

微量添加元素の局所構造解析

JASRI 大淵博宣

1. はじめに
2. Eu添加Ga_{0.99}Nについて
3. Artemisを使用した解析
 - ・ 構造モデルの作成
 - ・ 理論計算結果の比較
 - ・ カーブフィッティング
4. Eu添加AlGa_{0.99}Nについて
5. Artemisを使用した解析
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Artemisを用いた通常の解析

→既知の結晶構造を仮定してフィッティング

既知の結晶構造モデルでは
フィッティングできない例

1. 混晶： $A_{1-x}B_xC$ 、 $A_{1-x}B_xC_{1-y}D_y$ 等

Eu添加AlGa₂N

2. 点欠陥：異種原子(置換型)

Eu添加Ga₂N

格子間原子(進入型)

原子空孔等

3. 界面、表面：超薄膜、ナノ粒子等

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希土類添加半導体

発光特性:

- 希土類元素特有の4f殻内遷移
- 非常に鋭い発光ピーク
- 発光波長が温度に対し安定

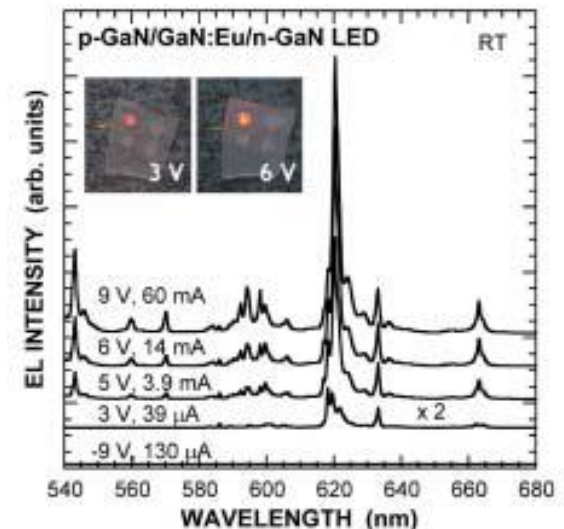
OMVPE法により
EuをGaNに添加



Eu添加GaN
赤色LED

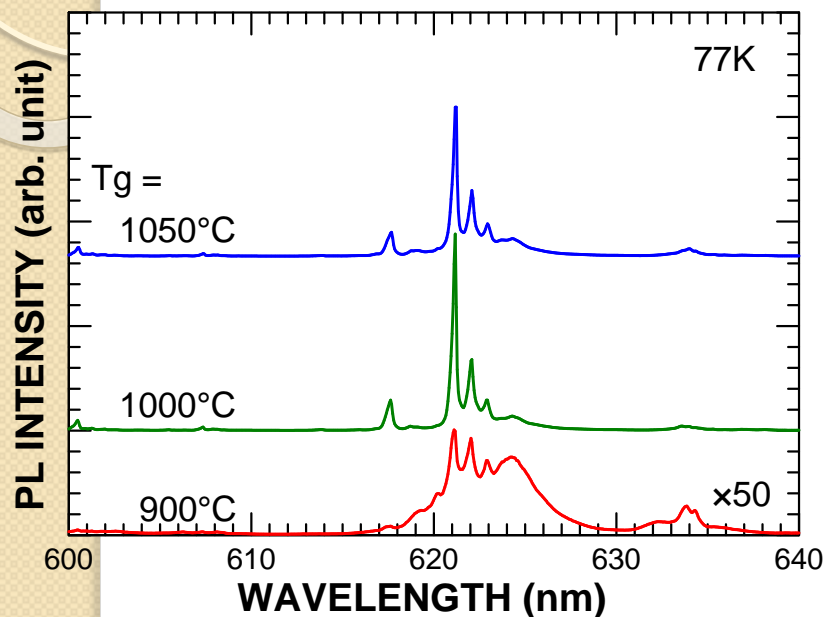


平成21年7月4日、朝日小学生新聞(1面)



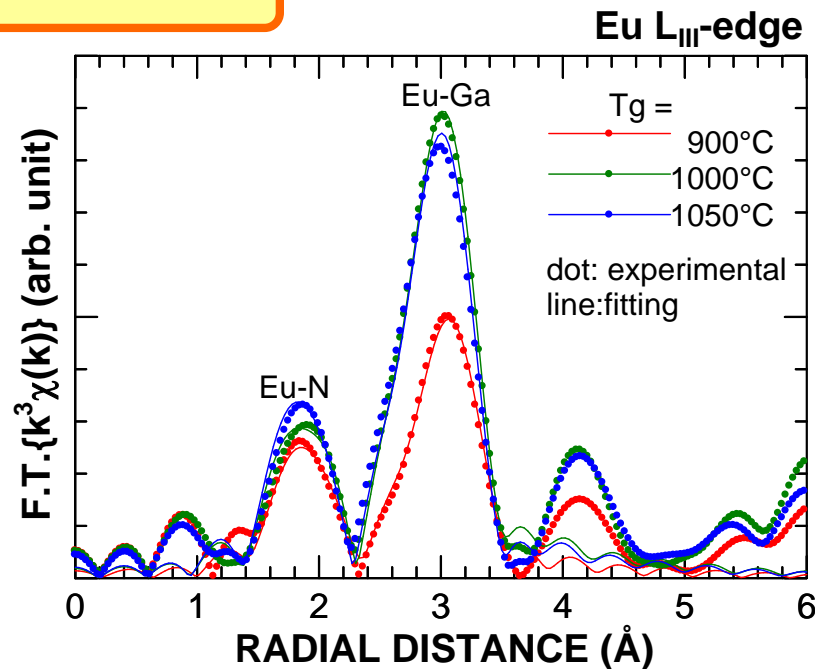
A. Nishikawa et al., Appl. Phys. Exp. **2**, 071004 (2009).

PLスペクトル



成長温度 1000°C で
発光強度が最大

動経分布

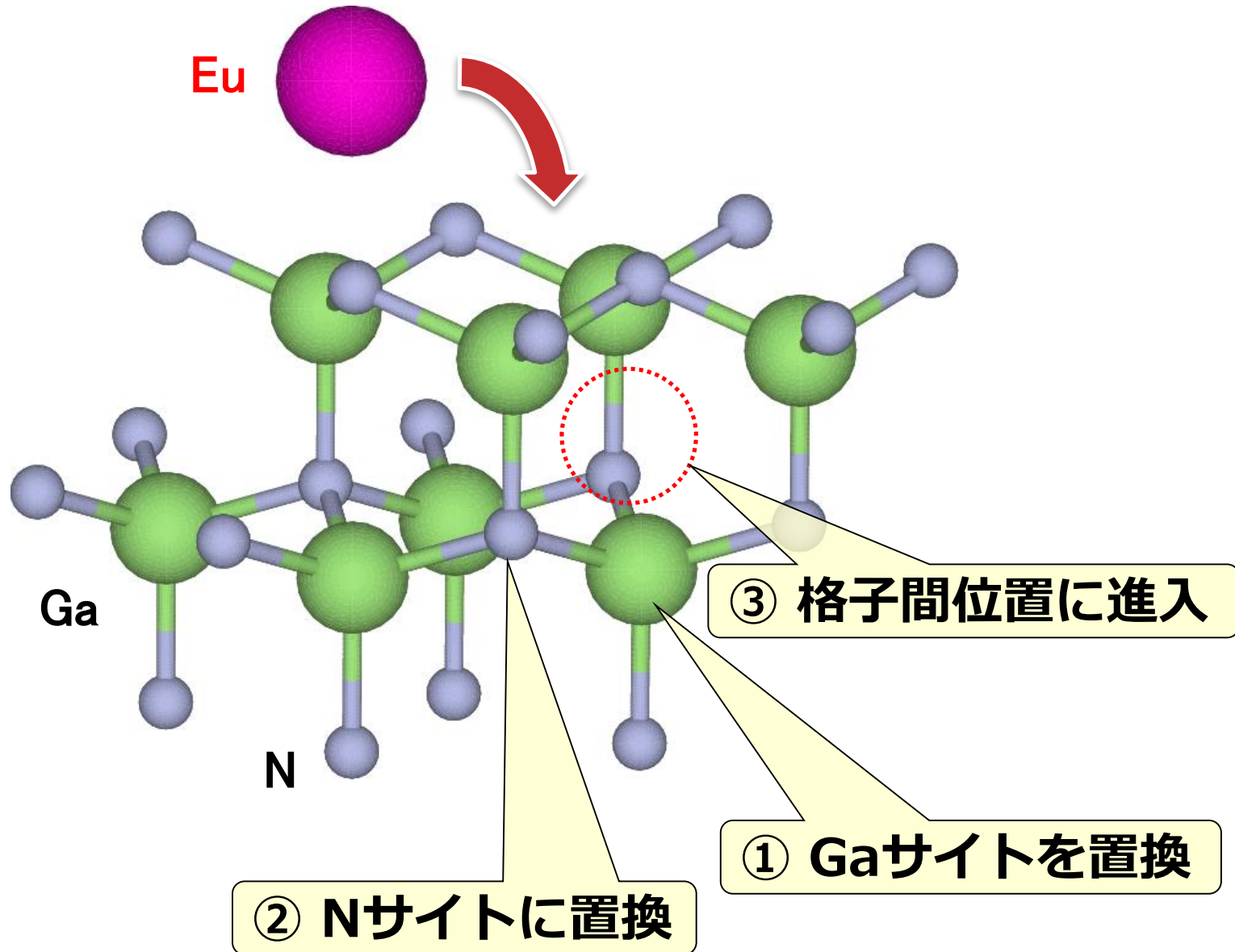


H. Ofuchi *et al.*, e-J. Surf. Sci. Nanotech. **9**, 51 (2011).

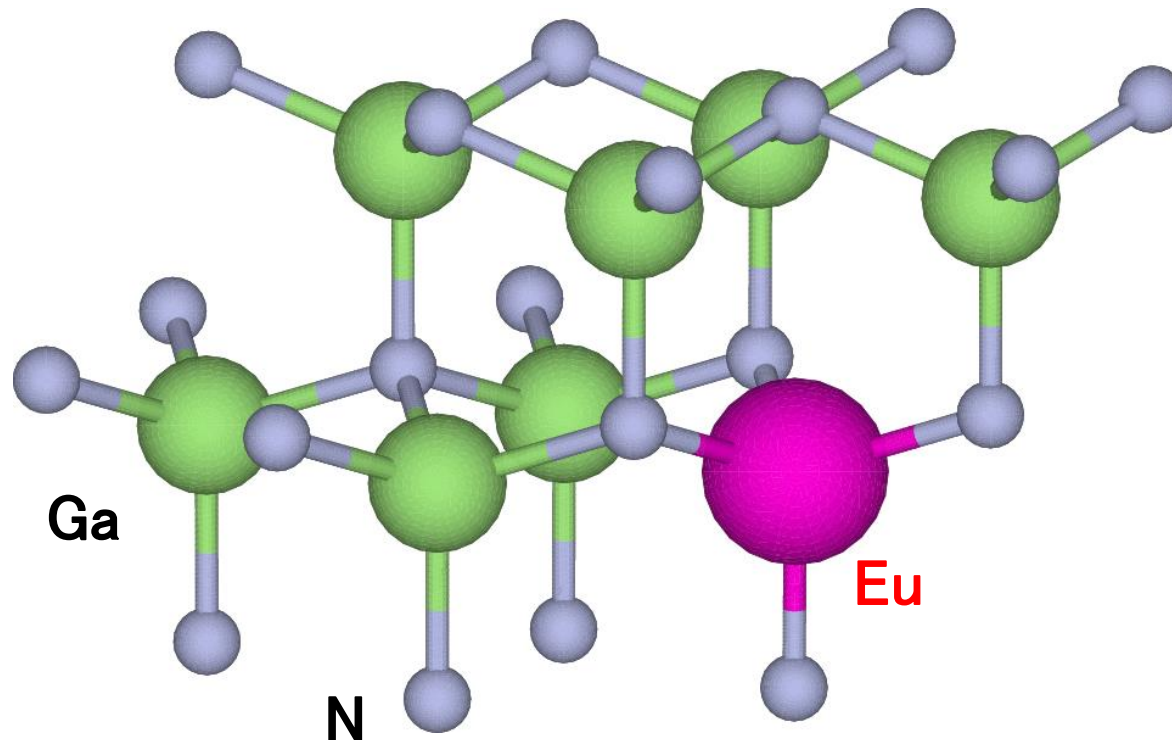
3 \AA 付近の第二近接
Gaに起因した
ピーク高さが変化

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 - **理論計算結果の比較**
 - **カーブフィッティング**
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仮定する構造モデル

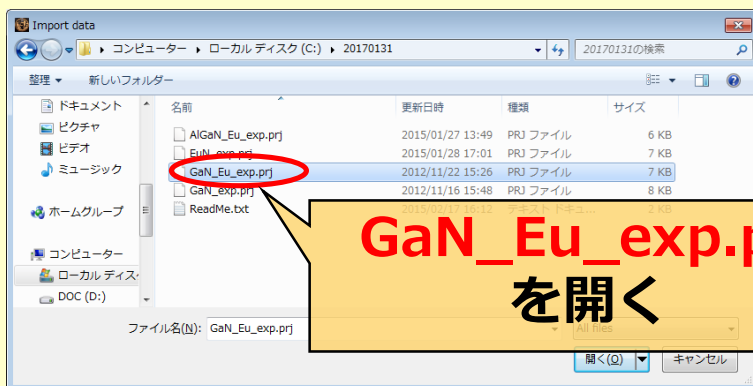
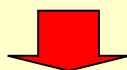
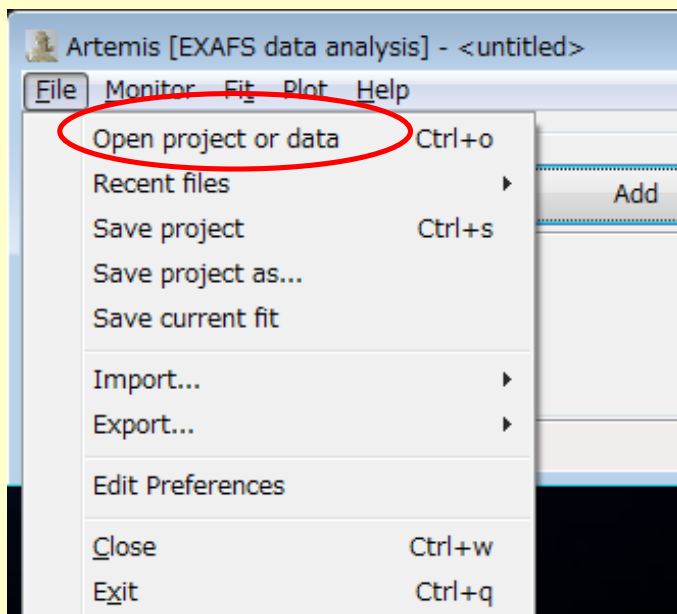


① Gaサイト置換型モデルの作成



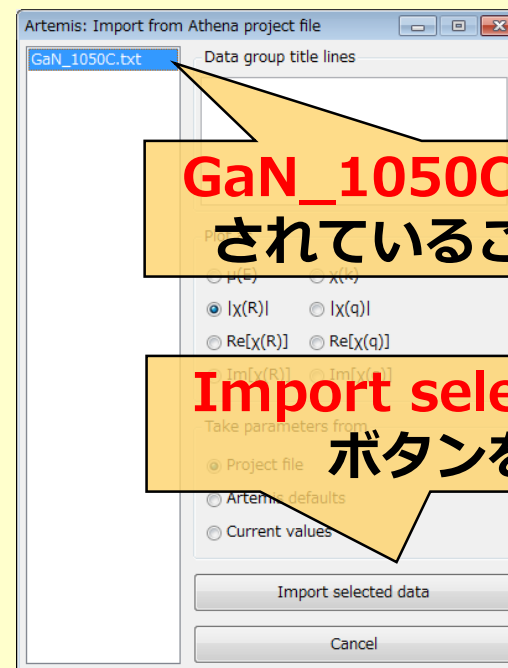
1. Athenaで解析したファイルを開く

- Ctrl-o または
- File - Open file(s)



GaN_Eu_exp.prj
を開く

2. データを選択



GaN_1050C.txtが選択
されていることを確認

Import selected data
ボタンを押す

実験データの確認

Artemis [Data] GaN_1050C.txt

Data Path Marks Actions Debug Help

GaN_1050C.txt CV 1 Path list

Data source
C:\20170131\GaN_Eu_exp.prj, 1

Plot this data set as
k123 R123 Rmr Rk kg

Title lines

Fourier transform parameters

kmin	3	kmax	10.5	dk	1
rmin	1.4	rmax	3.6	dr	0.0

Fitting k weights
 1 2 3 other

Other parameters
 Include in fit Plot after fit
 $\epsilon(k)$ 0 Plot with phase correction

Transferred data set "GaN_1050C.txt" to the plotting list.

Artemis [Plot]

k **R** **q**

k-weight
 0 1 2 3 kw

indic VP

Magnitude Real Imag

Plot $\chi(q)$
 Magnitude Real Imag

Plot fit Plot bkg
 Plot window Plot residual
 Plot running R-factor

kmin 0 kmax 15
rmin 0 rmax 6
qmin 0 qmax 15

Plotting list
 Data: GaN_1050C.txt

Freeze

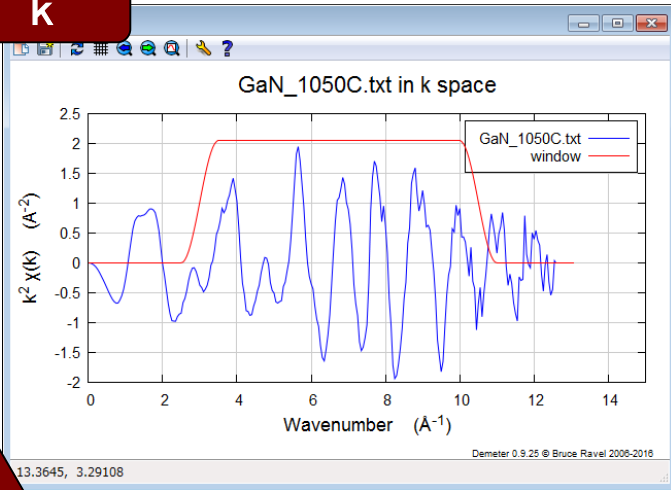
Save next plot to a file.

3を選択

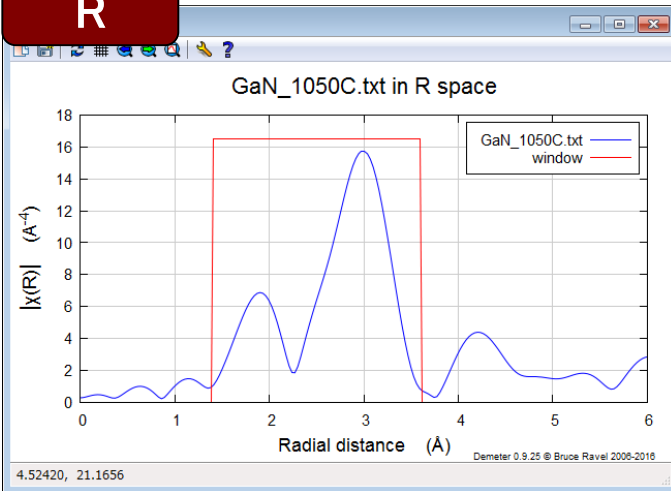
k-range: 3 - 10.5 \AA^{-1}

R-range: 1.4 - 3.6 \AA

k

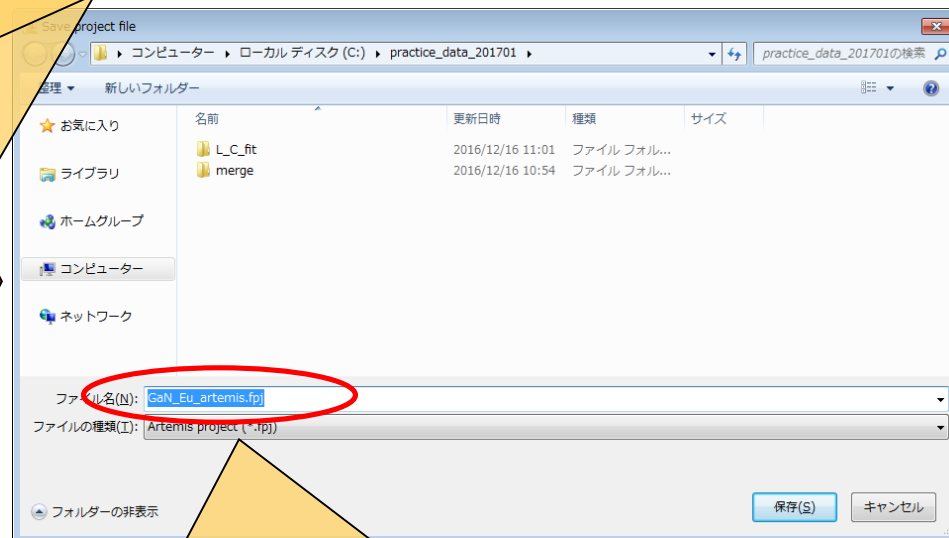
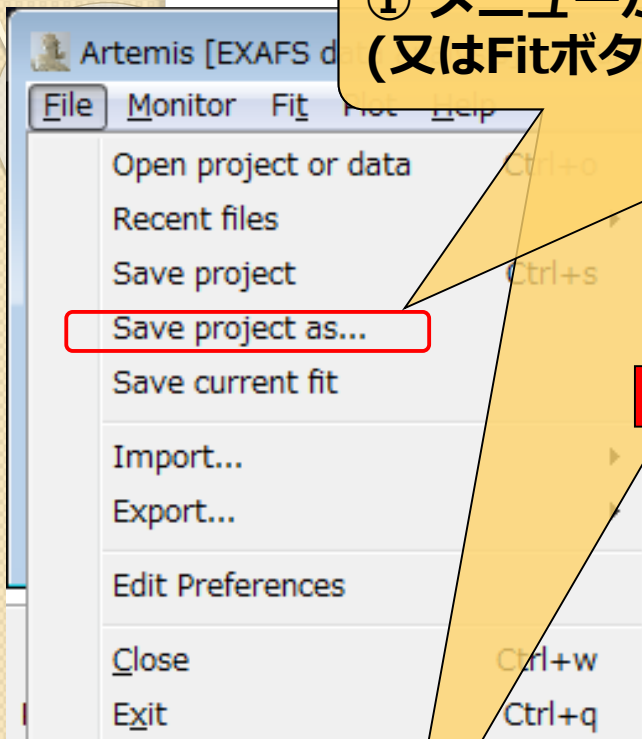


