是多解中的某一个解 数据操作窗口/Data/show Nidp

独立节点概念!!!







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多壳层拟合-Cu



拟合策略: 相同原子所有路径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△E0可设成统一 配位数可以通过模型限定或合理限定 △R可以用热膨胀或与结构关联起来 稳定性: 改变K、R的选取范围

放松对变量的限制 设定部分变量、放开部分变量





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🔛 Artemis [Plot. 1] 🍖 🏾 🎜 🇮 🍳 🍳 🕲



路径选取:增加了键长4-5.4A的3leg MS 共4条 参数设置:统一S02、△E0、sigma^2,△R=alpha*reff







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参数设置:将1st path的ss 设置成独立







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路径选取:增加了键长小于5.4A的 MS 共9条 参数设置:统一SO2、△EO、sigma^2,△R=alpha*reff; 1stpath sigma^2 独立;









▶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

 >注意点及小技巧
 >上机练习





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多权重拟合-NiO





不同原子对于k的响应不同; sigma^2、 $\triangle R$ 、 $\triangle E0$ 对k的响应为非线性;

Fitting k weights □ 1 🗹 2 🗹 3 🗔 other 数据操作窗口左下: 0







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多权重拟合-NiO













▶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

 ▶注意点及小技巧
 ▶上机练习





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多Feff拟合



例YBa2Cu3O7: Cu有两种占位

title YBCO space = P rmax = 7.	: Y Ba2 C M M M 2 a=3.8	си3 07 817 b=3.8	82 c=11.	671
core = cu	1			
atoms				
! At.type	x	У	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
0	0	0.5	0	01
0	0	0	0.1589	02
0	0	0.5	0.3780	03
0	0.5	0	0.3783	04



和数据分析讲习班 2014



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多Feff拟合



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		ر 🛃	His [.]				1		Hide "ybco-	atoms.inp″		
		m .	Tom									
		. 62	,									
	Core	E1 .	x	у	z		Core	E1 .	x	y	z	Tag
1		Y	0.5	0.5	0.5	1		Y	0.5	0.5	0.5	Y
2		Ba	0.5	0.5	0.184	2		Ba	0.5	0.5	0.184	Ba
3		Cu	0	0	0	3		Cu	0	0	0	cul
4		Cu	0	0	0.356	4	 Image: A set of the set of the	Cu	0	0	0.356	cu2
5		0	0	0.5	0	5		0	0	0.5	0	o1
6		0	0	0	0.158	6		0	0	0	0.158	٥2
7		0	0	0.5	0.379	7		0	0	0.5	0.379	٥3
8		0	0.5	0	0.377	8		0	0.5	0	0.377	o4

<u>Label</u>	Reff=1.927, nleg=2, degen=2		
N	2		
<u>S0²</u>	1/3*ampsite1		
<u>∆ eo</u>	enoto		
<u> </u>	alpha*reff		
<u> </u>	sssitel		





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多Feff拟合



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和数据分析讲习班X射线吸收谱学实验

•201*4*

<u>Label</u>	Reff=1.927, nleg=2, degen=2		
W		<u>Label</u>	Reff=1.846, nleg=2, degen=2
Ξ	2	<u>N</u>	2
<u>S0²</u>	1/3*ampsite1	S0²	2/2*:*-2
$\Delta E0$		<u></u>	2/3*ampsite2
		$\Delta E0$	enoto
$\Delta \mathbf{R}$	alpha*reff	$\Delta \mathbf{R}$	alpha*reff
$\sigma^{(2)}$	ersital	σ ²	
	3551(61	<u> </u>	sssiteZ

XAFS信号获取的信息为样品的统计平均值

修正拟合参数(占位1配位数*1/3,占位2配位数*2/3)









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guess parameters:

enots	<u>-23.43613266</u>
amp	= 1.48776701 #+/- 0.18008590 [1.00000]
enotni	= 0.30571123
delrni	= 0.01799916 #+/- 0.00786207 [0]
ssni	= 0.00792367 #+/- 0.00085477 [0.00300]
delrs	= 0.11081540 #+/- 0.02757453 [0]
ssS	= 0.01427525 #+/- 0.00171318 [0.00300]