R

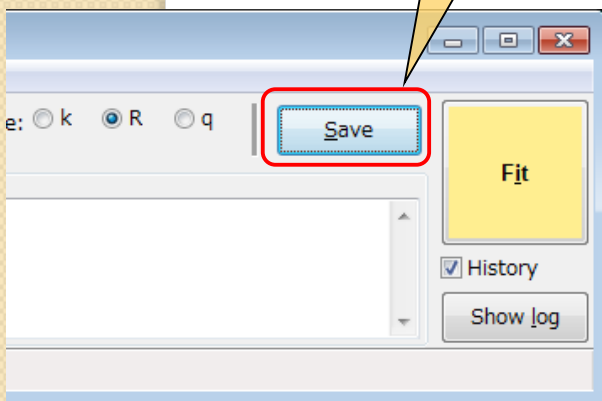


データの保存

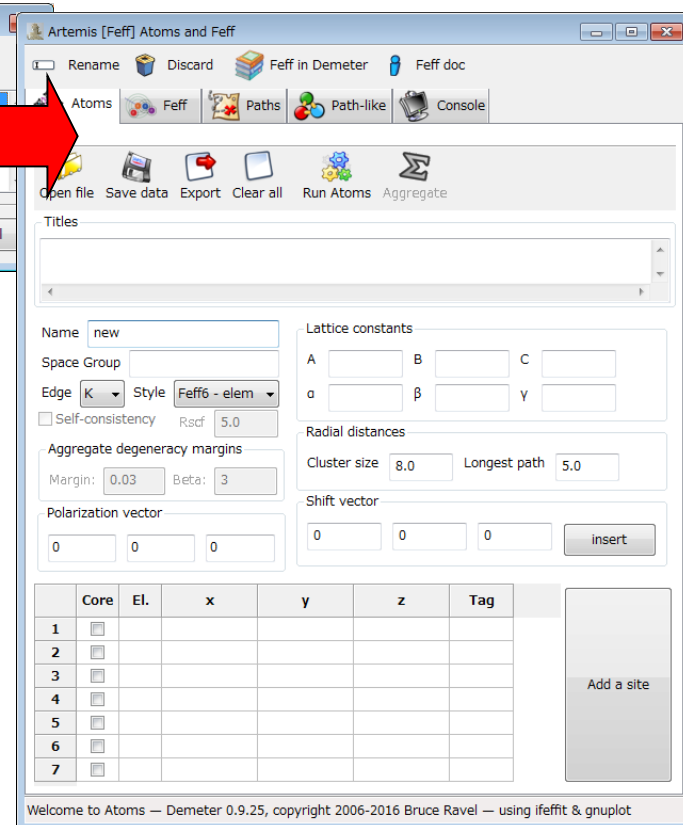
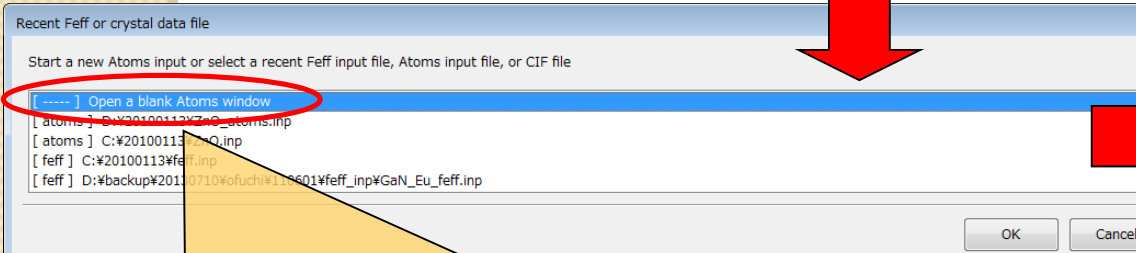
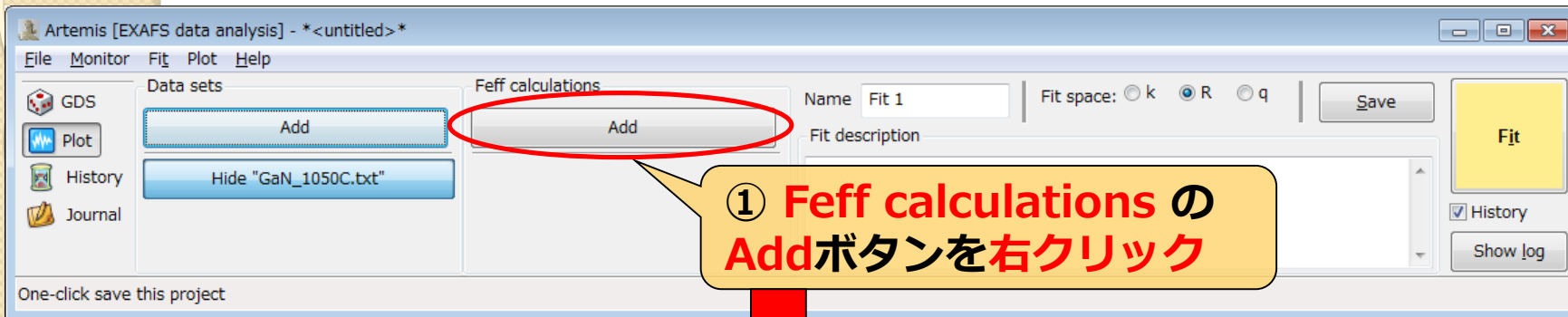
① メニューから **File – Save project as...** を選択
(又はFitボタン左の**Save**ボタンをクリック)



② ファイル名 **GaN_Eu_artemis.fpj** を
入力して保存
→ **この後は作業ごとに保存**



FEFFによる理論計算



結晶学データの入力 (Atoms)

Atoms: FEFF.inpを作成するプログラム

タイトル

① モデル名を入力
Ga-site

② 空間群を入力
P63mc (186)

③ Edgeを選択
K

⑤ 原子座標を入力
Ga: 0.33333, 0.66667, 0
N: 0.33333, 0.66667, 0.375

⑥ 中心原子を選択
Ga

④ 格子定数を入力
 $a = 3.186 \text{ \AA}$
 $b = 3.186 \text{ \AA}$
 $c = 5.176 \text{ \AA}$
 $\alpha = 90^\circ$
 $\beta = 90^\circ$
 $\gamma = 120^\circ$

クラスタの半径 (Å)

Shift vector:
原点の取り方によっては、修正することも

	Core	El.	x	y	z	Tag
1	<input checked="" type="checkbox"/>	Ga	0.33333	0.66667	0.00000	Ga1
2	<input type="checkbox"/>	N	0.33333	0.66667	0.37500	N1
3	<input type="checkbox"/>					
4	<input type="checkbox"/>					
5	<input type="checkbox"/>					
6	<input type="checkbox"/>					

各種ファイル (atoms.inp, feff.inp)、座標データファイル保存

① Feffウィンドウの**Atoms**タブを選択

② **Save data**アイコンをクリックし、**GaN_atoms.inp**で保存
→この後のモデル計算で使用

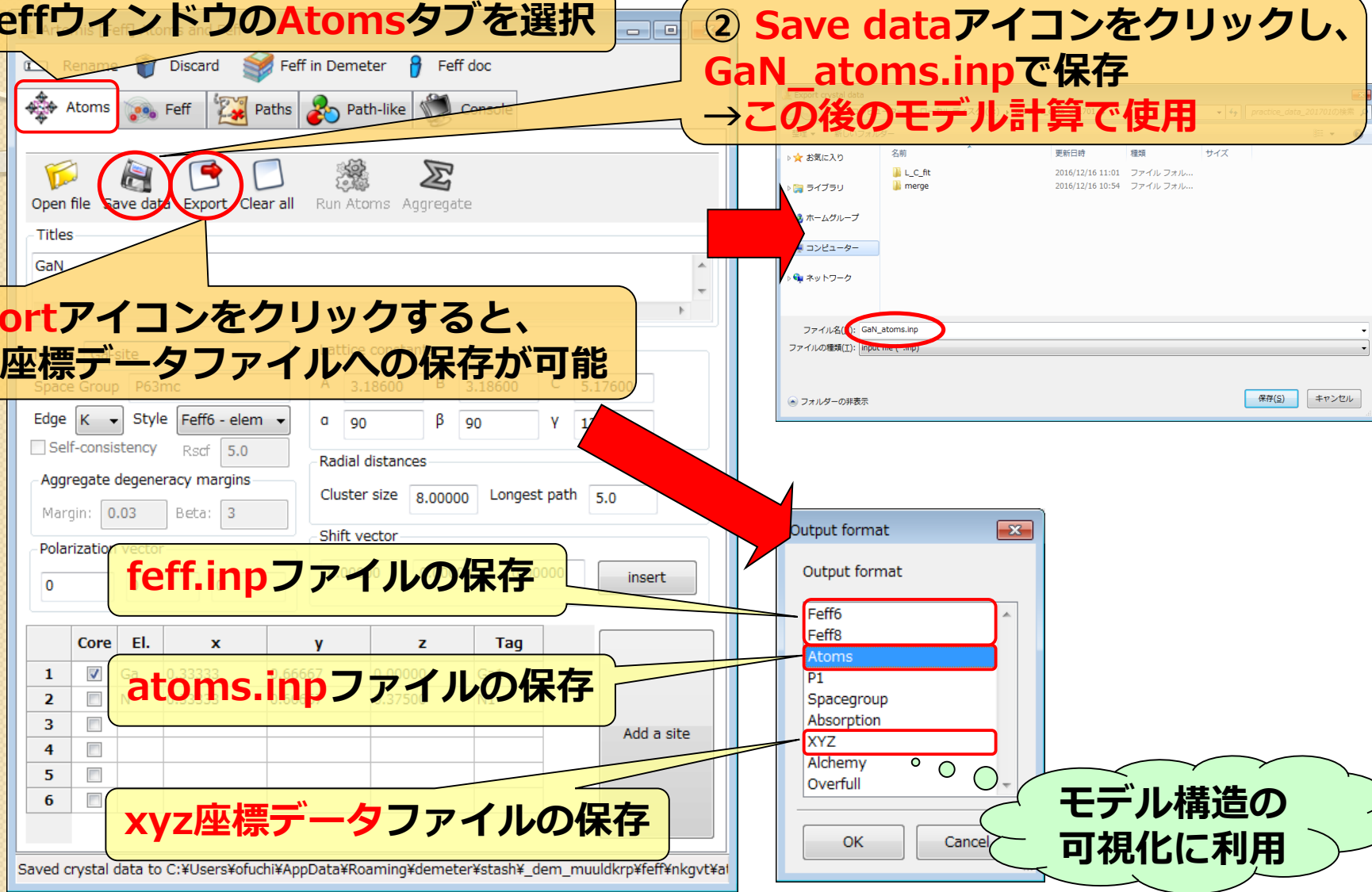
Exportアイコンをクリックすると、各種座標データファイルへの保存が可能

feff.inpファイルの保存

atoms.inpファイルの保存

xyz座標データファイルの保存

モデル構造の可視化に利用



Atoms計算 (Gaサイト置換型)

Artemis [Feff] Atoms and Feff

Rename Discard **Run Atoms をクリック**

Atoms Feff Paths Path-like Console

Open file Save data Export Clear all **Run Atoms** Aggregate

Titles
GaN

Name Ga-site
Space Group P63mc
Edge K Style Feff6 - elem
 Self-consistency Rscf 5.0

Aggregate degeneracy margins
Margin: 0.03 Beta: 3

Polarization vector
0 0 0

Lattice constants
A 3.18600 B 3.18600 C 5.17600
 α 90 β 90 γ 120

Radial distances
Cluster size 8.00000 Longest path 5.0

Shift vector
0.00000 0.00000 0.00000

	Core	El.	x	y	z	Tag
1	<input checked="" type="checkbox"/>	Ga	0.33333	0.66667	0.00000	Ga1
2	<input type="checkbox"/>	N	0.33333	0.66667	0.37500	N1
3	<input type="checkbox"/>					
4	<input type="checkbox"/>					
5	<input type="checkbox"/>					
6	<input type="checkbox"/>					

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: Ga-site Margin: 0.03 Beta: 3 nlegs: 4 6

Feff input file

```

* This feff6 file was generated by Demeter 0.9.25
* Demeter written by and copyright (c) Bruce Ravel, 2006-2016

* -----
* total mu*=1: 8.955 microns, unit edge step: 10.490 microns
* specific gravity: 6.111
* -----
* normalization correction: 0.00045 ang^2
* -----

TITLE GaN

HOLE      1  1.0  * FYI: (Ga K edge @ 10367 eV, second number is S0^2)
*          mphase,mpath,mfeff,mchi
CONTROL   1      1      1
PRINT     1      0      0

RMAX      5.0
*POLARIZATION 0.0  0.0  0.0

POTENTIALS
* ipot  Z      tag
  0     31     Ga
  1     31     Ga
  2      7      N

ATOMS      * this list contains 193 atoms
*  x      y      z      ipot tag      distance
  0.00000  0.00000  0.00000  0     Ga1      0.00000
  0.00000  0.00000  1.94100  2     N1.1     1.94100
  1.83942  0.00003  -0.64700  2     N1.2     1.94989
 -0.91974  -1.59297  -0.64700  2     N1.2     1.94989
 -0.91974  1.59303  -0.64700  2     N1.2     1.94994
  1.83942  0.00003  2.58800  1     Ga1.1     3.17509
 -0.91974  -1.59297  2.58800  1     Ga1.1     3.17509
  1.83942  0.00003  -2.58800  1     Ga1.1     3.17509
    
```

feff.inpの編集(Gaサイト置換型) SPRing 8

TITLE GaN

```
HOLE 1 1 0 * FYI: (Ga K edge @ 10367 eV, second number is  
* mphase,mpath,mfeff,mchi  
CONTROL 1 1 1 1  
PRINT 1 0 0 0  
RMAX 5.0  
*POLARIZATION 0.0 0.0 0.0
```

POTENTIALS

```
* ipot Z tag  
0 31 Ga  
1 31 Ga  
2 7 N
```

ATOMS * this list contains 183 atoms

```
* x y z ipot tag  
0.00000 0.00000 0.00000 0 Ga1
```

① HOLEを1(K-edge)から4(L₃-edge)に変更

TITLE GaN

```
HOLE 4 1.0 * FYI: (Ga K edge @ 10367 eV, second number is  
S0^2)  
* mphase,mpath,mfeff,mchi  
CONTROL 1 1 1 1  
PRINT 1 0 0 0  
RMAX 5.0  
*POLARIZATION 0.0 0.0 0.0
```

② 中心原子(ipot 0)をGa(Z=31)からEu(Z=63)に変更

POTENTIALS

```
* ipot Z tag  
0 63 Eu  
1 31 Ga  
2 7 N
```

③ 中心原子のtagをGa1からEu1に変更

ATOMS * this list contains 183 atoms

```
* x y z ipot tag distance  
0.00000 0.00000 0.00000 0 Eu1 0.00000
```

FEFF計算(Gaサイト置換型)

Artemis [Feff] Atoms and Feff

② Run Feffをクリック

Run Feff

Name: N-site Margin: 0.03 Beta: 3 nlegs: 4 6

Feff input file

```
* This feff6 file was generated by Demeter 0.9.25
* Demeter written by and copyright (c) Bruce Ravel, 2006-2016

* -----
* total mu*x=1: 0.153 microns, unit edge step: -1.872 microns
* specific gravity: 6.111
* -----
* normalization correction: 0.00520 ang^2
* -----

TITLE GaN

HOLE 4 1.0 * FYI: (N K edge @ 409.9 eV, second number is S0^2)
* mphase,mpath,mfeff,mchi
CONTROL 1 1 1 1
PRINT 1 0 0 0

RMAX 5.0
*POLARIZATION 0.0 0.0 0.0

POTENTIALS
* ipot Z tag
0 63 Eu
1 31 Ga
2 7 N

ATOMS * this list contains 183 atoms
* x y z ipot tag distance
0.00000 0.00000 0.00000 0 Eu1 0.00000
0.00000 0.00000 -1.94100 1 Ga1.1 1.94100
0.91974 1.59297 0.64700 1 Ga1.2 1.94989
-1.83942 -0.00003 0.64700 1 Ga1.2 1.94989
0.91974 -1.59303 0.64700 1 Ga1.2 1.94989
0.91974 1.59297 2.58900 2 N1.1 3.17503
-1.83942 -0.00003 2.58900 2 N1.1 3.17503
0.91974 1.59297 0.64700 1 Ga1.1 1.94100
```

Artemis [Feff] Atoms and Feff

Name of this Feff calculation: Ga-site

Description

```
## TITLE GaN
## This paths.dat file was written by Demeter 0.9.25
## The central atom is denoted by this token: @
## Cluster size = 5.00 A, containing 182 atoms
## 24 paths were found within 5.000 A
## Forward scattering cutoff 20.00
## Distance fuzz = 0.030 A
```

Scattering Paths

	Degen	Reff	Scattering path	Rank	L	Type
1	4.00	1.948	@ N1.1 @	100.00	2	single scattering
2	12.00	3.181	@ Ga1.1 @	100.00	2	single scattering
3	1.00	3.235	@ N1.3 @	7.11	2	single scattering
4	12.00	3.538	@ N1.1 N1.2 @	18.06	3	other double scatter in
5	24.00	3.538	@ N1.1 Ga1.1 @	18.65	3	other double scatter in
6	9.00	3.732	@ N1.4 @	43.14	2	single scattering
7	4.00	3.895	@ N1.1 @ N1.1 @	9.77	4	rattle
8	12.00	3.895	@ N1.1 @ N1.2 @	10.65	4	hinge
9	12.00	3.895	@ N1.1 Ga1.1 N1.1 @	4.27	4	dog-leg
13	36.00	4.431	@ N1.2 Ga1.1 @	9.52	3	other double scatter in
14	36.00	4.431	@ N1.2 N1.4 @	12.69	3	other double scatter in
15	36.00	4.431	@ Ga1.1 N1.4 @	9.69	3	other double scatter in
16	6.00	4.498	@ Ga1.3 @	20.47	2	single scattering
19	6.00	4.540	@ N1.6 @	16.18	2	single scattering
20	48.00	4.771	@ Ga1.1 Ga1.1 @	3.70	3	acute triangle
22	12.00	4.833	@ N1.2 N1.6 @	6.54	3	obtuse triangle
24	9.00	4.902	@ N1.7 @	19.15	2	single scattering

① 変更箇所の確認

- HOLE : 1(K-edge) → 4(L₃-edge)
- 中心原子(ipot 0) : Ga(Z=31) → Eu(Z=63)
- 中心原子のtag : Ga1 → Eu1

実験値と理論計算(Gaサイト置換型)の比較

Uegen	Reff	scattering path	Rank	L Type
1	4.00	1.948 @ N1.1 @	100.00	2 single scattering
2	12.00	3.181 @ Ga1.1 @	100.00	2 single scattering
3	1.00	3.235 @ N1.3 @	7.11	2 single scattering
4	12.00	3.938 @ N1.1 N1.2 @	18.06	3 other double scattering
5	24.00	3.938 @ N1.1 Ga1.1 @	18.65	3 other double scattering
6	9.00	3.732 @ N1.4 @	43.14	2 single scattering

① Ctrlキーを押しながら Path1-2,4-6を選択し、Dataウィンドウにドラッグ&ドロップ (Path3は寄与が低い)

Artemis [Data] GaN_1050C.txt

Data Path Marks Actions Debug Help

GaN_1050C.txt CV 1

Data source: C:\practice_data_201701\GaN_Eu_exp.prj, 1

Plot this data set as: k123, R123, Emr

Fourier transform parameters: kmin 3, kmax 10.5, dk 1, rmin 1.4, rmax 3.6, dr 0.0

② 各Pathのアイコンをクリック

③ Rをクリック

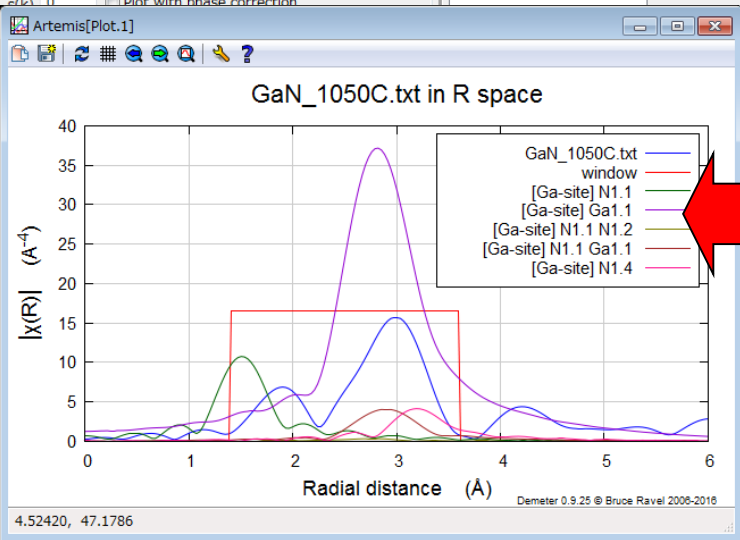
Artemis [Plot.1]

GaN_1050C.txt in R space

Plot x(q): Magnitude, Real, Imag.

Plot x(R): Magnitude, Real, Imag.

Plotting list: Data: GaN_1050C.txt, Path: [Ga-site] N1.1 from GaN_1050C.txt, Path: [Ga-site] Ga1.1 from GaN_1050C.txt, Path: [Ga-site] N1.1 N1.2 from GaN_1050C.txt, Path: [Ga-site] N1.1 Ga1.1 from GaN_1050C.txt, Path: [Ga-site] N1.4 from GaN_1050C.txt



Pathの足し合わせ(Gaサイト置換型)

① すべてのPathをチェック

**② Dataウィンドウのメニューから
Action
- Make sum of marked paths and plot in R
を選択**

③ VPath名にGa-siteと入力

④ DataとVPath以外のチェックを外す

⑤ Rをクリック

⑥ 選択したPathの足し合わせを表示

Artemis [Data] GaN_1050C.txt
Data Path Marks Actions Debug Help

CV 1

Path name: Ga-site

Artemis [Plot]

[Ga-site]

k R q

Plotting list

- Data: GaN_1050C.txt
- Path: [Ga-site] N1.1 from GaN_1050C.txt
- Path: [Ga-site] Ga1.1 from GaN_1050C.txt
- Path: [Ga-site] N1.1 N1.2 from GaN_1050C.txt
- Path: [Ga-site] N1.1 Ga1.1 from GaN_1050C.txt
- Path: [Ga-site] N1.4 from GaN_1050C.txt
- VPath: Ga-site

Freeze Clear

Save next plot to a file.

Artemis[Plot.1]

GaN_1050C.txt in R space

Y-axis: $|X(R)|$ (\AA^{-4})

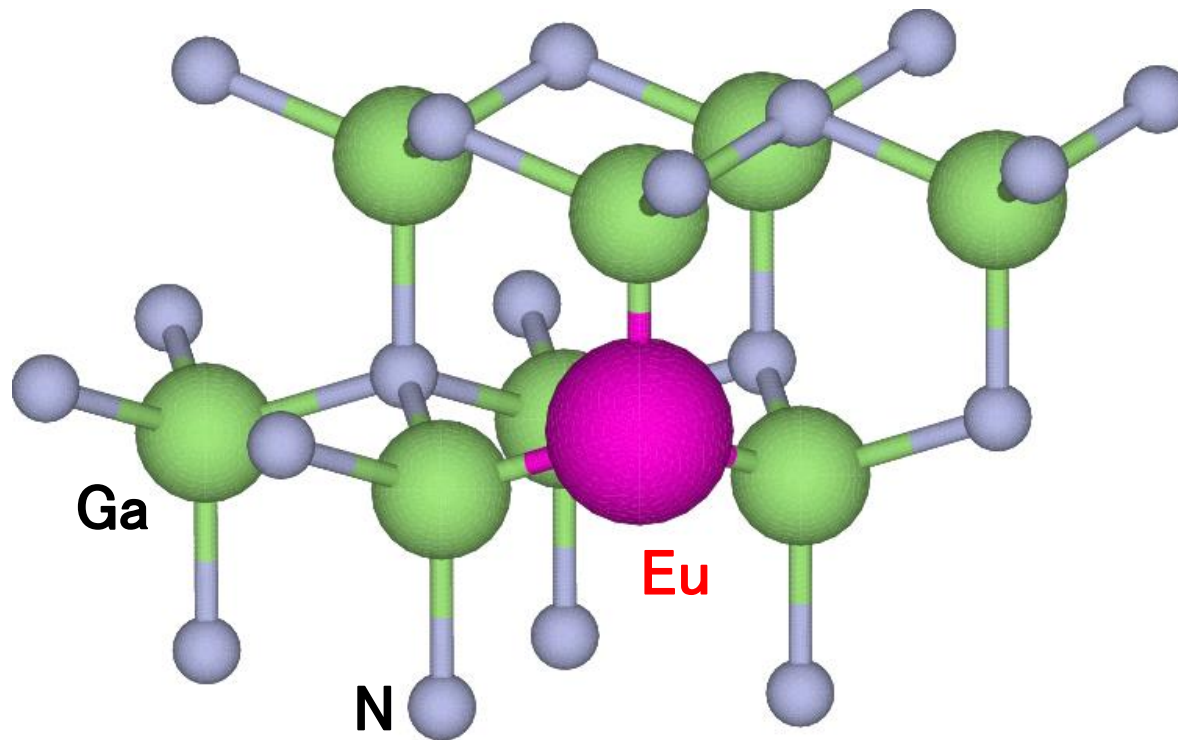
X-axis: Radial distance (\AA)

Legend: GaN_1050C.txt (blue), window (red), Ga-site (green)

1.76834, 23.2809

Demeter 0.9.25 © Bruce Ravel 2006-2016

② Nサイト置換型モデルの作成



feff.inpの作成(Nサイト置換型)

① Feff calculationsのAddボタンをクリック

② 先程保存したGaN_atoms.inpファイルを開く

③ モデル名を入力N-site

④ Nにcoreのチェックを入れる

⑤ Run Atomsをクリック

	Core	El.	x	y	z	Tag
1	<input type="checkbox"/>	Ga	0.33333	0.66667	0.00000	Ga1
2	<input checked="" type="checkbox"/>	N	0.33333	0.66667	0.37500	N1
3	<input type="checkbox"/>					
4	<input type="checkbox"/>					
5	<input type="checkbox"/>					
6	<input type="checkbox"/>					

FEFF計算(Nサイト置換型)

Artemis [Feff] Atoms and Feff

② Run Feffをクリック

Run Feff

Name: Ga-site Margin: 0.03 Beta: 3 nlegs: 4 6

Feff input file

```

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* -----
* total mu*x=1: 8.955 microns, unit edge step: 10.490 microns
* specific gravity: 6.111
* -----
* normalization correction: 0.00045 ang^2
* -----

TITLE GaN

HOLE      4 1.0 * FYI: (Ga K edge @ 10367 eV, second number is S0^2)
* mphase,mpath,mfeff,mchi
CONTROL   1 1 1 1
PRINT     1 0 0 0

RMAX      5.0
*POLARIZATION 0.0 0.0 0.0

POTENTIALS
* ipot  Z      tag
  0     63     Eu1
  1     31     Ga
  2     7      N

ATOMS      * this list contains 188 atoms
* x      y      z      ipot tag      distance
0.00000  0.00000  0.00000  0     Eu1      0.00000
0.00000  0.00000  1.94100  2     N1.1     1.94100
1.83942  0.00003  -0.64700  2     N1.1     1.94989
-0.91974 -1.59297  -0.64700  2     N1.2     1.94989
-0.91974  1.59303  -0.64700  2     N1.2     1.94989
1.83942  0.00003  2.58800  1     Ga1.1     3.17503
-0.91974 -1.59297  2.58800  1     Ga1.1     3.17503
1.83942  0.00003  0.00000  1     Ga1.1     3.17503
    
```

① 変更箇所の確認

- HOLE : 1(K-edge) → **4(L₃-edge)**
- 中心原子(ipot 0) : N(Z=7) → **Eu(Z=63)**
- 中心原子のtag : N1 → **Eu1**

Artemis [Feff] Atoms and Feff

Name of this Feff calculation: N-site

Description

```

# TITLE GaN
# This paths.dat file was written by Demeter 0.9.25
# The central atom is denoted by this token: @
# Cluster size = 5.00 A, containing 182 atoms
# 24 paths were found within 5.000 A
# Forward scattering cutoff 20.00
# Distance fuzz = 0.030 A
    
```

Scattering Paths

	Degen	Reff	Scattering path	Rank	L	Type
1	4.00	1.948	@ Ga1.1 @	100.00	2	single scattering
2	12.00	3.181	@ N1.1 @	76.89	2	single scattering
3	1.00	3.235	@ Ga1.3 @	7.12	2	single scattering
4	12.00	3.538	@ Ga1.1 Ga1.2 @	7.15	3	other double scatter in
5	24.00	3.538	@ Ga1.1 N1.1 @	13.86	3	other double scatter in
6	9.00	3.732	@ Ga1.4 @	44.81	2	single scattering
7	4.00	3.895	@ Ga1.1 @ Ga1.1 @	4.62	4	rattle
8	12.00	3.895	@ Ga1.1 @ Ga1.2 @	5.72	4	hinge
13	36.00	4.431	@ Ga1.2 N1.1 @	9.81	3	other double scatter in
14	36.00	4.431	@ Ga1.2 Ga1.4 @	3.55	3	other double scatter in
15	36.00	4.431	@ N1.1 Ga1.4 @	6.31	3	other double scatter in
16	6.00	4.498	@ N1.3 @	14.35	2	single scattering
19	6.00	4.540	@ Ga1.6 @	17.68	2	single scattering
20	48.00	4.771	@ N1.1 N1.1 @	5.91	3	acute triangle
23	12.00	4.833	@ N1.1 Ga1.6 @	4.22	3	obtuse triangle
24	9.00	4.902	@ Ga1.7 @	21.36	2	single scattering

実験値と理論計算(Nサイト置換型)の比較

Artemis [Feff] Atoms and Feff

Atoms Feff Paths Path-like Console

Name of this Feff calculation: N-site

Description

```

TITLE GaN
This paths.dat file was written by Demeter 0.9.25
The central atom is denoted by this token: @
Cluster size = 5.00 Å, containing 182 atoms
24 paths were found within 5.000 Å
Forward scattering cutoff 20.00
Distance fuzz = 0.030 Å
    
```

Scattering Paths

Order	Qmag	Qerr	Scattering path	Rank	L Type
1	4.00	1.348	@ Ga1.1 @	100.00	2 single scattering
2	12.00	3.181	@ N1.1 @	78.89	2 single scattering
3	1.00	3.235	@ Ga1.3 @	7.12	2 single scattering
4	12.00	3.538	@ Ga1.1 Ga1.2 @	7.15	2 other double scattering
5	24.00	3.538	@ Ga1.1 N1.1 @	13.86	2 other double scattering
6	9.00	3.732	@ Ga1.4 @	44.91	2 single scattering
7	4.00	3.895	@ Ga1.1 @ Ga1.1 @	4.62	2 rattle
8	12.00	3.895	@ Ga1.1 @ Ga1.2 @	5.72	2 hinge
13	36.00	4.431	@ @ @ 1 @	9.81	2 other double scattering
14	36.00	4.431	@ Ga1.2 @ Ga1.4 @	3.55	2 other double scattering
15	36.00	4.431	@ N1.1 @ Ga1.1 @	6.31	2 other double scattering
16	4.00	4.438	@ N1.3 @	14.36	2 single scattering
19	6.00	4.540	@ Ga1.5 @	17.68	2 single scattering

① Ctrlキーを押しながら Path1-2,6を選択し、Dataウィンドウにドロップ (Path3-5は寄与が低い)

Artemis [Data] GaN_1050C.txt

Data Path Marks Actions Debug Help

GaN_1050C.txt CV 1

Data source

C:\practice_data_201701\GaN_Eu_exp.prj, 1

Plot this data set as

k123 R123 Rmr Rk

Title lines

Other transform parameters

kmin 3 kmax 10.5 dk 1

rmin 1.4 rmax 3.6 dr 0.0

Fitting k weights

1 2 3 other 0.5

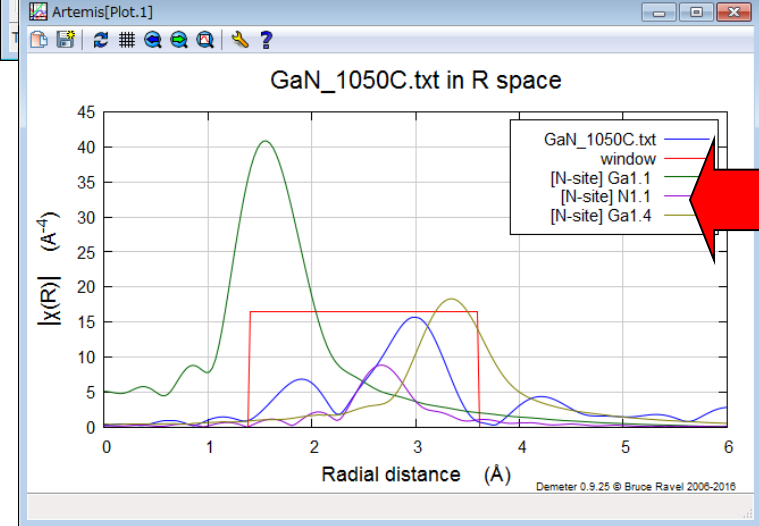
Other parameters

Include in fit Plot after fit Fit background

② [N-site]のアイコンをクリック

④ Rをクリック

③ DataとPath:[N-site]以外のチェックを外す



Plotting list

- Data: GaN_1050C.txt
- Path: [Ga-site] N1.1 from GaN_1050C.txt
- Path: [Ga-site] Ga1.1 from GaN_1050C.txt
- Path: [Ga-site] N1.1 N1.2 from GaN_1050C.txt
- Path: [Ga-site] N1.1 Ga1.1 from GaN_1050C.txt
- Path: [Ga-site] N1.4 from GaN_1050C.txt
- VPath: Ga-site
- Path: [N-site] Ga1.1 from GaN_1050C.txt
- Path: [N-site] N1.1 from GaN_1050C.txt
- Path: [N-site] Ga1.4 from GaN_1050C.txt

Freeze Clear

Save next plot to a file.

Pathの足し合わせ(Nサイト置換型)

① [N-site]をすべてチェック

② Dataウィンドウのメニューから Action - Make sum of marked paths and plot in R を選択

③ VPath名に N-siteと入力

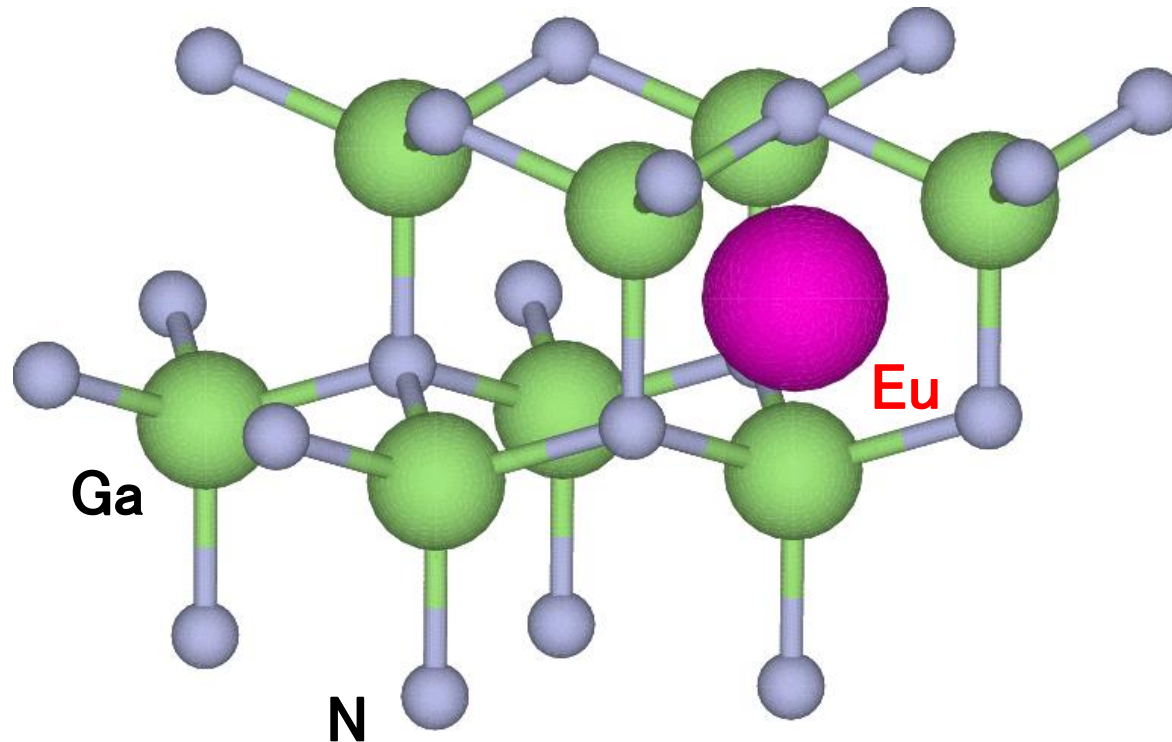
④ DataとVPath:N-site以外のチェックを外す

⑤ Rをクリック

⑥ 選択したPathの足し合わせを表示

The plot shows $|X(R)|$ vs Radial distance (Å) for GaN_1050C.txt in R space. The plot includes three data series: GaN_1050C.txt (blue line), window (red line), and N-site (green line). The x-axis ranges from 0 to 6 Å, and the y-axis ranges from 0 to 45. A red box highlights the region between approximately 1.5 Å and 3.5 Å on the x-axis.

③ 進入型モデルの作成



feff.inpの作成(進入型)

① Feff calculationsのAddボタンをクリック

② 先程保存したGaN_atoms.inpファイルを開く

③ モデル名を入力interstitial

④ Gaにcoreのチェックを入れる

⑤ Run Atomsをクリック

Core	El.	x	y	z	Tag
<input checked="" type="checkbox"/>	Ga	0.33333	0.66667	0.00000	Ga1
<input type="checkbox"/>	N	0.33333	0.66667	0.37500	N1
<input type="checkbox"/>					
<input type="checkbox"/>					
<input type="checkbox"/>					
<input type="checkbox"/>					

feff.inpの編集(進入型)

```
HOLE 4 1.0
```

① HOLEを1(K-edge)から4(L3-edge)に変更

```
* mphase, mpaen, mfeff, mona
```

```
CONTROL 1 1 1 1
```

```
PRINT 1 0 0 0
```

```
RMAX 5.0
```

```
*POLARIZATION 0.0 0.0 0.0
```

② 中心原子(ipot 0)をGa(Z=31)からEu(Z=63)に変更

```
POTENTIALS
```

```
* ipot Z tag
```

```
0 63 Eu
```

```
1 31 Ga
```

```
2 7 N
```

③ 原点のipot 0を
散乱原子Gaのipot 1に変更

```
ATOMS * this list contains 183 atoms
```

```
* x y z ipot tag distance
```

```
0.00000 0.00000 0.00000 1 Ga1 0.00000
```

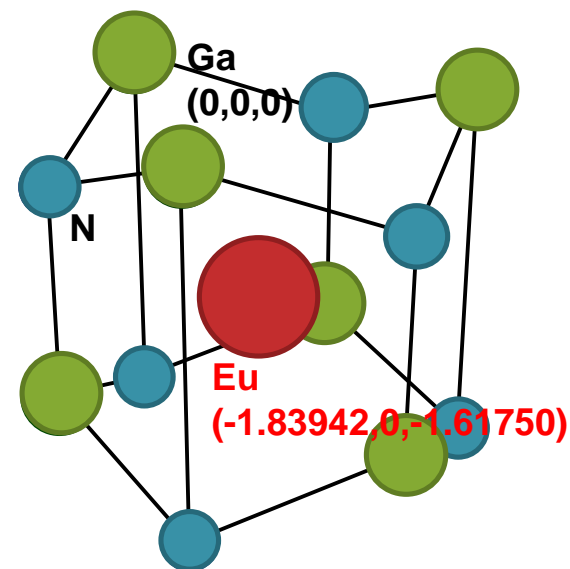
```
-1.83942 0.00000 -1.61750 0 Eu1 0.00000
```

```
0.00000 0.00000 1.94100 2 N1.1 1.94100
```

```
1.83942 0.00003 -0.64700 2 N1.2 1.94989
```

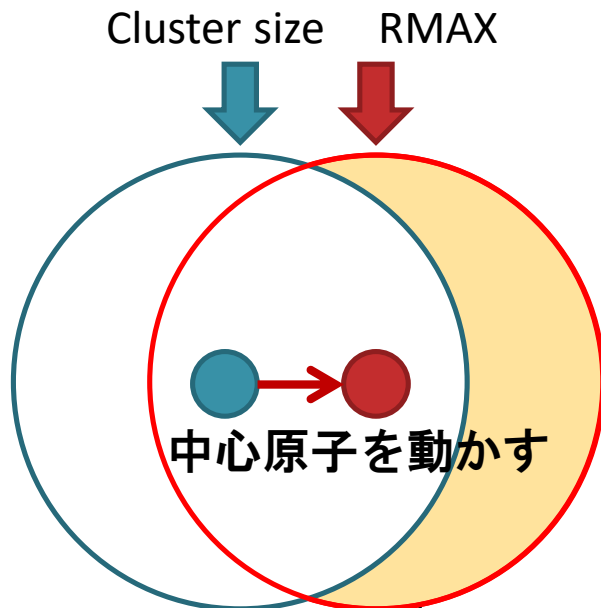
④ 進入原子Euの座標を追加

(-1.83942 0.00000 -1.61750 0 Eu1)



中心原子の座標変更時の注意点

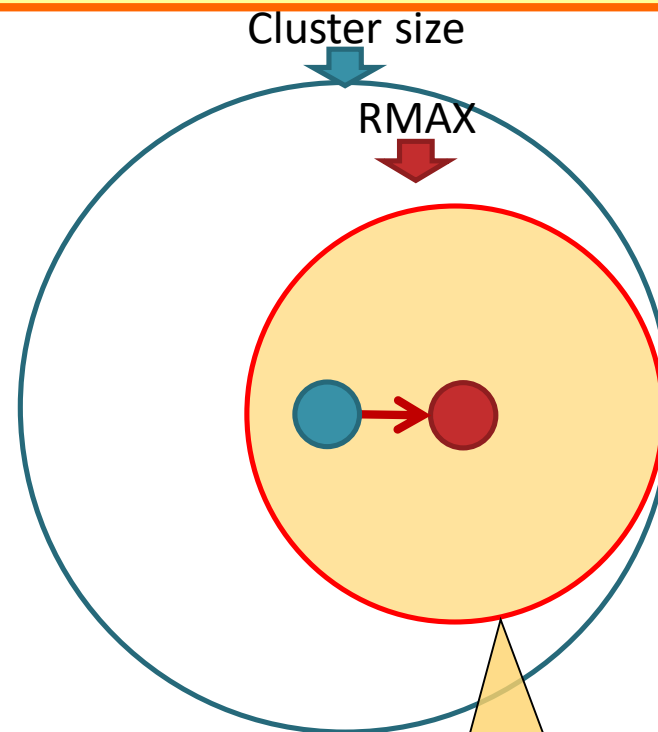
Cluster size = RMAXの場合



この領域の原子座標が feff.inp にない

RMAX内にあるべき一部の原子を含まずに計算

Cluster size > RMAXの場合



Cluster size内にある原子を含む

FEFF計算(進入型)

Artemis [Feff] Atoms and Feff

② Run Feffをクリック

Run Feff

Name: interstitial Margin: 0.03 Beta: 3 nlegs: 4 6

Feff input file

```
* This feff6 file was generated by Demeter 0.9.25
* Demeter written by and copyright (c) Bruce Ravel, 2006-2018

* -----
* total mu*x=1: 8.955 microns, unit edge step: 10.490 microns
* specific gravity: 6.111
* -----
* normalization correction: 0.00045 ang^2
* -----

TITLE GaN
HOLE 4 1.0 * FYI: (Ga K edge @ 10387 eV, second number is S0^2)
* mphase,mpath,mfeff,mchi
CONTROL 1 1 1 1
PRINT 1 0 0 0
RMAX 5.0
*POLARIZATION 0.0 0.0 0.0

POTENTIALS
* ipot Z tag
0 63 Eu
1 31 Ga
2 7 N

ATOMS * this list contains 183 atoms
* x y z ipot tag distance
0.00000 0.00000 0.00000 1 Ga1 0.00000
-1.83942 0.00000 -1.61750 0 Eu1 0.00000
0.00000 0.00000 1.34100 2 N1.1 1.34100
1.83942 0.00003 -0.64700 2 N1.2 1.94989
-0.31974 -1.59297 -0.64700 2 N1.2 1.94989
-0.31974 1.59303 -0.64700 2 N1.2 1.94989
1.83942 0.00000 0.00000 2 N1.1 1.34100
-0.91974 0.00000 0.00000 2 N1.2 1.94989
```