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	Type	Name	
1	guess	amp1	1.00000
2	guess	enot	0
3	def	delr1	reff*alpha
4	guess	ss1	0.00300
5	def	delr2	reff*alpha
6	guess	alpha	0.00500
7	guess	ss2	0.00300
8	guess	amp2	1

guess	parameters:

amp1	<u>= -0.4003</u> 956
enot	<u>= 6.57718523 #+/- 3.510053</u>
ss1	= 0.01180511 #+/- 0.0230933
alpha	$= -0.03166901 \ \# +/- \ 0.007023$
alpha ss2	= -0.03166901 # +/- 0.007023 $= 0.00406466 # +/- 0.0015860$
alpha ss2 amp2	= -0.03166901 # +/- 0.007023 $= 0.00406466 # +/- 0.0015860$ $= 1.11763518 # +/- 0.33260$



和数据分析讲习班X射线吸收谱学实验





<u>ss1</u>

alpha

<u>ss2</u>

=

=

=

0.19461402

-<u>0.03403929</u>

0.00454527

0.00300

0.00500

0.00300

3*amp1

reff*alpha

ss1

delr2

alpha

ss2

amp2

delr2 =	-0.06951845
amp2 =	1.24804377

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4

5

6

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9

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guess

guess

guess

guess

guess

def

def





重金属的相移因子存在突变,会使得其配位峰在R空间表现出峰的劈裂

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🌉 Artemis [Log] 4SS 🛛

GDS: 'ampcu'

This is a guess parameter which is not used in the math expressions for any def or path parameters.

GDS: 'sscu'

This is a guess parameter which is not used in the math expressions for any def or path parameters.

GDS: 'enotcu'

This is a guess parameter which is not used in the math expressions for any def or path parameters.











良好的数据 准确的模型





Beijing Synchrotron Radiation Facility 北京同步辐射装置

上机练习: C0304 拟合演示

Reference

Depero L.E., Levrangi P., Sberveglieri G.: "Structural Models for Cobalt-Tin Oxide Thin Films", J. Solid State Chem. 116 (1995) 256-264.

Data

Published Crystallographic Data

Space Group: F-43m

Cell Parameters:

Lattice Constant [nm]	Angle [°]	Constants' Ratio	Volume V [nm ³]
a = 0.8083	a = 90	a/b = 1.000	0.52810
b = 0.8083	β = 90	b/c = 1.000	
c = 0.8083	y = 90	c/a = 1.000	

Standardized Crystallographic Data

Space Group: F-43m

Cell Parameters:

	Uni	it Cell			Niggli-re	duced Cell	
Lattice Constant [nm]	Angle [°]	Constants' Ratio	Volume V [nm ³]	Lattice Constant [nm]	Angle [°]	Constants' Ratio	Volume I⁄ [nm ³]
a = 0.8083 b = 0.8083 c = 0.8083	a = 90 $\beta = 90$ y = 90	a/b = 1.000 b/c = 1.000 c/a = 1.000	0.5281	a = 0.57155 b = 0.57155 c = 0.57155	a = 60. $\beta = 60.$ y = 60.	a/b = 1.000 b/c = 1.000 c/a = 1.000	0.13202

Atom Coordinates:

Site	Element	Wyckoff Symbol	Symmetry	x	y	z	Occupation	Coordination Number	Atomic Environment Type
01	0	16 <i>e</i>	.3 <i>m</i>	0.140	0.140	0.140	1		
Co1	Со	16e	.3 <i>m</i>	0.375	0.375	0.375	1		
02	0	16 <i>e</i>	.3 <i>m</i>	0.610	0.610	0.610	1		
Co2	Со	4ď	-43m	3/4	3/4	3/4	1		
Co3	Со	4a	-43m	0	0	0	1		

Note: Atom coordinates assigned by the editor.

http://www.springermaterials.com/docs/VSP/datasheet/lpf-sd/01101000/LPFSD_1101456.html