Artemis [Feff] Atoms and Feff

Name of this Feff calculation: interstitial

Description

```
# TITLE GaN
# This paths.dat file was written by Demeter 0.9.25
# The central atom is denoted by this token: @
# Cluster size = 5.00 A, containing 183 atoms
# 70 paths were found within 5.000 A
# Forward scattering cutoff 20.00
# Distance fuzz = 0.030 A
```

Scattering Paths

Degen	Reff	Scattering path	Rank	L	Type
1	3.00	2.080 @ N1.2 @	100.00	2	single scattering
2	3.00	2.080 @ Ga1.1 @	100.00	2	single scattering
3	3.00	2.449 @ Ga1 @	65.94	2	single scattering
4	3.00	2.449 @ N1.3 @	62.02	2	single scattering
6	24.00	3.240 @ Ga1 N1.2 @	11.19	3	other double scatter
7	6.00	3.673 @ N1.2 N1.2 @	11.83	3	other double scatter
8	6.00	3.673 @ Ga1.1 Ga1.1 @	3.89	3	other double scatter
9	3.00	3.805 @ N1.2 @	19.41	2	single scattering
10	3.00	3.805 @ Ga1.1 @	22.62	2	single scattering
11	12.00	3.852 @ Ga1 Ga1.1 @	5.46	3	other double scatter
12	12.00	3.852 @ N1.2 N1.3 @	16.65	3	other double scatter
13	12.00	3.945 @ N1.2 Ga1.1 @	8.00	3	obtuse triangle
14	6.00	4.012 @ N1.1 @	33.30	2	single scattering
15	6.00	4.012 @ Ga1.4 @	39.38	2	single scattering
18	12.00	4.024 @ N1.2 Ga1.2 @	94.75	3	non-forward linear
20	6.00	4.030 @ Ga1.1 N1.6 Ga1.1 @	3.03	4	dog-leg
21	3.00	4.030 @ N1.2 Ga1.2 N1.2 @	28.65	4	forward triangle
22	3.00	4.030 @ N1.1 N1.6 Ga1.1 @	11.46	4	forward triangle
24	6.00	4.042 @ N1.6 N1.6 @	5.48	3	other double scatter

- ① 変更箇所の確認
- HOLE : 1(K-edge) → 4(L₃-edge)
 - 中心原子(ipot 0) : Ga(Z=31) → Eu(Z=63)
 - 中心原子のipot : 0 → 1
 - 進入原子Euの座標を追加

実験値と理論計算(進入型)の比較 SPring 8



Artemis [Feff] Atoms and Feff

Rename Discard Feff in Demeter Feff doc

Atoms Feff Paths Path-like Console

① Path 1-4,9-10,12を選択し、Dataウィンドウにドラッグ&ドロップ (Path6-8,11は寄与が低い)

Order	Begen	neff	Scattering path	Rank	Contribution	Type
1	3.00	2.080	@ N1.2 @	100.00	2	single soat
2	3.00	2.080	@ Ga1.1 @	100.00	2	single soat
3	3.00	2.449	@ Ga1 @	85.94	2	single soat
4	3.00	2.449	@ N1.3 @	82.02	2	single soat
6	24.00	3.240	@ Ga1 N1.2 @	11.19	3	other doubl
7	6.00	3.673	@ N1.2 N1.2 @	11.83	3	other doubl
8	6.00	3.673	@ Ga1.1 Ga1.1 @	3.89	3	other doubl
9	3.00	3.805	@ N1.2 @	19.41	2	single soat
10	3.00	3.805	@ Ga1.1 @	22.62	2	single soat
11	12.00	3.852	@ Ga1 Ga1.1 @	5.46	3	other doubl
12	12.00	3.852	@ N1.2 N1.3 @	16.65	3	other doubl
13	12.00	3.945	@ N1.2 Ga1.1 @	8.00	3	obtuse
14	6.00	4.012	@ N1.1 @	38.30	2	single
15	6.00	4.012	@ Ga1.4 @	39.38	2	single
18	12.00	4.024	@ N1.2 Ga1.2 @	94.75	3	non-fo
20	6.00	4.030	@ Ga1.1 N1.6 Ga1.1 @	3.03	2	dog-le
21	3.00	4.030	@ N1.2 Ga1.2 N1.2 @	28.65	2	forwar
22	3.00	4.030	@ Ga1.1 N1.6 Ga1.1 @	11.46	2	forwar
24	6.00	4.042	@ N1.6 N1.6 @	5.49	3	other

② [interstitial]のアイコンをクリック

④ Rをクリック

Artemis [Data] GaN_1050C.txt

Data Path Marks Actions Debug Help

GaN_1050C.txt CV 1

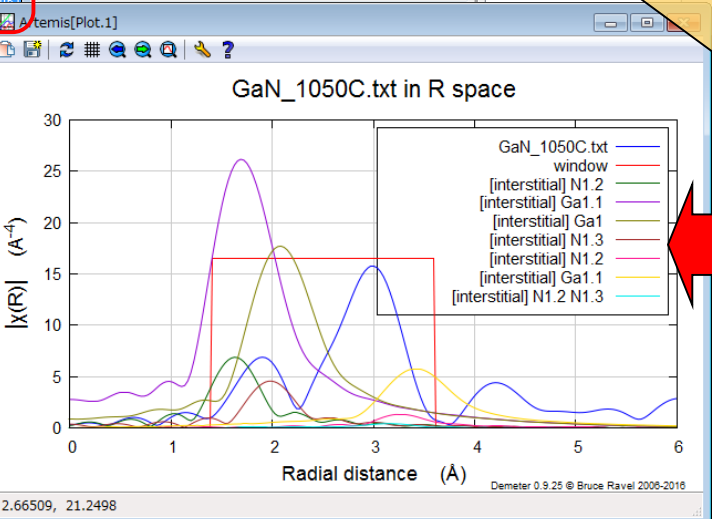
Data source: Artemis [Data] GaN_1050C.txt

Fourier transform parameters: kmin 3, kmax 10.5, dk 1, rmin 1.4, rmax 3.6, dr 0.0

Fitting k weights: 1, 2, 3, other 0.5

Other parameters: Include in fit, Plot after fit, Fit background, e(k) 0, Plot with phase correction

③ DataとPath:[interstitial]以外のチェックを外す



Plotting list

- Path: [N-site] Ga1.4 from GaN_1050C.txt
- VPath: N-site
- Path: [interstitial] N1.2 from GaN_1050C.txt
- Path: [interstitial] Ga1.1 from GaN_1050C.txt
- Path: [interstitial] Ga1 from GaN_1050C.txt
- Path: [interstitial] N1.3 from GaN_1050C.txt
- Path: [interstitial] N1.2 from GaN_1050C.txt
- Path: [interstitial] Ga1.1 from GaN_1050C.txt
- Path: [interstitial] N1.2 N1.3 from GaN_1050C.txt

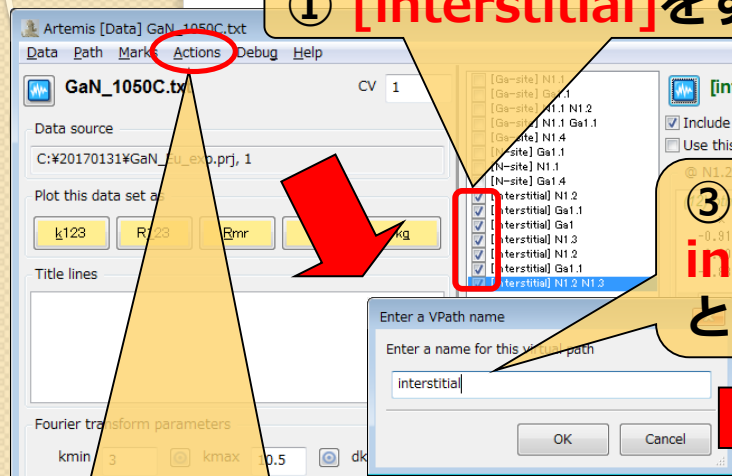
Freeze

Clear

Save next plot to a file.

Pathの足し合わせ(進入型)

① [interstitial]をすべてチェック



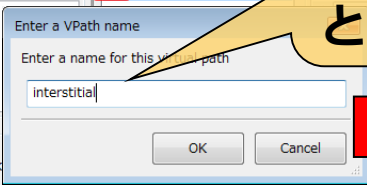
② Dataウィンドウのメニューから

Action

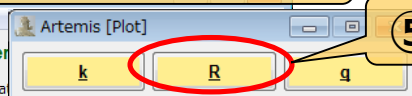
— Make sum of marked paths and plot in R を選択

④ DataとVPath:interstitial以外のチェックを外す

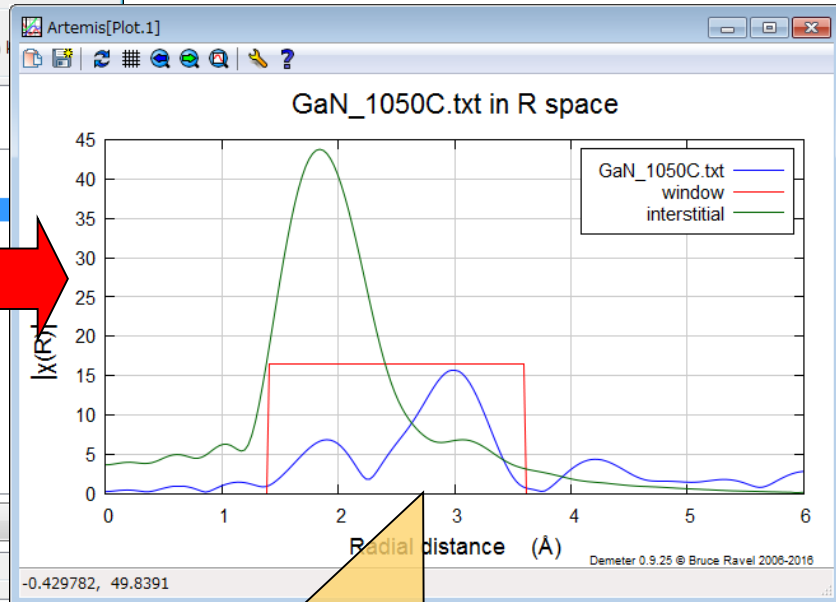
③ VPath名にinterstitialと入力



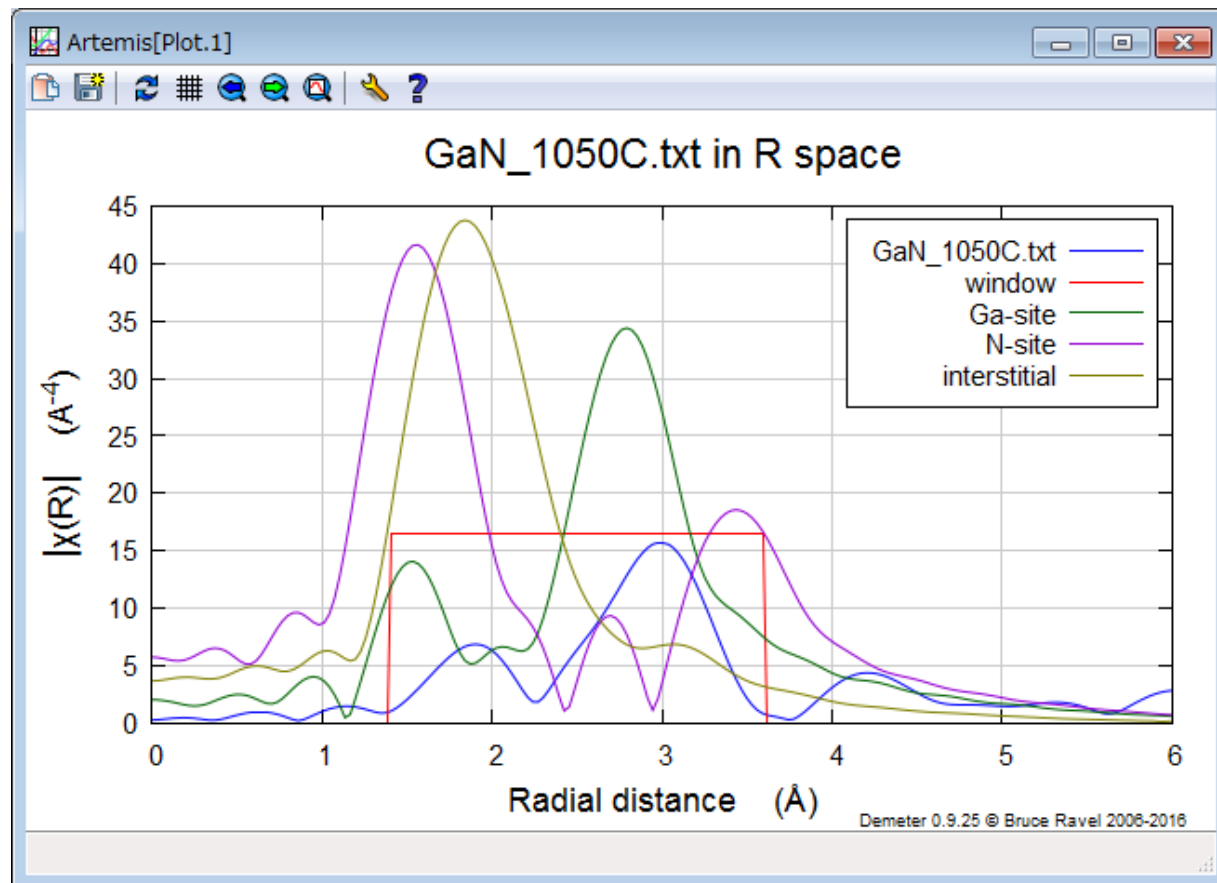
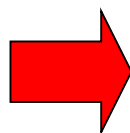
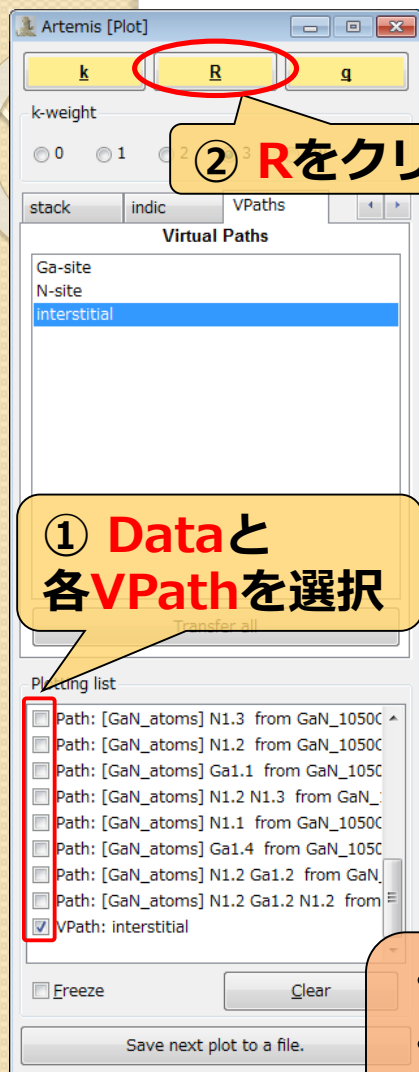
⑤ Rをクリック



⑥ 選択したPathの足し合わせを表示

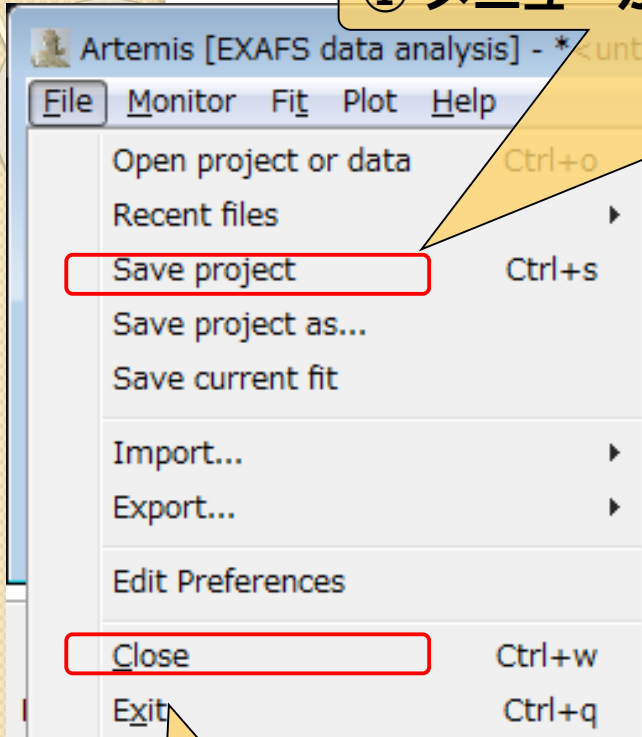


各モデルの理論計算結果の比較



- ピーク形状はGaサイト置換型が実験データに最も近い
- ピーク位置の違いは中心原子の原子半径の違いによる局所的な歪緩和の影響

① メニューから **File – Save project** を選択し、ファイルを保存

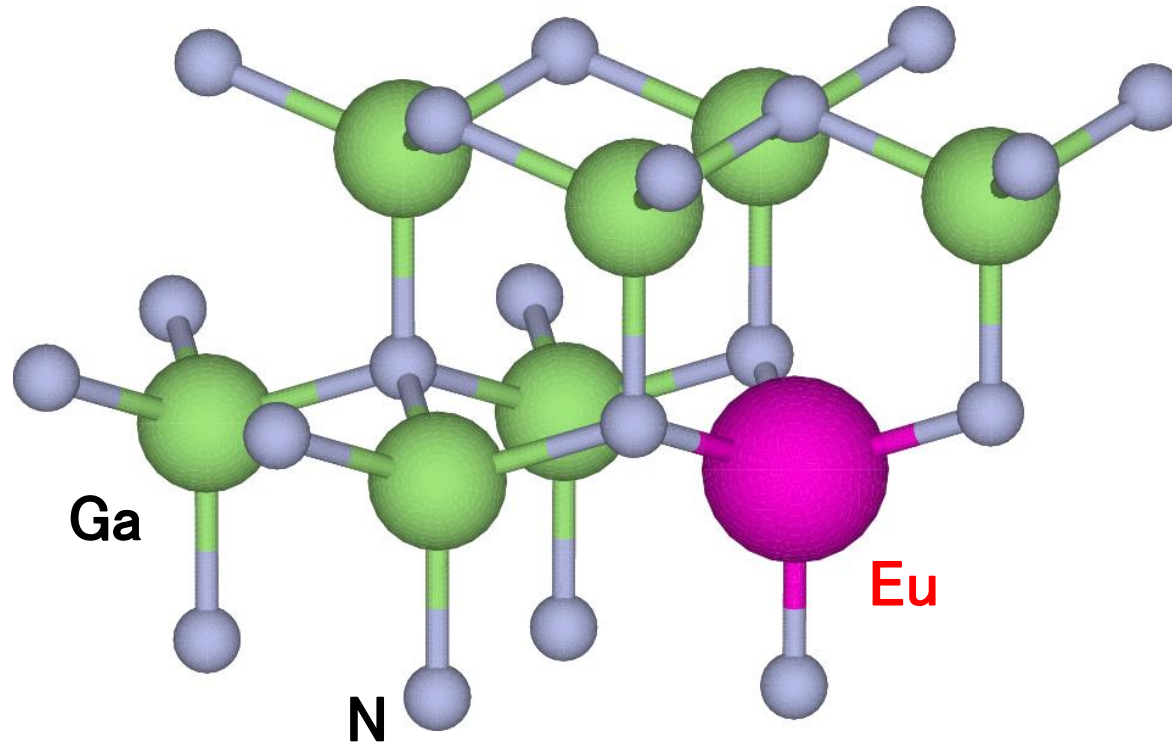


② メニューから **File – Exit** を選択し、一旦Artemisを終了する

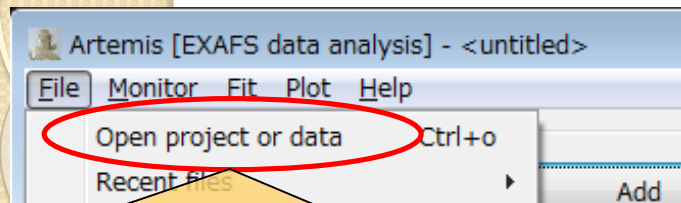
途中休憩(10分)



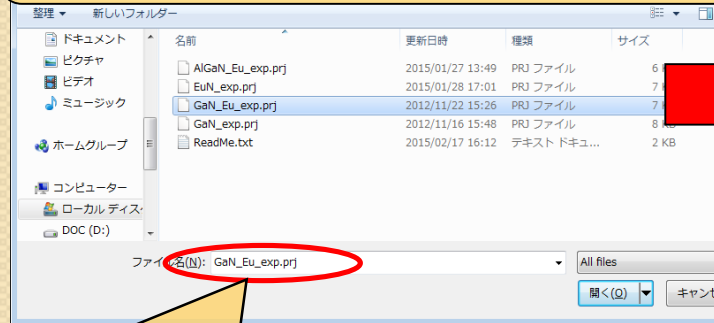
カーブフィッティング (Gaサイト置換型)



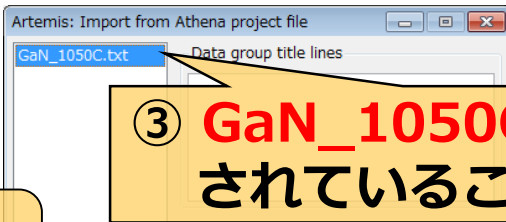
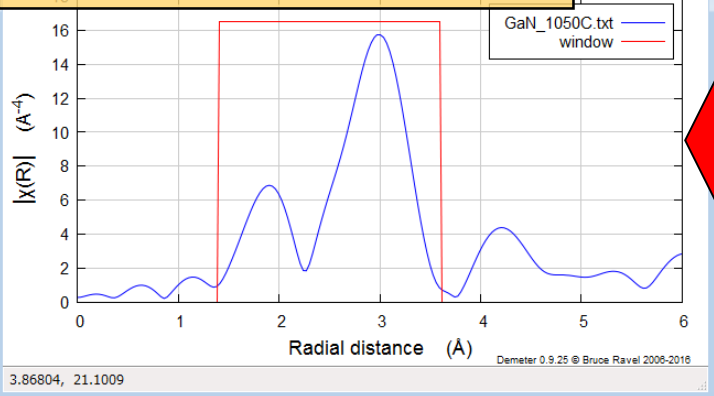
実験データの読み込み



① メニューから **File - Open project or data** を選択

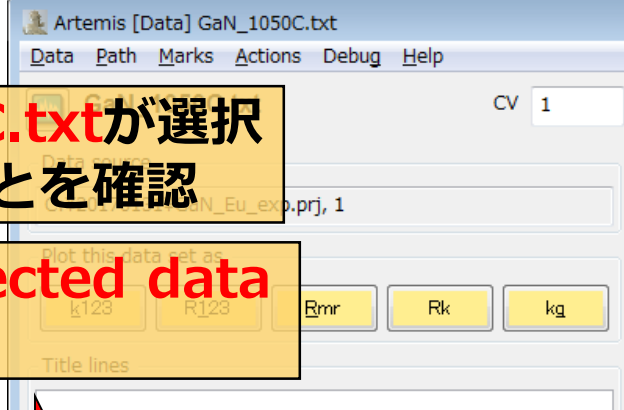


② **GaN_Eu_exp.prj** を開く



③ **GaN_1050C.txt** が選択されていることを確認

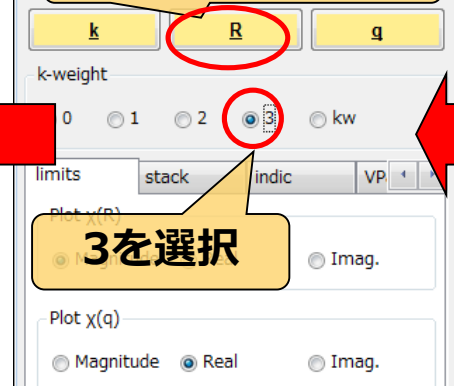
④ **Import selected data** ボタンを押す



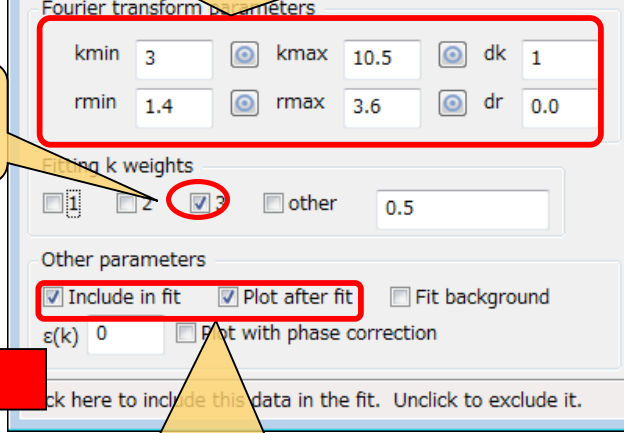
k-range : 3 - 10.5 Å⁻¹
R-range: 1.4 - 3.6 Å

Fitting k weightsは 3 を選択

④ **R** をクリック



④ **3** を選択



Include in fit と **Plot after fit** をチェック

feff.inpの作成(Gaサイト置換型) SPring 8

① Feff calculationsのAddボタンをクリック

② 先程保存したGaN_atoms.inpファイルを開く

③ モデル名を入力Ga-site

④ Gaにcoreのチェックを入れる

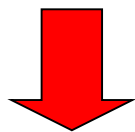
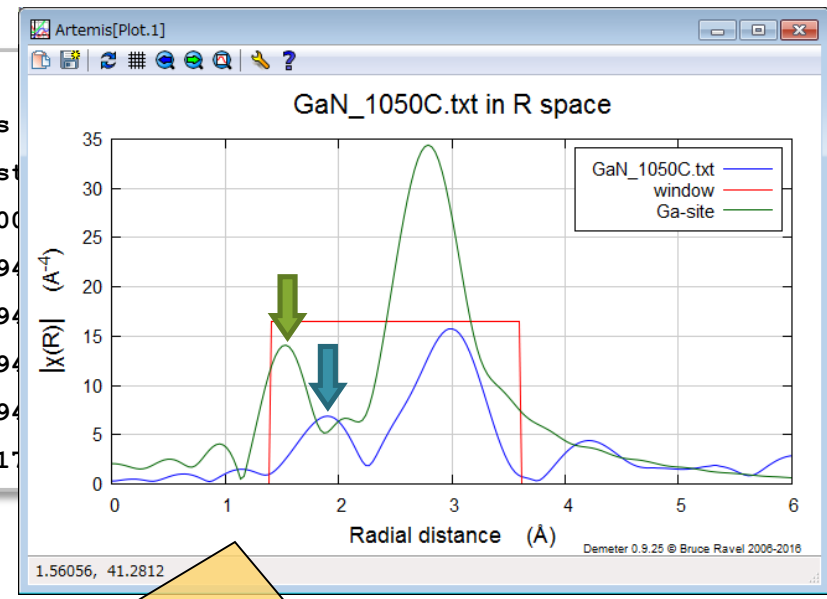
⑤ Run Atomsをクリック

Core	El.	x	y	z	Tag
<input checked="" type="checkbox"/>	Ga	0.33333	0.66667	0.00000	Ga1
<input type="checkbox"/>	N	0.33333	0.66667	0.37500	N1
<input type="checkbox"/>					
<input type="checkbox"/>					
<input type="checkbox"/>					
<input type="checkbox"/>					

feff.inpの編集(Gaサイト置換型) SPring 8

```

ATOMS          * this list contains 183 atoms
*   x           y           z       ipot tag       dist
0.00000      0.00000      0.00000  0   Ga1        0.00000
0.00000      0.00000      1.94100  2   N1.1       1.94100
1.83942      0.00003      -0.64700  2   N1.2       1.94100
-0.91974     -1.59297     -0.64700  2   N1.2       1.94100
-0.91974      1.59303     -0.64700  2   N1.2       1.94100
1.83942      0.00003      2.58800  1   Ga1.1      3.17509
    
```



中心原子の原子半径の違いによる
最近接原子のピーク位置のずれ

```

ATOMS          * this list contains 183 atoms
*   x           y           z       ipot tag       distance
0.00000      0.00000      0.00000  0   Eu1        0.00000
0.00000      0.00000      2.20000  2   N1.1       2.20000
2.07536      0.00003     -0.72999  2   N1.2       2.20000
-1.03771     -1.79730     -0.72999  2   N1.2       2.20000
-1.03769      1.79732     -0.72997  2   N1.2       2.20000
1.83942      0.00003      2.58800  1   Ga1.1      3.17509
    
```

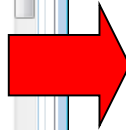
最近接原子間距離が2.2 Åに
なるようxyz座標を変更

feff計算(Gaサイト置換型)

② Save fileをクリックし、GaN-site.inpで保存
→この後のEu添加AlGaNのカーブフィッティングで利用

③ Run Feffをクリック

```
Feff input file
* This feff6 file was generated by Demeter 0.9.25
* Demeter written by and copyright (c) Bruce Ravel, 2006-2018
* -----
* total mu*k=1: 8.955 microns, unit edge step: 10.490 microns
* specific gravity: 6.111
* -----
* normalization correction: 0.00045 ang^2
* -----
TITLE GaN
HOLE 4 1.0 * FYI: (Ga K edge @ 10367 eV, second number is 10^2)
* mphase,mpath,mfeff,mchi
CONTROL
PRINT 1 0 0 0
RMAX 5.0
*POLARIZATION 0.0 0.0 0.0
POTENTIALS
* ipot Z tag
0 63 Eu
1 31 Ga
2 7 N
ATOMS * this list contains 183 atoms
* x y z ipot tag distance
0.00000 0.00000 0.00000 0 Eu1 0.00000
0.00000 0.00000 2.20000 2 N1_1 2.20000
2.07536 0.00003 -0.72989 2 N1_2 2.20000
-1.03771 -1.79730 -0.72989 2 N1_2 2.20000
-1.03769 1.79732 -0.72987 2 N1_3 2.20000
1.83942 0.00003 2.58800 1 Ga1.1 3.17509
-0.91974 -1.53247 2.58800 1 Ga1.1 3.17509
1.83942 0.00003 -2.58800 1 Ga1.1 3.17509
```



Name of this Feff calculation: Ga-site

Description

```
# TITLE GaN
# This paths.dat file was written by Demeter 0.9.25
# The central atom is denoted by this token: @
# Cluster size = 5.00 A, containing 182 atoms
# 22 paths were found within 5.000 A
# Forward scattering cutoff 20.00
# Distance fuzz = 0.030 A
```

Scattering Paths

	Degen	Reff	Scattering path	Rank	L	Type
1	4.00	2.200	@ N1.1 @	100.00	2	single scattering
2	12.00	3.181	@ Ga1.1 @	100.00	2	single scattering
3	1.00	3.235	@ N1.3 @	7.10	2	single scattering
4	24.00	3.630	@ N1.2 Ga1.1 @	11.31	3	other double scattering
5	9.00	3.732	@ N1.4 @	43.10	2	single scattering
6	12.00	3.996	@ N1.1 N1.2 @	10.67	3	other double scattering
7	12.00	4.079	@ N1.2 Ga1.1 N1.2 @	3.48	4	dog-leg
11	4.00	4.400	@ N1.1 @ N1.1 @	5.23	4	rattle
12	12.00	4.400	@ N1.2 @ N1.2 @	5.13	4	hinge
13	36.00	4.431	@ Ga1.1 N1.4 @	9.63	3	other double scattering
14	6.00	4.498	@ Ga1.3 @	20.47	2	single scattering
15	6.00	4.540	@ N1.6 @	16.16	2	single scattering
16	36.00	4.562	@ N1.2 N1.4 @	9.20	3	other double scattering
17	36.00	4.626	@ N1.2 Ga1.1 @	7.58	3	other double scattering
18	48.00	4.771	@ Ga1.1 Ga1.1 @	3.66	3	acute triangle
21	9.00	4.902	@ N1.7 @	19.13	2	single scattering
22	12.00	4.893	@ N1.2 N1.6 @	5.24	3	obtuse triangle

① 変更箇所の確認

- HOLE : 1(K-edge) → 4(L₃-edge)
- 中心原子(ipot 0) : Ga(Z=31) → Eu(Z=63)
- 中心原子のtag : Ga1 → Eu1
- 最近接原子Nのxyz座標を変更

実験値と理論計算(Gaサイト置換型)の比較

Artemis [Feff] Atoms and Feff

Atoms Feff Paths Path-like Console

Name of this Feff calculation: Ga-site

Description

```

# TITLE GaN
# This paths.dat file was written by Demeter 0.9.25
# The central atom is denoted by this token: @
# Cluster size = 5.000 Å, containing 182 atoms
# 22 paths were found within 5.000 Å
# Forward scattering cutoff 20.00
# Distance fuzz = 0.030 Å
    
```

Degen	Reff	Scattering path	Rank	L Type
1	4.00	@ N1.1 @	100.00	2 single scattering
2	12.00	@ Ga1.1 @	100.00	2 single scattering
3	1.00	@ N1.3 @	7.10	2 single scattering
4	24.00	@ N1.2 @ Ga1.1 @	11.31	3 other double scatterin
5	9.00	@ N1.4 @	43.10	2 single scattering

① Ctrlキーを押しながら
Path1-2,5を選択し、
Dataウィンドウに
ドラッグ&ドロップ
(Path3-4は寄与が低い)

Artemis [Data] GaN_1050C.txt

Data Path Marks Actions Debug Help

GaN_1050C.txt CV 1

Data source
C:\20170131\GaN_Eu_exp.prj, 1

Plot this data set as
k123 R123 Emr Rk

Title lines

Fourier transform parameters

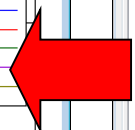
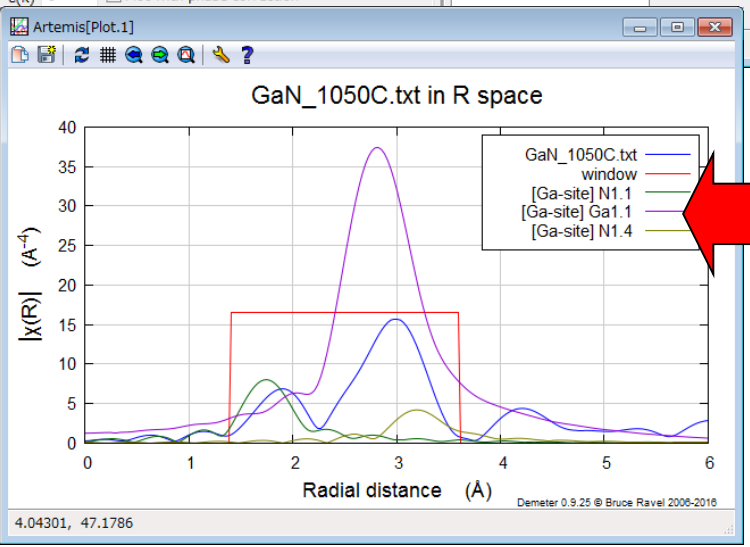
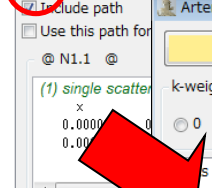
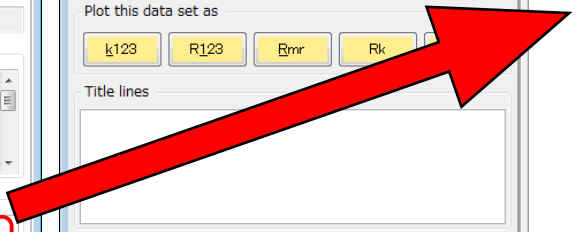
kmin 3 kmax 10.5 dk 1
rmin 1.4 rmax 3.6 dr 0.0

Fitting k weights
 1 2 3 other 0.5

Other parameters
 Include in fit Plot after fit Fit background
 $\epsilon(k)$ 0 Plot with phase correction

② 各Pathのアイコンをクリック

③ Rをクリック



Pathの足し合わせ(Gaサイト置換型)

① すべてのPathをチェック

② Dataウィンドウのメニューから Action - Make sum of marked paths and plot in R を選択

③ VPath名に Ga-site と入力

④ DataとVPath以外のチェックを外す

⑤ Rをクリック

⑥ 選択したPathの足し合わせを表示

The plot window shows the resulting intensity $|x(R)|$ versus Radial distance (Å). The legend indicates three data series: GaN_1050C.txt (blue line), window (red line), and Ga-site (green line). The Ga-site curve shows a prominent peak at approximately 3.0 Å.

パラメータの設定(Gaサイト置換型)

① [Ga-site]N1.1の $S0^2, \Delta E0, \Delta R, \sigma^2$ をそれぞれ amp, enot, delr, ss に設定

$S0^2$	amp
$\Delta E0$	enot
ΔR	delr
σ^2	ss

② 各パラメータを右クリック → Guess をクリック

③ [Ga-site]Ga1.1では amp, enot, delr2, ss2 に設定し、右クリック → Guess をクリック

$S0^2$	amp
$\Delta E0$	enot
ΔR	delr2
σ^2	ss2

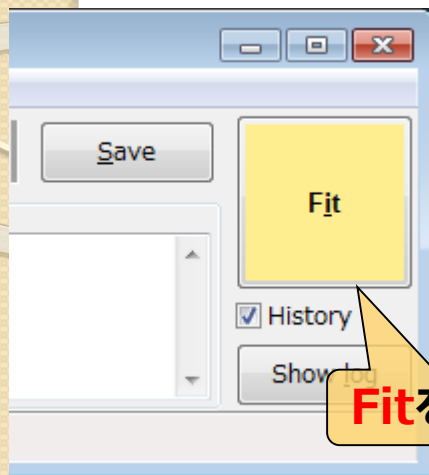
④ [Ga-site]N1.4では amp, enot, delr3, ss3 に設定し、右クリック → Guess をクリック

$S0^2$	amp
$\Delta E0$	enot
ΔR	delr3
σ^2	ss3

⑤ GDSウィンドウでパラメータを確認

	Type	Name	Math expr
1	guess	amp	1.00000
2	guess	enot	0
3	guess	delr	0
4	guess	ss	0.00300
5	guess	delr2	0
6	guess	ss2	0.00300
7	guess	delr3	0
8	guess	ss3	0.00300
9	guess		
10	guess		
11	guess		
12	guess		

フィッティング結果(Gaサイト置換型)



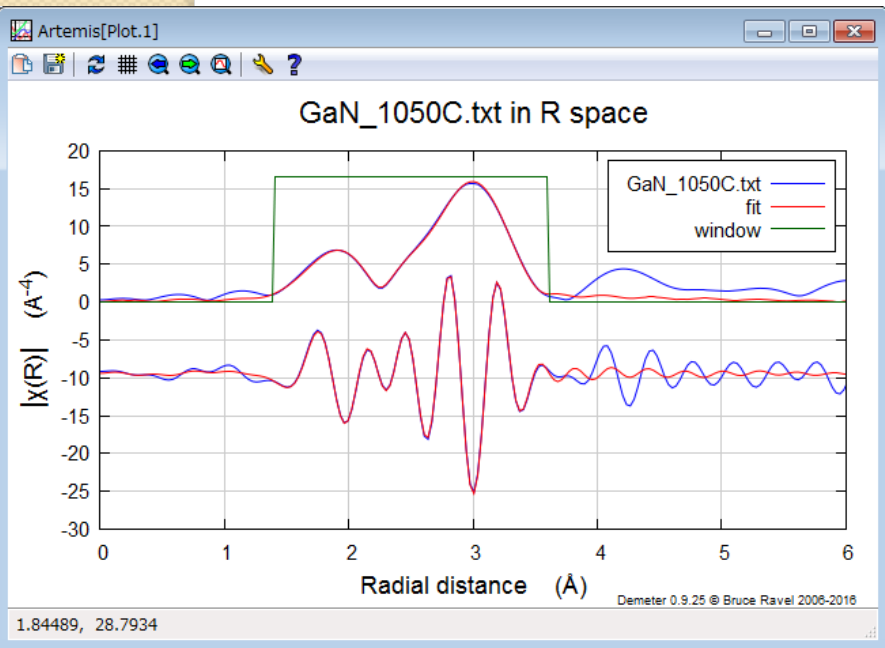
Fitを実行

Artemis [Log] Fit 1

```
=====  
Independent points      : 10.3310547  
Number of variables     : 8  
Chi-square              : 5.4634211  
Reduced chi-square     : 2.3437550  
R-factor                : 0.0006214  
Number of data sets    : 1  
=====  
Penalty of 27.0 sigma2 for [Ga-site] N1.4 is negative.  
Used 8 of 10331 independent points for a penalty of 12.923  
1 correlation above 0.950 for a penalty of 3.000  
***** Note: happiness is a semantic parameter and should *****  
***** NEVER be reported in a publication -- NEVER! *****  
  
GUESS parameters:  
-----  
amp      = 0.74996652  # +/- 0.05804875  [1.00000]  
enot     = 10.37764629 # +/- 0.65383701  [0]  
delr     = 0.02085513  # +/- 0.00442518  [0]  
ss       = -0.00028036 # +/- 0.00067503  [0.00300]  
delr2    = 0.08882057  # +/- 0.00433079  [0]  
ss2      = 0.00375538  # +/- 0.00061790  [0.00300]  
delr3    = 0.02958280  # +/- 0.01271497  [0]  
ss3      = -0.00137958 # +/- 0.00164492  [0.00300]  
  
Correlations between variables:  
-----  
-----  
-----
```

良くフィットしているように見えるが、
ss,ss3の値がマイナスになっている

ampとの相互作用の影響



標準試料からampを求める

FEFFによる計算から得られる $\text{amp}(S_0^2) = 0.70 \sim 1.05$

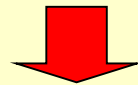
G. G. Li et al., PRB 52, 6332 (1995).

guess parameters:

amp	=	0.74996652	# +/-	0.05804875	[1.00000]
enot	=	10.37764629	# +/-	0.65383701	[0]
delr	=	0.02085513	# +/-	0.00442518	[0]
ss	=	-0.00028036	# +/-	0.00067503	[0.00300]
delr2	=	0.08882057	# +/-	0.00433079	[0]
ss2	=	0.00375538	# +/-	0.00061790	[0.00300]
delr3	=	0.02958280	# +/-	0.01271497	[0]
ss3	=	-0.00137958	# +/-	0.00164492	[0.00300]

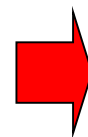
ampの値が0.75と
やや小さい値

構造が既知の標準試料からampの値を求める



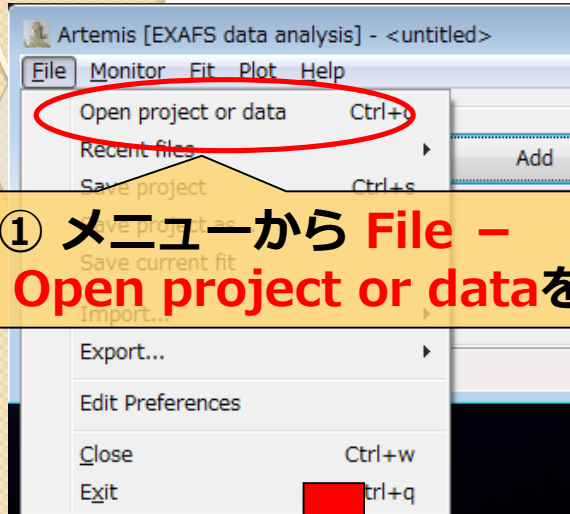
未知試料のampに用いる

標準試料EuN(NaCl型)
からampを求める

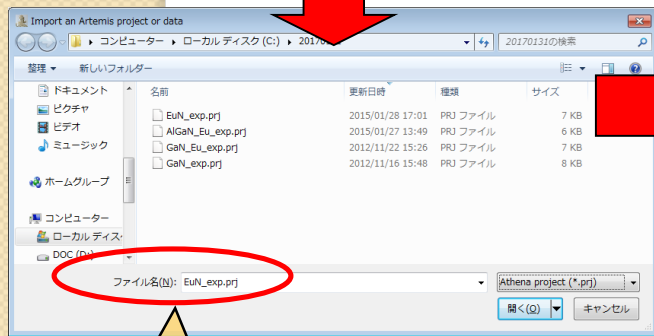


未知試料Eu添加GaNの
ampに用いる

実験データの読み込み(EuN)