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Artemis [Feff] Atoms and Feff	
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🐳 💽 Feff 🔯 Paths 🗞 Path-like 👹 Console	
Open file Save file Clear all Template Run Feff	
Name: col Margin: 0.03 Beta: 3	
Feff input file	
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HOLE 1 1.0 * FYI: (Co K edge @ 7709 eV, second number is SO ²) * mphase, mpath, mfeff, mchi CONTROL 1 1 1 1 FRINT 1 0 0 0 RMAX 5.0	
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POTENTIALS * ipot Z tag 0 27 co 1 27 co 2 8 o	
ATOMS * this list contains 325 atoms	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	
	>

改变吸收原子选择,点击run atoms,将feff文件保存co1.inp, co2.inp, co3.inp;



上机练习: C0304 拟合演示

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和数据分析讲习班 X射线吸收谱学实验

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[Artemis [EXAFS data analysis] - *co3o4-2*	
File Monitor Fit Plot Help Image: Show "co3o4" Image: File Monitor Fit Plot Help Image: Show "co3o4" Image: Fit Plot Help Image: Fit Plot He	Fit listory how log
Use this space to fully describe this fitting model.	

Data sets Add已处理好的Co3O4.prj Feff calculation Add 保存的 co1.inp , co2.inp , co3.inp

弹出下述窗口



上机练习:C0304 拟合演示





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上机练习: C0304 拟合演示

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Data Fath Marks Actions Debug Help	
Co304 std CV 1	Path list Drag paths from a Feff interpretation list and drop them in this space to add paths to this data set
Plot this data set as k123 R123 Rmr Rk kq Title lines	Import crystal data or a Feff calculation
	<u>Start a quick first shell fit</u>
	Import a structural unit
Fourier transform parameters kmin 2.726 Imax 13.149 Imax 1 rmin 0.95 rmax 3.406 Imax 0.0	<u>Import an empirical standara</u>
Fitting k weights I	
Other parameters ✓ Include in fit ♥ Plot after fit Fit background ε (k)	

此时自由节点数为16.3



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	🥦 Feff	P:	aths 🥉) Path-	like 関	Console			
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Descrip	otion								
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# Clust # Clust # Z5 pa # Forwa # Angle Scatter 0000 0001 0002 0003 0004 0005 0006 0007 0008	ths were f rd scatter fuz = 3. Degen 4.000 12.000 12.000 12.000 12.000 24.000 12.000 12.000 12.000 12.000	Reff 1.9600 3.3510 3.3510 3.5000 3.5604 3.6092 3.8673 3.9200	Scatter @ 02.1 @ Co2.1 @ Co2.1 @ Co2.1 @ Co1.1 @ Co1.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1	ing pat @ @ @ 02.1 Co2.1 Co2.1	€ € 02.1 € 02.1 € 02.1 €	Rank 100.00 89.68 81.61 26.88 13.38 31.20 5.36 3.97	Legs 2 2 2 2 3 3 4 4 4	Type single scattering single scattering single scattering other double scattering other double scatterin obtuse triangle dog-leg rattle hinge	١g
Clust # Angle # Angle \$ Scatter 00000 0001 0002 0003 0004 0005 0006 0007 0008 0007 0008	ths were f rd scatter fuzz = 3. Degen 4.000 12.000 4.000 12.000 24.000 12.000 4.000 12.000 24.000 12.000 4.000	Reff 1.9600 3.3510 3.3939 3.5000 3.5604 3.9200 3.9201 4.1110	Scatter @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1	ing pat @ @ @ 02.1 Co2.1 Co2.1	e e 02.1 @ 02.1 @ 02.1 @	Rank 100,00 89,68 81,61 26,88 13,38 31,20 5,36 3,97 5,56 31,53	Legs 2 2 2 2 3 3 4 4 4 4 3	Type single scattering single scattering single scattering other double scatterin obtuse triangle dog-leg rattle hinge other double scatterin	ıg
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Clust # Clust # Clust # Z5 pa # Forwa # Angle Scatter 0000 0001 0002 0004 0005 0006 0007 0008 0009 0010 0012	ths were f rd scatter fuzz = 3. Degen 4.000 12.000 12.000 12.000 12.000 12.000 12.000 4.000 12.000 4.000 12.000 48.000 12.000 48.000 12.000 48.000 24.000	Reff 1.9600 3.3510 3.3510 3.5000 3.5604 3.6092 3.8673 3.9200 3.9201 4.1110 4.2679 4.3261	Scatter @ 02.1 @ Co2.1 @ Co2.1 @ Co2.1 @ Co2.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.1 @ 02.2 @ Co2.1 @ 02.2	ring pat @ @ @ 02.1 Co2.1 Co2.1 Co2.1 Co2.1 01.1 01.1 02.2	e e 02.1 e 02.1 e 02.1 e e	Rank 100.00 89.68 81.61 26.88 13.38 31.20 5.36 3.97 5.56 31.53 45.22 22.64	Legs 2 2 2 3 3 4 4 4 3 2 3 3	Type single scattering single scattering single scattering other double scattering obtuse triangle dog-leg rattle hinge other double scattering other double scattering other double scattering	ıg
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Co3.inp