① メニューから **File - Open project or data** を選択

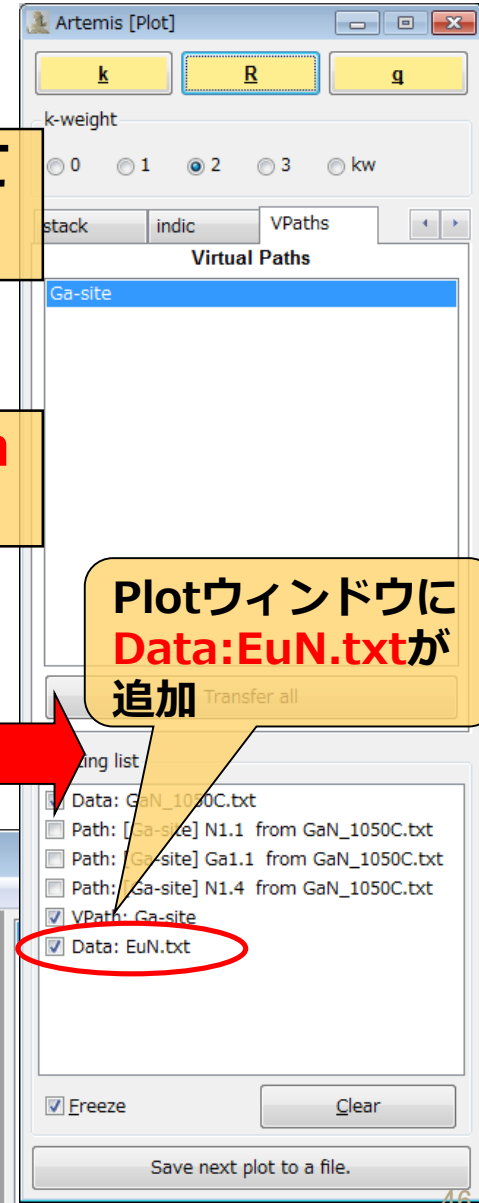
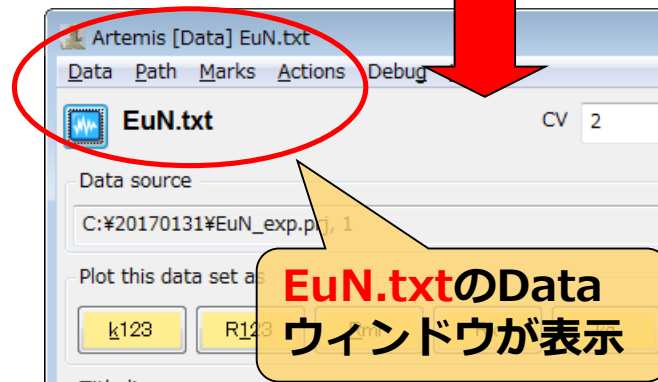


② **EuN_exp.prj** を開く



③ **EuN.txt** が選択されていることを確認

④ **Import these data** ボタンを押す



Plotウィンドウに **Data:EuN.txt** が追加

実験データの確認 (EuN)

The image shows the Artemis software interface for processing EuN data. The main window is titled 'Artemis [Data] EuN.txt'. The 'EuN.txt' section shows the data source as 'C:\¥20170131¥EuN_exp.prj, 1' and the CV value as 3. The 'Fourier transform parameters' section is highlighted with a red box, showing 'kmin 3', 'kmax 10.5', 'dk 1', 'rmin 1.4', 'rmax 4', and 'dr 0.0'. The 'Fitting k weights' section has '3' selected, and the 'Other parameters' section has 'Include in fit' and 'Plot after fit' checked. The 'Plotting list' at the bottom shows 'Data: EuN.txt' selected. Two plots are shown: 'EuN.txt in k space' and 'EuN.txt in R space'. A red arrow points from the 'k' and 'R' labels to the respective plots. A red box highlights the 'k' and 'R' labels in the top right corner.

k

R

3を選択

Fitting k weightsは3を選択

Include in fitとPlot after fitをチェック

Data:EuN.txtのみ選択

k-range: 3 - 10.5 Å⁻¹
R-range: 1.4 - 4.0 Å

Artemis [Data] EuN.txt

Data source: C:\¥20170131¥EuN_exp.prj, 1

CV 3

Fourier transform parameters

kmin 3 kmax 10.5 dk 1

rmin 1.4 rmax 4 dr 0.0

Fitting k weights

3

Other parameters

Include in fit Plot after fit

Plotting list

Data: EuN.txt

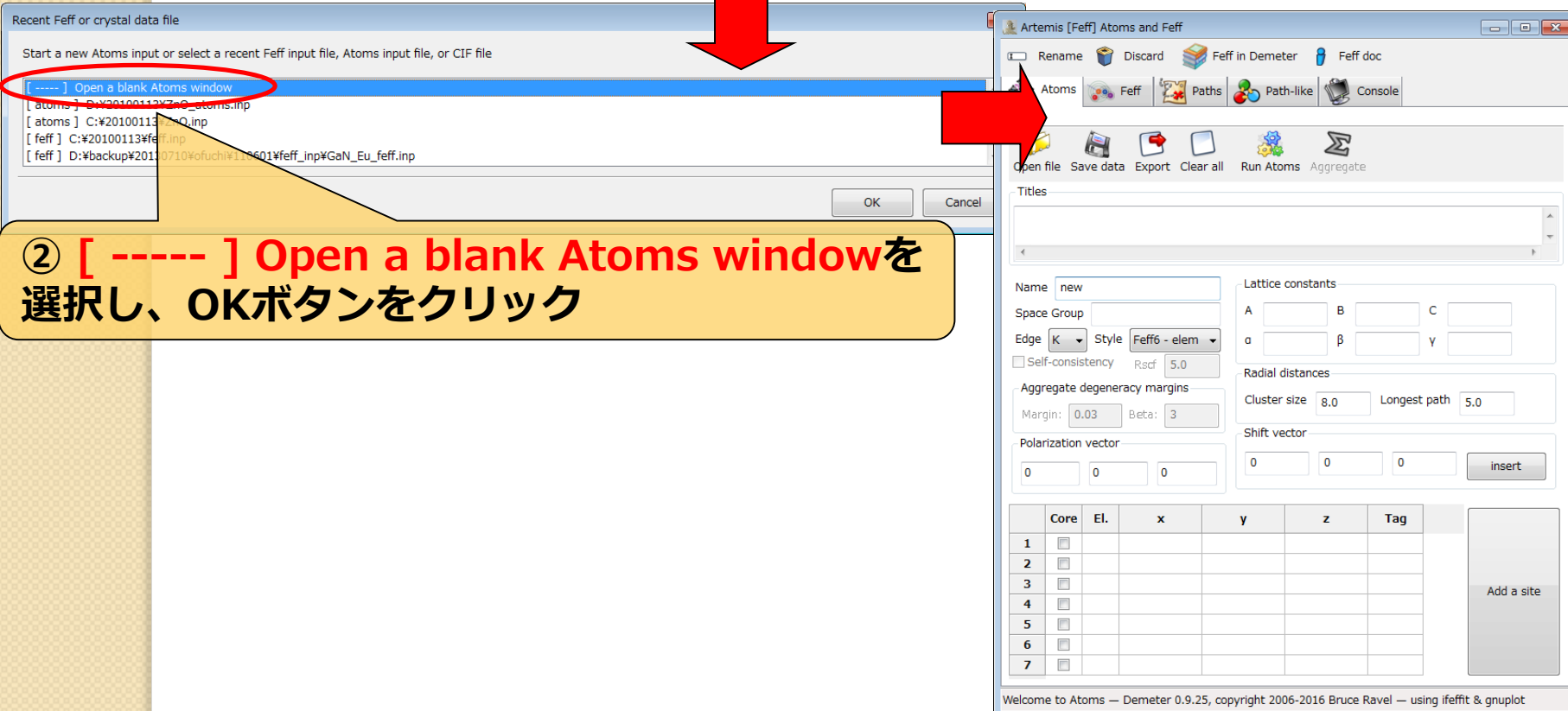
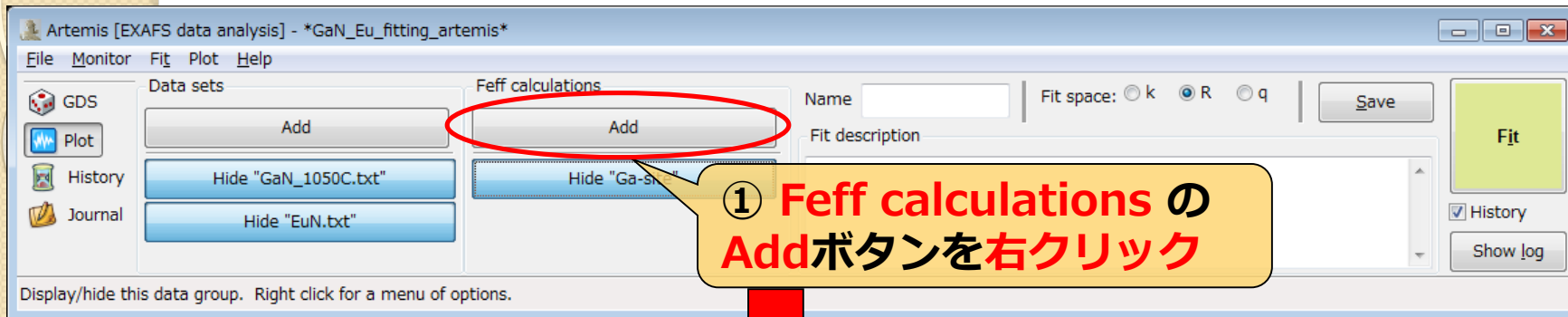
Artemis [Plot]

Artemis [Plot.1]

EuN.txt in k space

EuN.txt in R space

FEFFによる理論計算(EuN)



結晶学データの入力(EuN)

① モデル名を入力
EuN

② 空間群を入力
Fm-3m (225)

③ Edgeを選択 (L3)

⑤ 原子座標を入力
Eu: 0, 0, 0
N: 0.5, 0.5, 0.5

⑥ 中心原子Euを選択

⑦ 入力が終わったら
Run Atomsを押す

④ 格子定数を入力
 $a = 5.014 \text{ \AA}$
 $b = 5.014 \text{ \AA}$
 $c = 5.014 \text{ \AA}$
 $\alpha = 90^\circ$
 $\beta = 90^\circ$
 $\gamma = 90^\circ$

Artemis [Feff] Atoms of Feff in Demeter

Rename Discard

Atoms Paths Path like Console

Open file Save data Export Clear all Run Atoms Aggregate

Titles

EuN

Name: EuN

Space Group: NaCl

Edge: L3 Style: Feff6 - elem

Self-consistency Rscf: 5.0

Aggregate degeneracy margins

Margin: 0.03 Beta: 3

Polarization vector

0 0 0

Lattice constants

A: 5.014 B: 5.014 C: 5.014

α : 90 β : 90 γ : 90

Radial distances

Cluster size: 8.00000 Longest path: 5.0

Shift vector

0.00000 0.00000 0.00000 insert

	El.	x	y	z	Tag
1	<input checked="" type="checkbox"/> Eu	0	0	0	Eu1
2	<input type="checkbox"/> N	0.5	0.5	0.5	N1
3	<input type="checkbox"/>				
4	<input type="checkbox"/>				
5	<input type="checkbox"/>				
6	<input type="checkbox"/>				

Add a site

Pathの選別(EuN)

① Run Feffをクリック

Artemis [Data] EuN.txt

CV 2

[EuN] N1.1

[EuN] Eu1.1

Include path Plot after fit

Use this path for phase corrected plotting.

@ N1.1 @

(1) single scattering, high (100.00)

x	y	z	ipot	label
2.507000	0.000000	0.000000	2	'N1.1
0.000000	0.000000	0.000000	0	'abs

Label Reff=2.507, nleg=2, degen=6

N 6

S0 1

ΔE0

ΔR

σ^2 |

Ei

3rd

4th

EuN.txt

Artemis [Feff] Atoms and Feff

Name of this Feff calculation: EuN

Description

|| TITLE EuN

|| This paths.dat file was written by Demeter 0.9.25

|| The central atom is denoted by this token: @

|| Cluster size = 5.00 Å, containing 146 atoms

|| 5 paths were found within 5.000 Å

|| Forward scattering cutoff 20.00

|| Distance fuzz = 0.030 Å

Scattering Paths

Degen	Reff	Scatter. loc. path	Bank	Type
1	6.00	2.507 @ N1.1 @	100.00	2 single scattering
2	12.00	3.545 @ Eu1.1 @	100.00	2 single scattering
3	24.00	4.280 @ N1.1 @	11.43	2 other double scattering
4	48.00	4.280 @ N1.1 @	11.43	2 other double scattering
5	8.00	4.342 @ N1.1 @	24.74	2 single scattering

② Ctrlキーを押しながらPath1-2を選択し、EuN.txtのDataウィンドウにドラッグ&ドロップ

パラメータの設定(EuN)

② [EuN]N1.1は
amp_1,enot_1,
delr_1,ss_1に設定し、
右クリック→Guessをクリック

amp_1
enot_1
delr_1
ss_1

② [EuN]Eu1.1は
amp_1,enot_1,
delr_12,ss_12に設定し、
右クリック→Guessをクリック

amp_1
enot_1
delr_12
ss_12

③ GDSウィンドウで
パラメータを確認

Artemis [GDS] Guess, Def, Set parameters

	Type	Name	Math expression	Evaluated
1	guess	amp	1.00000	0.74997 +/- 0.05805
2	guess	enot	0	10.37765 +/- 0.65384
3	guess	delr	0	0.02086 +/- 0.00443
4	guess	ss	0.00300	-0.00028 +/- 0.00068
5	guess	delr2	0	0.08882 +/- 0.00433
6	guess	ss2	0.00300	0.00376 +/- 0.00062
7	guess	delr3	0	0.02958 +/- 0.01271
8	guess	ss3	0.00300	-0.00138 +/- 0.00164
9	guess	amp_1	1.00000	
10	guess	enot_1	0	
11	guess	delr_1	0	
12	guess	ss_1	0.00300	
13	guess	delr_12	0	
14	guess	ss_12	0.00300	

amp: 0.74996652 +/- 0.05804875

パラメータの設定(EuN)

Artemis [GDS] Guess, Def, Set parameters

Type	Name	Math expression	Evaluated
1	set	amp_1	
2	guess	enot	0
3	guess	delr	0
4	guess	ss	0.00300
5	guess	delr2	0
6	guess	ss2	0.00300
7	guess	delr3	0
8	guess	ss3	0.00300
9	guess	amp_1	1.00000
10	guess	enot	0
11	guess	delr_1	0
12	guess	ss_1	0.00300
13	guess	delr_12	0
14	guess	ss_12	0.00300

amp: 0.74996652 +/- 0.05804875

Artemis [Plot]

Plotting list

- Data: GaN_1050C.txt
- Data: EuN.txt

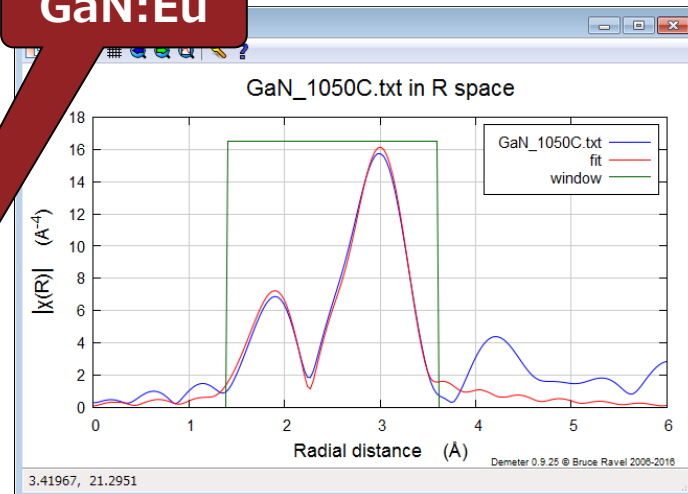
① ampをGuessからsetに変更し、Math expressionをamp_1にする。

④ Rをクリック

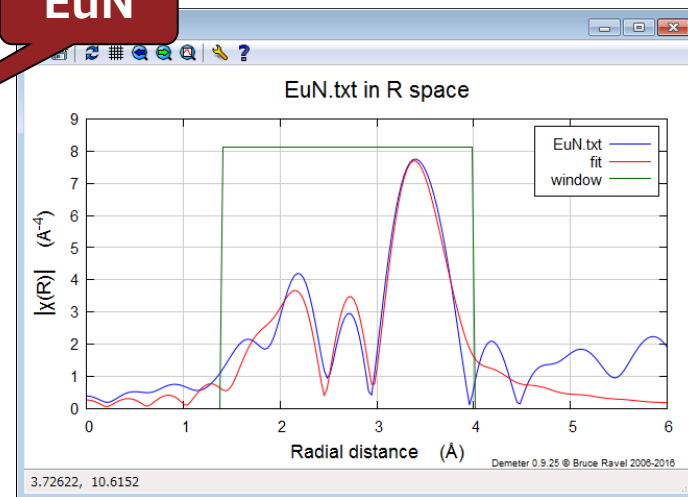
② Fitを実行

③ Plotウィンドウで表示させたい方のDataをチェック

GaN:Eu

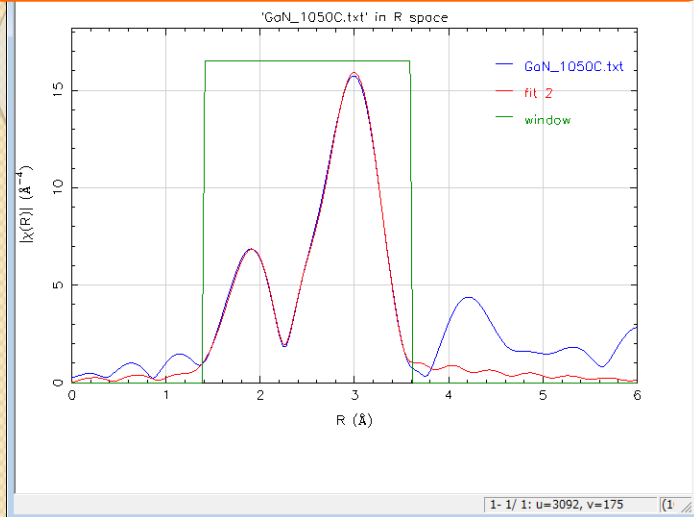


EuN



フィッティング結果の比較

EuNのampを用いない場合



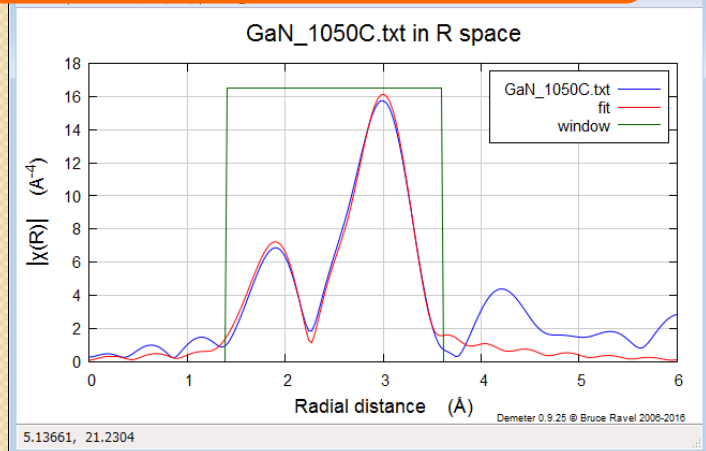
```
Used 8 of 10.331 independent points for a penalty of 12.923
1 correlation above 0.950 for a penalty of 3.000
**** Note: happiness is a semantic parameter and should ****
**** NEVER be reported in a publication -- NEVER! ****
```

guess parameters:

amp	=	0.74996652	# +/-	0.05804875	[1.00000]
enot	=	10.37764629	# +/-	0.65383701	[0]
delr	=	0.02085513	# +/-	0.00442518	[0]
ss	=	-0.00028036	# +/-	0.00067503	[0.00300]
delr2	=	0.08882057	# +/-	0.00433079	[0]
ss2	=	0.00375538	# +/-	0.00061790	[0.00300]
delr3	=	0.02958280	# +/-	0.01271497	[0]
ss3	=	-0.00137958	# +/-	0.00164492	[0.00300]

Correlations between variables:

EuNのampを用いた場合



ss,ss3が適切な値になっている

guess parameters:

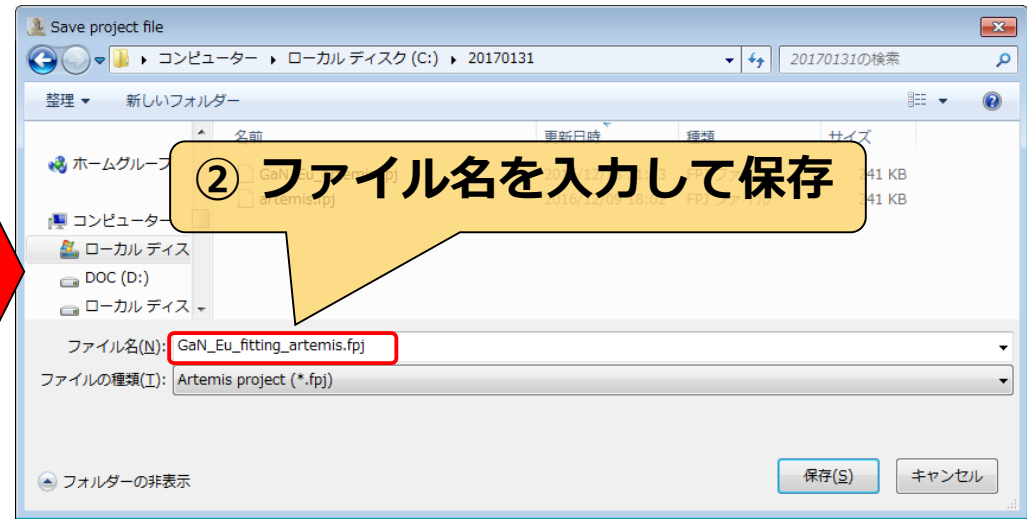
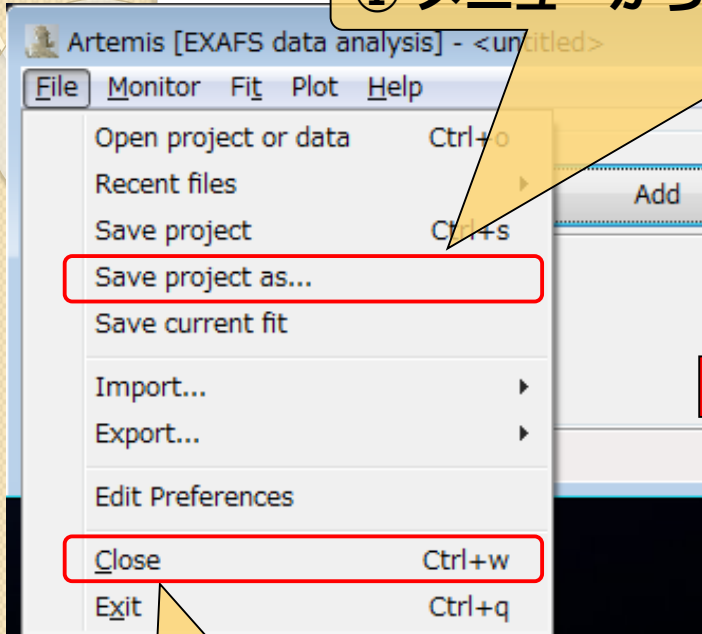
enot	=	9.91720870	# +/-	8.44328009	[0]
delr	=	0.02446667	# +/-	0.05415436	[0]
ss	=	0.00181247	# +/-	0.00466043	[0.00300]
delr2	=	0.09108411	# +/-	0.04941993	[0]
ss2	=	0.00602794	# +/-	0.00194021	[0.00300]
delr3	=	0.01747184	# +/-	0.25998001	[0]
ss3	=	0.00593208	# +/-	0.01826127	[0.00300]
amp_1	=	0.83311901	# +/-	0.14346732	[1.00000]
enot_1	=	6.12654442	# +/-	1.32206759	[0]
delr_1	=	-0.02608589	# +/-	0.01937029	[0]
ss_1	=	0.00953596	# +/-	0.00309390	[0.00300]
delr_12	=	0.01492827	# +/-	0.00993911	[0]
ss_12	=	0.00634620	# +/-	0.00123201	[0.00300]

amp_1=0.833

後のフィッティングで使用

データの保存(Gaサイト置換型) SPring 8

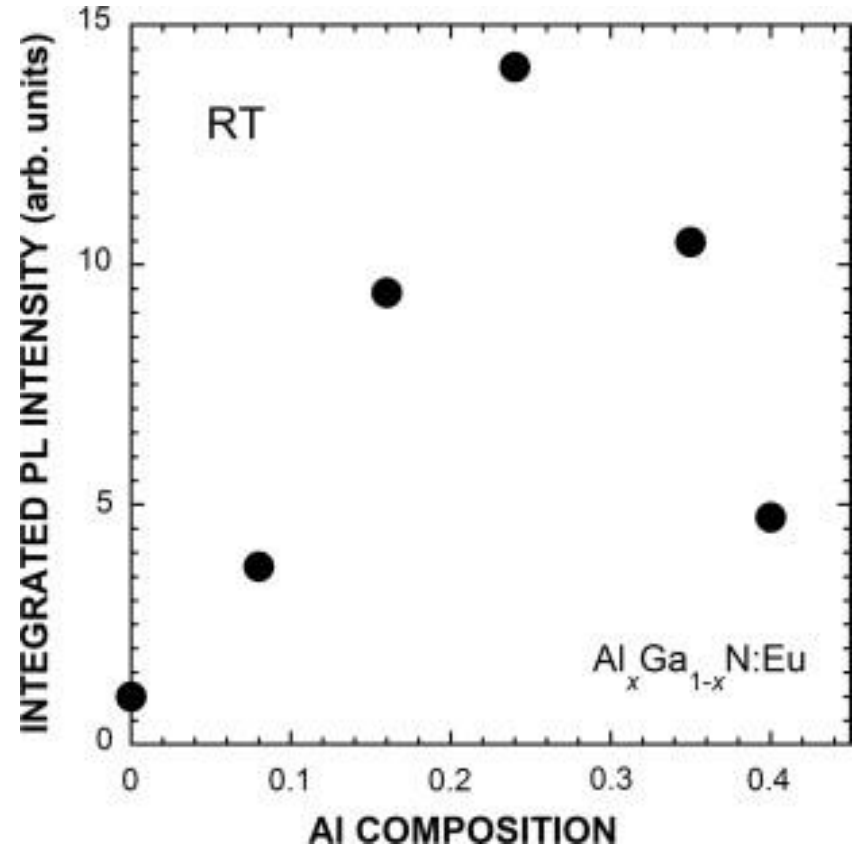
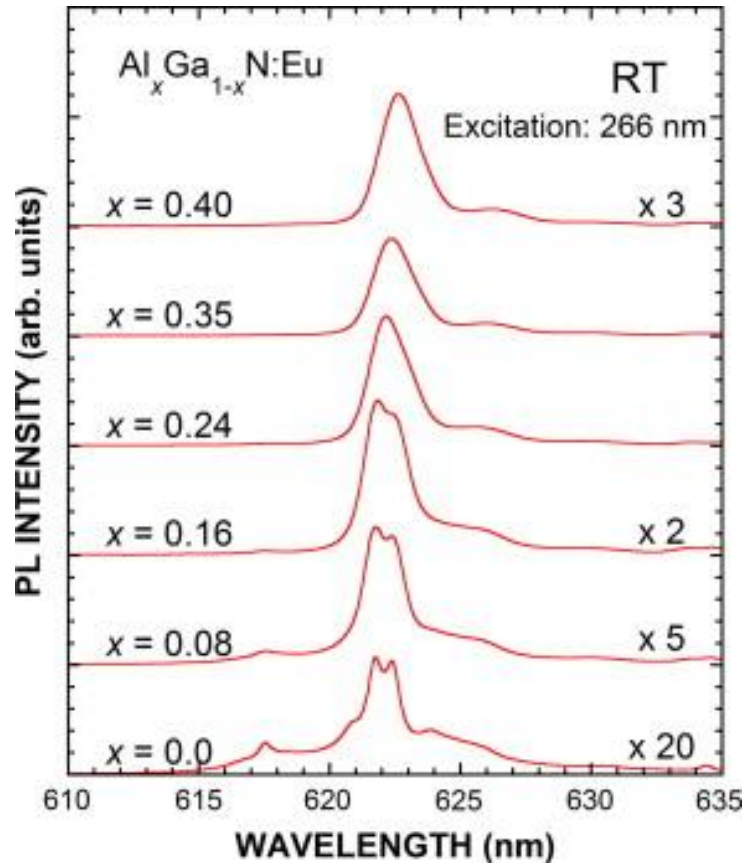
① メニューから **File – Save project as...** を選択



③ メニューから **File – Colse** を選択し、
一旦データを閉じる

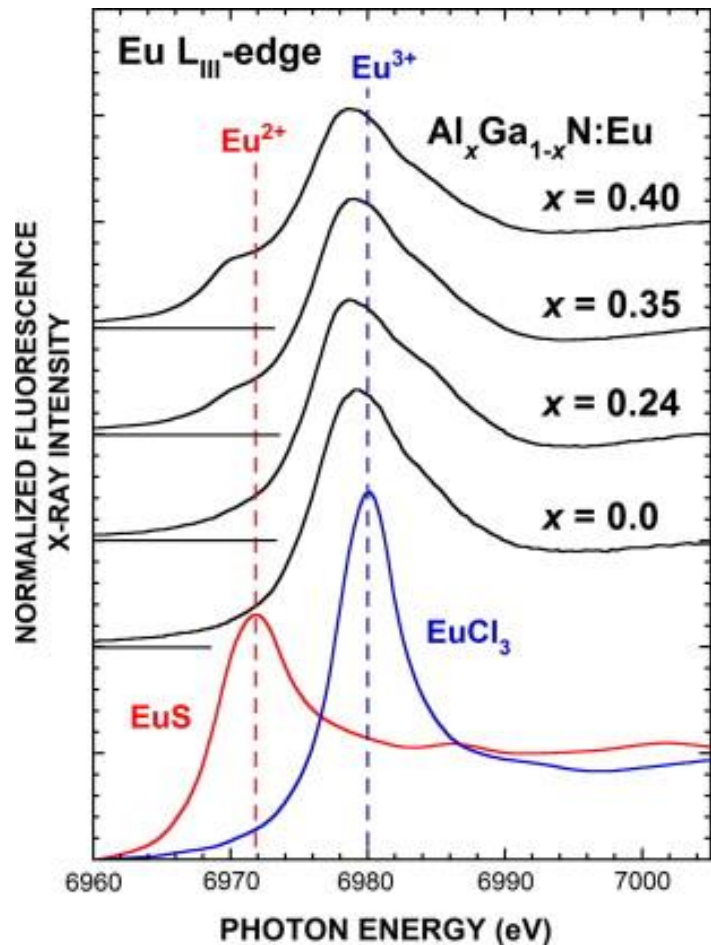
1. はじめに
2. Eu添加GaNについて
3. Artemisを使用した解析
 - ・ 構造モデルの作成
 - ・ 理論計算結果の比較
 - ・ カーブフィッティング
- 4. Eu添加AlGaNについて**
5. Artemisを使用した解析
 - ・ 構造モデルの作成
 - ・ 理論計算結果の比較
 - ・ カーブフィッティング

Eu添加AlGa_xN

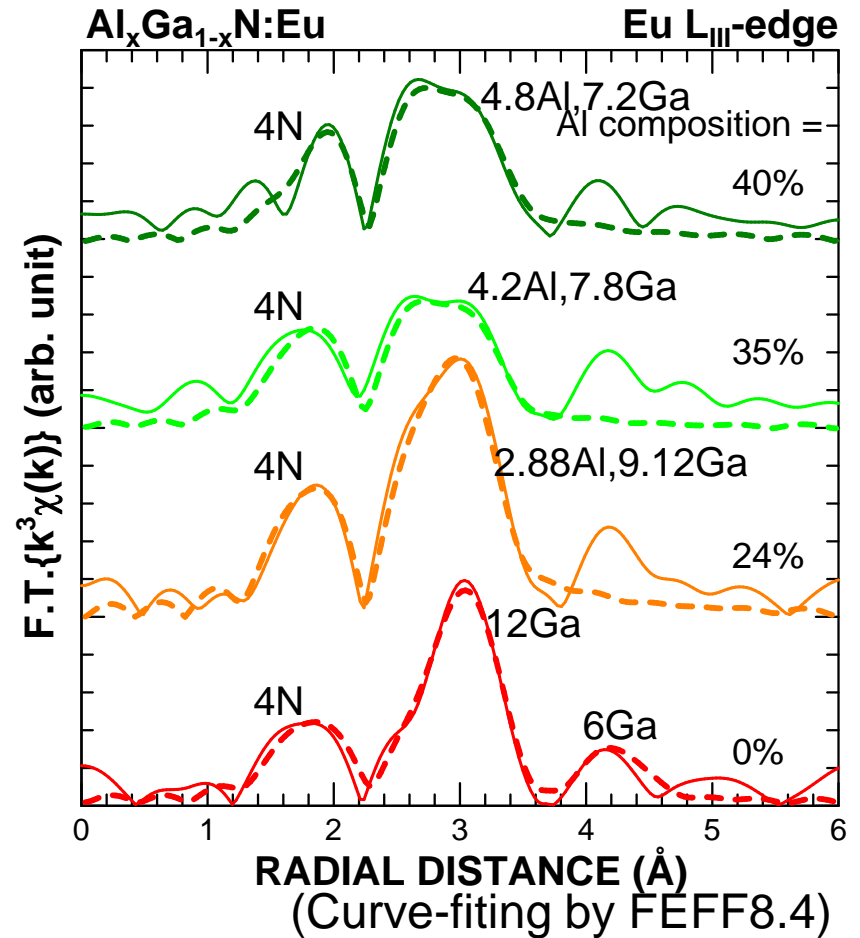


Al組成 $x=0.24$ で
発光強度が最大

Eu添加AlGa_N



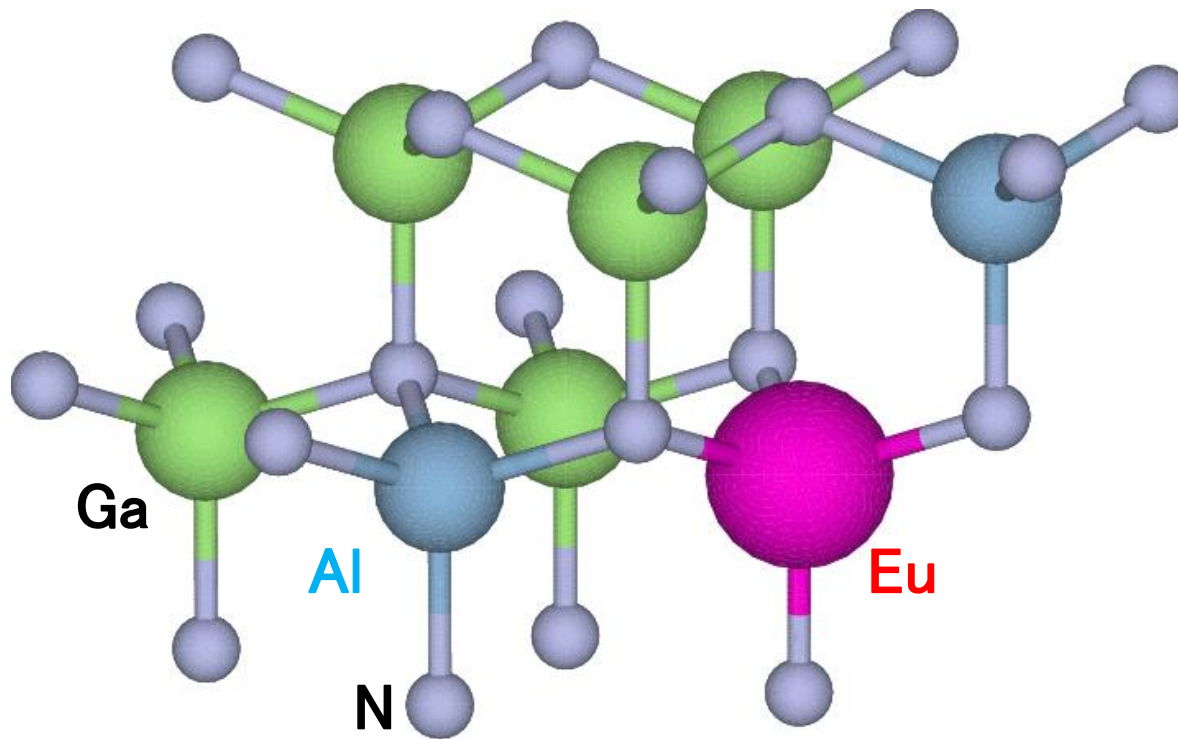
A. Koizumi *et al.*, Opt. Mat. **41**, 75 (2015).



H. Ofuchi *et al.*, E-MRS2011, **VII1** (2011).

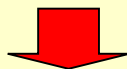
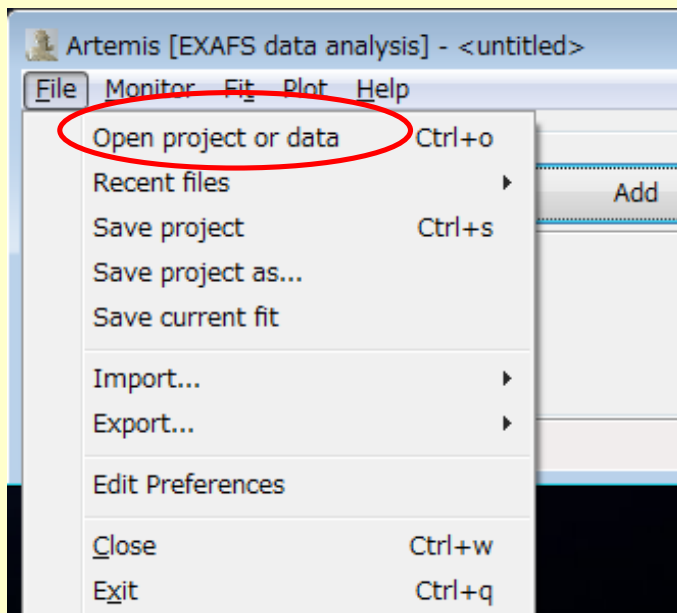
1. はじめに
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4. Eu添加AlGaNについて
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 - ・ カーブフィッティング

III族サイト置換型モデルの作成

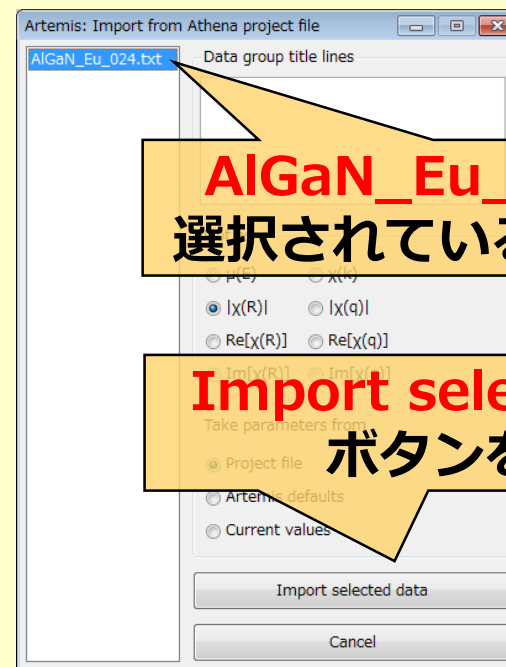


1. Athenaで解析したファイルを開く

- Ctrl-o または
- File - Open file(s)

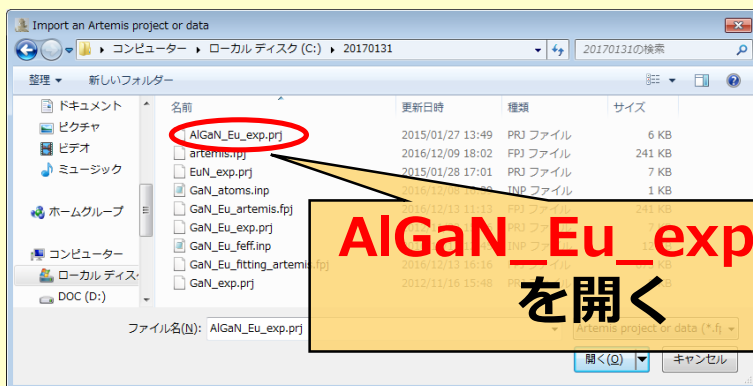


2. データを選択



AlGaN_Eu_024.txtが
選択されていることを確認

Import selected data
ボタンを押す



AlGaN_Eu_exp.prj
を開く

実験データの確認

Artemis [Data] AlGa_N_Eu_024.txt

Data source: C:\%20130110\AlGa_N_Eu_exp.prj, 1

Plot this data set as: k123, R123, Rmr, Rk, kg

Fourier transform parameters:

kmin	3	kmax	10.5	dk	1
rmin	1.4	rmax	3.6	dr	0.0

Fitting k weights: 1 2 3

Other parameters: Include in fit Plot after fit

Transferred data set "AlGa_N_Eu_024.txt" to the plotting list.

k-range: 3 – 10.5 Å⁻¹
R-range: 1.4 – 3.6 Å

Fitting k weightsは3を選択

Include in fitとPlot after fitをチェック

Artemis [Plot]

k R q

k-weight: 0 1 2 3 kw

3を選択

Do stacked plot:

Starting value: 0

Downward offset: 0

Invert paths: Never Only |χ(R)| |χ(R)| + |χ(q)|

Stack data sets:

Downward offset: 0

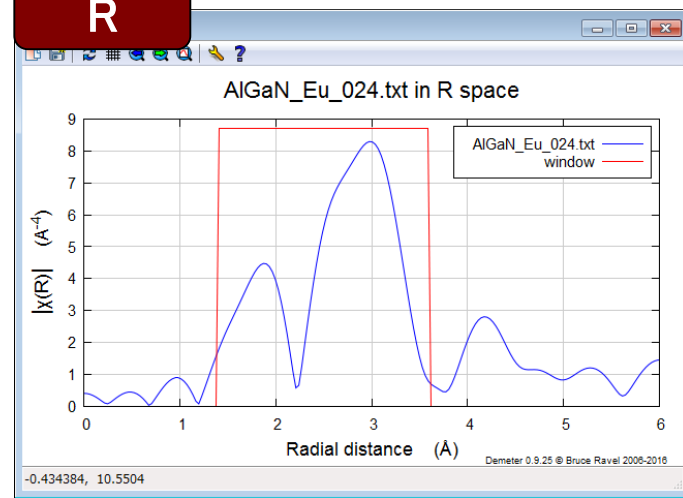
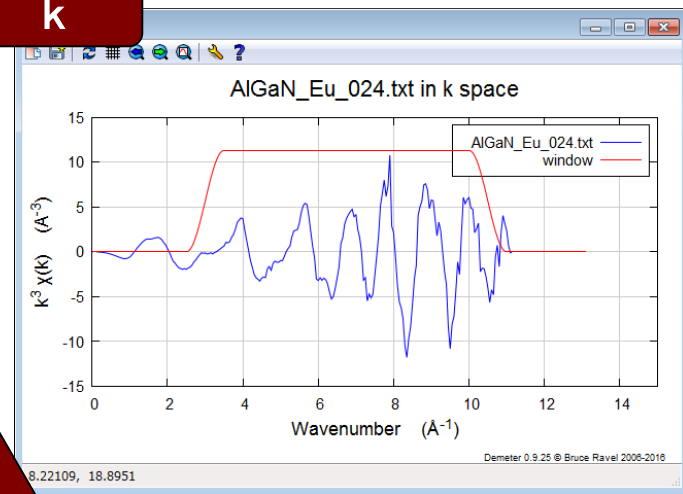
Plotting list: Data: AlGa_N_Eu_024.txt

Freeze Clear

Save next plot to a file.

k

R



feff計算(Ⅱ族サイト置換型)