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和数据分析讲习班X射线吸收谱学实验

2014
上机练习: C0304 拟合演示

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ing 2	Data Path Marks Actions Debug Help			
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Plot with phase correction

可以发现其中Co1与Co2是等效的,选定拟合范围内的单散路径; 取Co1 0000,0001路径: Co3 0001,0003路径:



ipot label

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single scattering, medium (9.22)

-1.899510 -1.899510 2 '01.2

数据分析讲习班

ε(k) 0





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上机练习:C0304 拟合演示

	Type	Name	∎ath expression	Evaluated 🔷	🤪 Vse best fit
1	guess	amp1	1.00000		🙆 Reset all
2	guess	eOo	0		
3	guess	delr1	0		🁋 Highlight
4	guess	ss1	0.00300		🗑 Evaluate
5	guess	amp2	1.00000		
6	guess	eOco	0		🐼 Import GDS
7	guess	delr2	0		Import obs
8	guess	ss2	0.00300		📑 Export GDS
9	guess	amp3	1.00000		<u> </u>
10	guess	delr3	0		📡 Discard all
11	guess	ss3	0.00300		
12	guess	amp4	1.00000		200 KK4 🐟
13	guess	delr4	0		
14	guess	ss4	0.00300		
15	guess			~	
<					



将Co-O键的 ΔEO 都定义为eOo,将Co-Co键的的 ΔEO 都定义为eOco, 共计14个变量,点击fit,进行拟合;





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上机练习: C0304 拟合演示

修正配位数:

(4X2+6)/3 ≈5 Co-O: 1.96A (12X2+6)/3=10Co-Co: 3.35A Co-Co: 2.86A 6/3 = 2 (2X2+12)/3 ≈5 Co-O: 3.29



和数据分析讲习班X射线吸收谱学实验 2014

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上机练习:C0304 拟合演示









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l j	<u>guess parameters:</u>					
V	amp1	=	0.83174481	# +/-	0.08238543	[1.00000]
	eOo	=	1.08015878	# +/-	1.42360753	[0]
	delr1	=	-0.04007808	# +/-	0.00633760	[0]
	ss1	=	0.00306295	# +/-	0.00073505	[0.00300]
	amp2	=	0.68725780	# +/-	0.63433740	[1.00000]
	eOco	=	0.77772083	# +/-	3.80396605	[0]
	delr2	=	0.02189250	# +/-	0.04425948	[0]
	ss2	=	0.00727293	# +/-	0.00647593	[0.00300]
	amp3	= [1.72326511	# +/-	0.77381487	[1.00000]
	delr3	=	0.00231561	# +/-	0.02508694	[0]
	ss3	=	0.00359278	# +/-	0.00215945	[0.00300]
	amp4	= (0.11528173	# +/-	0.38697501	[1.00000]
	delr4	=	0.01077481	# +/-	0.06934321	[0]
	ss4	=	-0.00601522	# +/-	0.01031920	[0.00300]

拟合结果可以看到,其中ss4异常,amp3,amp4 数值离合理值0.7-1很大; 可能存在的原因:未考虑3.4-3.6A 对拟合区域的影响;未考虑多散的影响;



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