Artemis [Feff] Atoms and Feff

② Run Feffをクリック

Run Feff

Name: Ga-site Margin: 0.03 Beta: 3 nlegs: 4 6

Feff input file

```

TITLE GaN
HOLE 4 1.0 * FYI: (Ga K edge @ 10367 eV, second number is S0^2)
* mphase,mpath,mfeff,mchi
CONTROL 1 1 1 1
PRINT 1 0 0 0

RMAX 5.0
*POLARIZATION 0.0 0.0 0.0

POTENTIALS
* ipot Z tag
0 63 Eu
1 31 Ga
2 7 N
3 13 Al

ATOMS
* this list contains 183 atoms
* x y z ipot tag distance
0.00000 0.00000 0.00000 0 Eu1 0.00000
0.00000 0.00000 2.20000 2 Ni.1 2.20000
2.07536 0.00003 -0.72399 2 Ni.2 2.20000
-1.03771 -1.73730 -0.72399 2 Ni.2 2.20000
-1.03769 -1.73732 -0.72397 2 Ni.2 2.20000
1.83842 0.00003 2.58800 1 Ga1.1 3.17509
-0.31974 -1.53237 2.58800 1 Ga1.1 3.17509
1.83842 0.00003 -2.58800 1 Ga1.1 3.17509
-0.31974 -1.53237 -2.58800 1 Ga1.1 3.17509
-0.31974 1.53303 2.58800 1 Ga1.1 3.17512
-0.31974 1.53303 -2.58800 1 Ga1.1 3.17512
2.75916 1.53300 0.00000 3 Al1.2 3.17600
-2.75916 1.53300 0.00000 3 Al1.2 3.17600
0.00000 3.18600 0.00000 3 Al1.2 3.17600
2.75916 -1.53300 0.00000 1 Ga1.2 3.17600
-2.75916 -1.53300 0.00000 1 Ga1.2 3.17600
    
```

Artemis [Feff] Atoms and Feff

Name of this Feff calculation: GaN_Eu_feff

Description

```

# TITLE GaN
# This paths.dat file was written by Demeter 0.9.25
# The central atom is denoted by this token: @
# Cluster size = 5.00 A, containing 182 atoms
# 29 paths were found within 5.000 A
# Forward scattering cutoff 20.00
# Distance fuzz = 0.030 A
    
```

Scattering Paths

Degen	Reff	Scattering path	Rank	L	Type
1	4.00	2.200 @ Ni.1 @	100.00	2	single scattering
2	9.00	3.179 @ Ga1.1 @	100.00	2	single scattering
3	3.00	3.186 @ Al1.2 @	31.57	2	single scattering
4	1.00	3.235 @ Ni.3 @	9.46	2	single scattering
5	18.00	3.628 @ Ni.2 Ga1.1 @	11.31	2	other double scatter
6	6.00	3.633 @ Ni.2 Al1.2 @	6.35	2	other double scatter
7	9.00	3.732 @ Ni.4 @	57.41	2	single scattering
8	12.00	3.996 @ Ni.1 Ni.2 @	14.23	2	other double scatter
9	9.00	4.078 @ Ni.2 Ga1.1 Ni.2 @	3.48	2	dog-leg
14	4.00	4.400 @ Ni.1 @ Ni.1 @	6.98	2	rattle
15	12.00	4.400 @ Ni.2 @ Ni.2 @	6.85	2	hinge
16	24.00	4.430 @ Ga1.1 Ni.4 @	8.56	2	other double scatter
17	12.00	4.432 @ Al1.2 Ni.4 @	5.44	2	other double scatter
18	6.00	4.498 @ Ga1.3 @	27.25	2	single scattering
19	6.00	4.540 @ Ni.6 @	21.53	2	single scattering
20	36.00	4.562 @ Ni.2 Ni.4 @	12.27	2	other double scatter
21	24.00	4.625 @ Ni.2 Ga1.1 @	8.74	2	other double scatter
22	12.00	4.629 @ Ni.2 Al1.2 @	4.37	2	other double scatter
23	12.00	4.631 @ Ni.1 Ni.2 @	3.66	2	obtuse triangle

① 変更箇所の確認

- HOLE : 1(K-edge) → 4(L₃-edge)
- 中心原子(ipot 0) : Ga(Z=31) → Eu(Z=63)
- 中心原子のtag : Ga1 → Eu1
- 最近接原子Nのxyz座標を変更
- 一部の第二近接原子GaをAl(ipot 3)に置き換える

実験値と理論計算(互換型)の比較

Dege	Path	Scattering path	Rank	Type
1	4.00	2.200 @ N1.1 @	100.00	single scattering
2	3.00	3.175 @ Ga1.1 @	100.00	single scattering
3	3.00	3.186 @ Al1.2 @	31.57	single scattering
4	1.00	3.235 @ N1.3 @	9.46	single scattering
5	18.00	3.628 @ N1.2 Ga1.1 @	11.31	other double scatter
6	6.00	3.633 @ N1.2 Al1.2 @	6.35	other double scatter
7	3.00	3.732 @ N1.4 @	57.41	single scattering
8	12.00	3.996 @ N1.1 N1.2 @	14.23	other double scatter
9	3.00	4.078 @ N1.2 @ N1.1 N1.2 @	3.43	dog-leg
14	4.00	4.400 @ N1.1 @	6.98	rattle
15	12.00	4.400 @ N1.1 N1.2 @	6.85	hinge
16	24.00	4.432 @ Ga1.1 N1.4 @	8.56	other double scatter
17	12.00	4.432 @ Al1.2 N1.4 @	5.44	other double scatter
8	9.00	4.498 @ Ga1.3 @	27.25	single scattering

① Ctrlキーを押しながら Path1-3,7を選択し、Dataウィンドウにドロップ (Path4-6は寄与が低い)

Artemis [Data] AlGaEu_024.txt

Data source: C:\20170131\AlGaEu_exp.prj, 1

Plot this data set as: k123, R123, Rmr, Rk

Fourier transform parameters: kmin 3, kmax 10.5, dk 1, rmin 1.4, rmax 3.6, dr 0.0

② 各Pathのアイコンをクリック

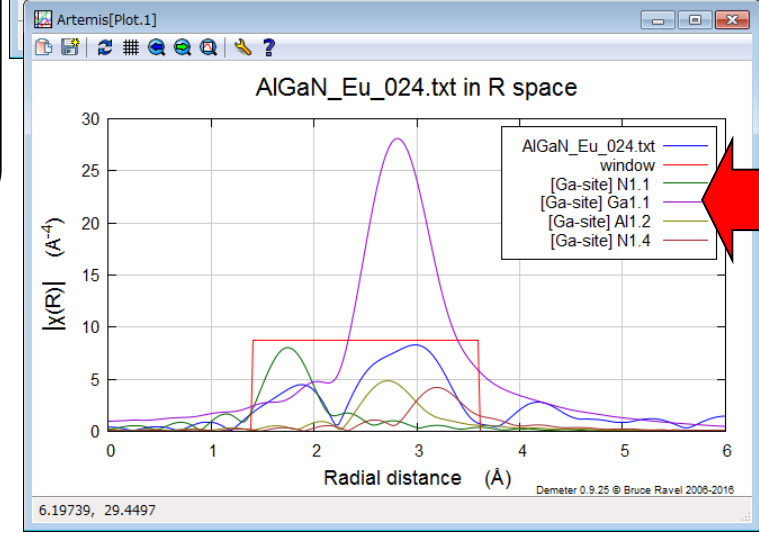
③ Rをクリック

Artemis [Ga-site] AlGaEu_024.txt

Include path: [Ga-site] N1.1, [Ga-site] Ga1.1, [Ga-site] Al1.2, [Ga-site] N1.4

Plot x(q): Magnitude, Real, Imag.

Plot x(q): Magnitude, Real, Imag.



Artemis [Plot.1]

Plotting list: Data: AlGaEu_024.txt, Path: [Ga-site] N1.1 from AlGaEu_024.txt, Path: [Ga-site] Ga1.1 from AlGaEu_024.txt, Path: [Ga-site] Al1.2 from AlGaEu_024.txt, Path: [Ga-site] N1.4 from AlGaEu_024.txt

Pathの足し合わせ(Ⅲ族サイト置換型)

① すべてのPathをチェック

② Dataウィンドウのメニューから Action - Make sum of marked paths and plot in R を選択

③ VPath名に Ga-site と入力

④ DataとVPath以外のチェックを外す

⑤ Rをクリック

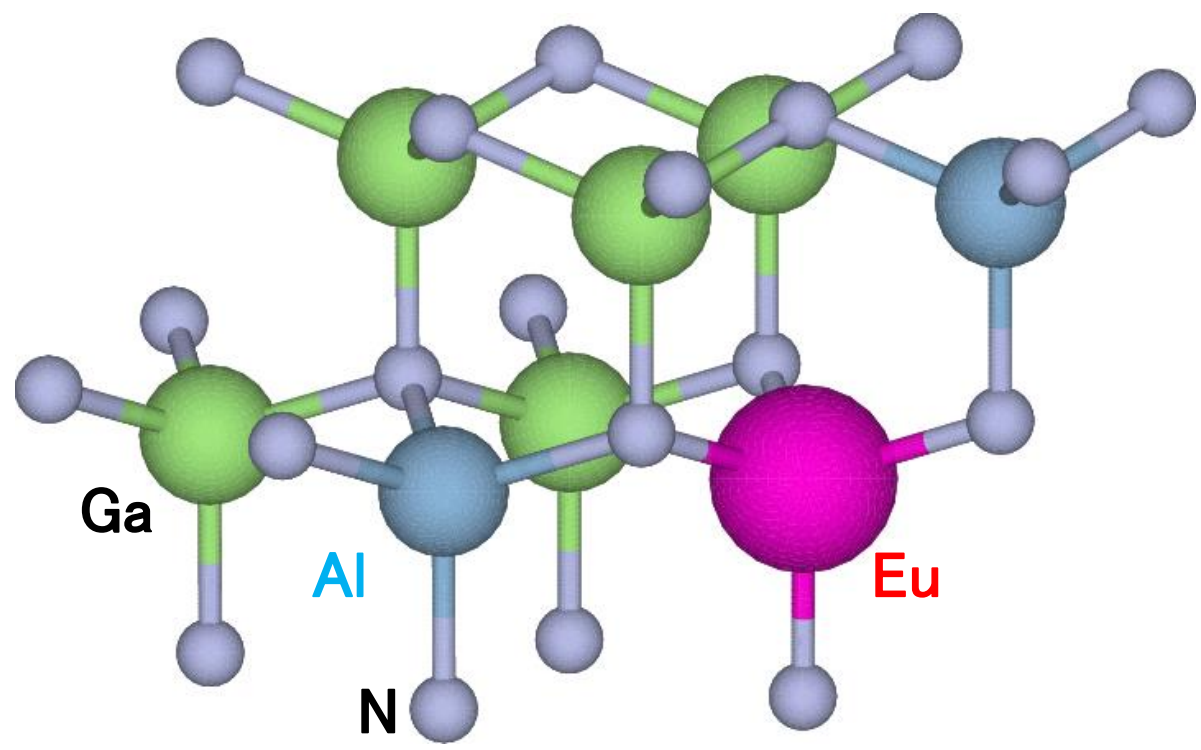
⑥ 選択したPathの足し合わせを表示

The plot window shows the resulting plot with the following legend:

- AIGaN_Eu_024.txt (Blue line)
- window (Red line)
- Ga-site (Green line)

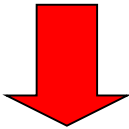
The plot axes are labeled $|x(R)|$ (Y-axis) and Radial distance (Å) (X-axis). The plot shows a prominent peak at approximately 3.0 Å.

カーブフィッティング (Ⅲ族サイト置換型(Eu添加AlGaN))



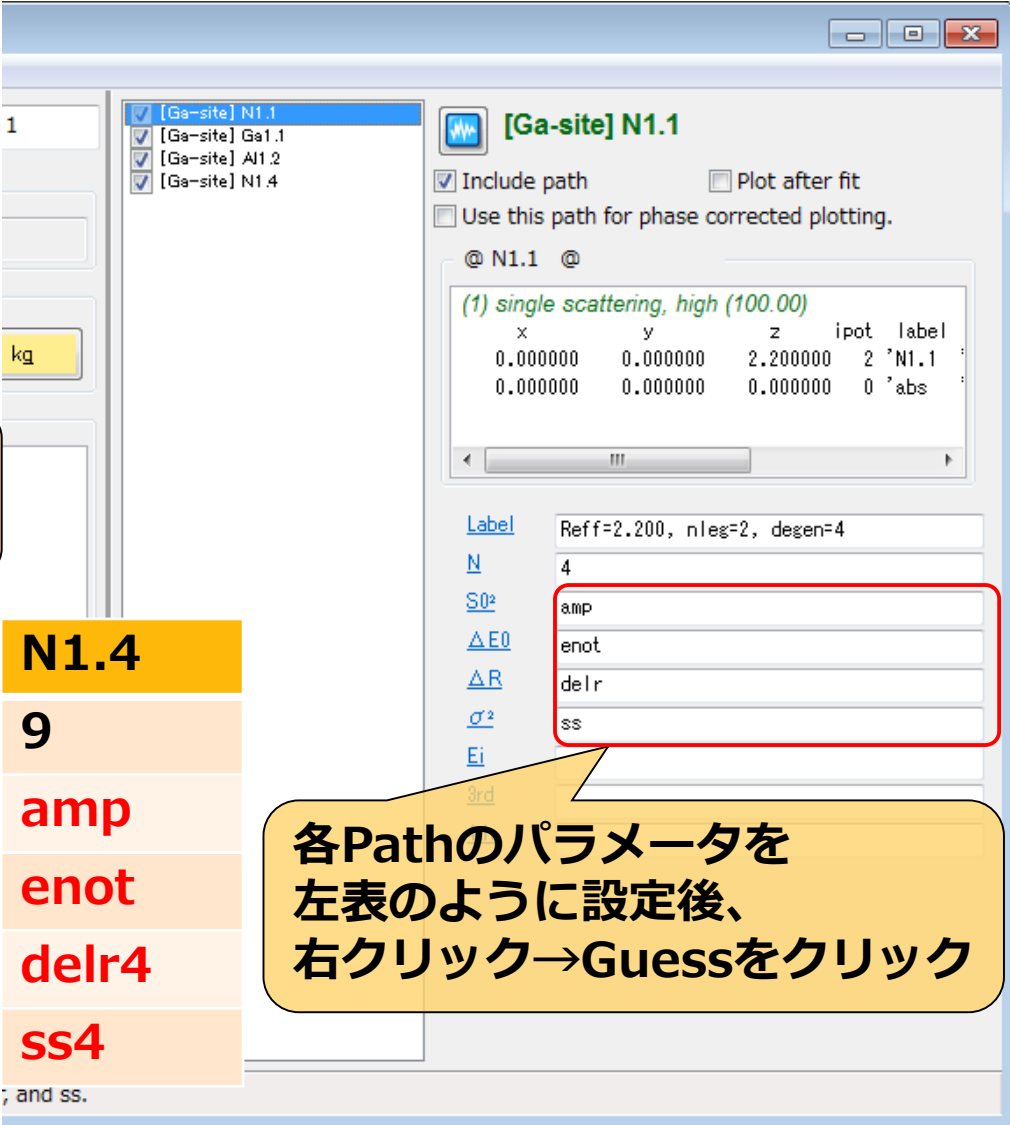
パラメータの設定(Ⅲ族サイト置換型)

第二近接原子の配位数 : 12
 Ga組成 : 0.76
 Al組成 : 0.24



Gaの配位数 : $12 \times 0.76 = 9.12$
 Alの配位数 : $12 \times 0.24 = 2.88$

	N1.1	Ga1.1	Al1.2	N1.4
N	4	9.12	2.88	9
S0 ²	amp	amp	amp	amp
ΔE0	enot	enot	enot	enot
ΔR	delr	delr2	delr3	delr4
σ ²	ss	ss2	ss3	ss4



[Ga-site] N1.1

Include path Plot after fit

Use this path for phase corrected plotting.

@ N1.1 @

(1) single scattering, high (100.00)

x	y	z	ipos	label
0.000000	0.000000	2.200000	2	'N1.1
0.000000	0.000000	0.000000	0	'abs

Label Reff=2.200, nleg=2, degen=4

N 4

S0² amp

ΔE0 enot

ΔR delr

σ² ss

Ei

3rd

and ss.

各Pathのパラメータを左表のように設定後、右クリック→Guessをクリック

パラメータの変更(卍族サイト置換型)

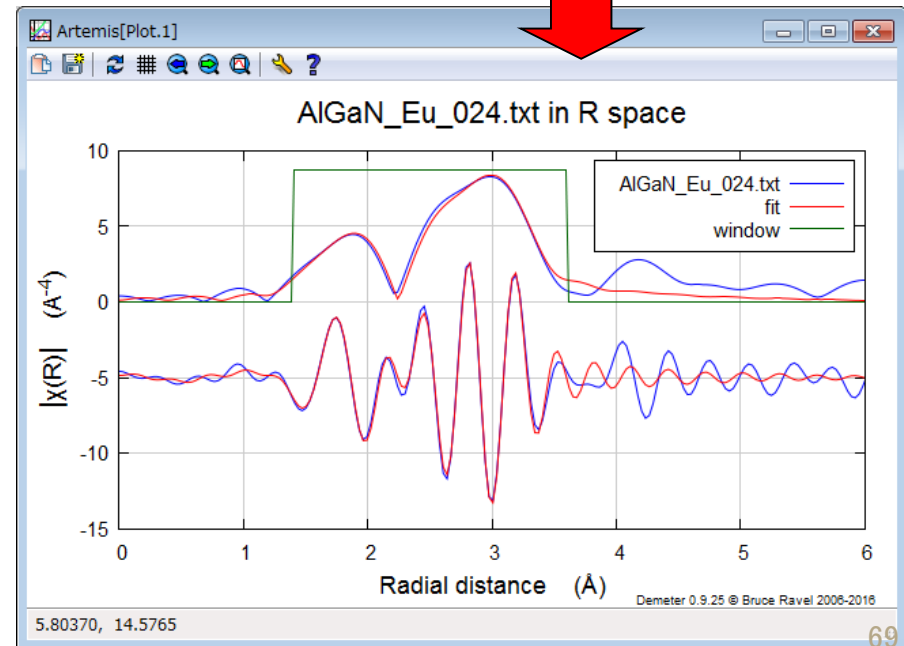
Artemis [GDS] Guess, Def, Set parameters

	Type	Name	Math expression	Evaluated
1	set	amp	0.833	
2	guess	enot	0	
3	guess	delr	0	
4	guess	ss	0.00300	
5	guess	delr2	0	
6	guess	ss2	0.00300	
7	guess	delr3	0	
8	guess	ss3	0.00300	
9	guess	delr4	0	
10	guess	ss4	0.00300	
11	guess			
12	guess			

Use best fit
Reset all
Highlight
Evaluate
Import GDS
Export GDS
Discard all
Add GDS
About: GDS



① ampをGuessからsetに変更し、
Math expressionを0.833に変更



フィッティング結果(Ⅱ族サイト置換型)

```

Independent points      : 10.3310547
Number of variables    : 9
Chi-square             : 78.3027993
Reduced chi-square     : 58.8276350
R-factor               : 0.0085126
Number of data sets   : 1
    
```

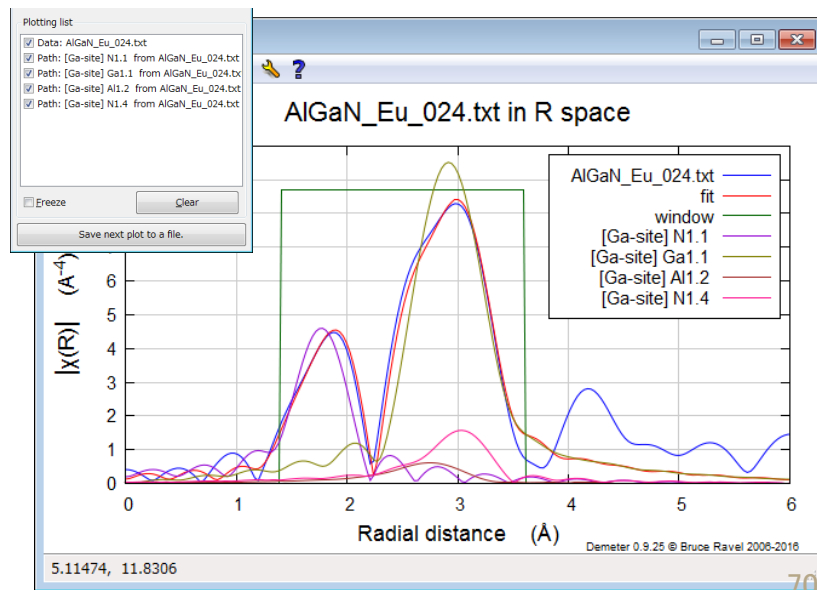
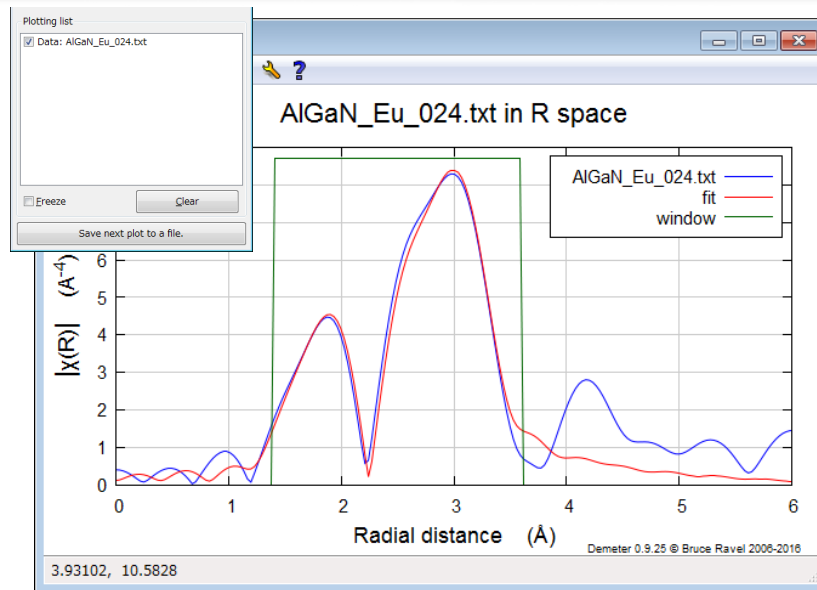
```

Happiness = 75.46/100          color = #FEC684
Used 9 of 10.331 independent points for a penalty of 24.539
***** Note: happiness is a semantic parameter and should *****
***** NEVER be reported in a publication -- NEVER! *****
    
```

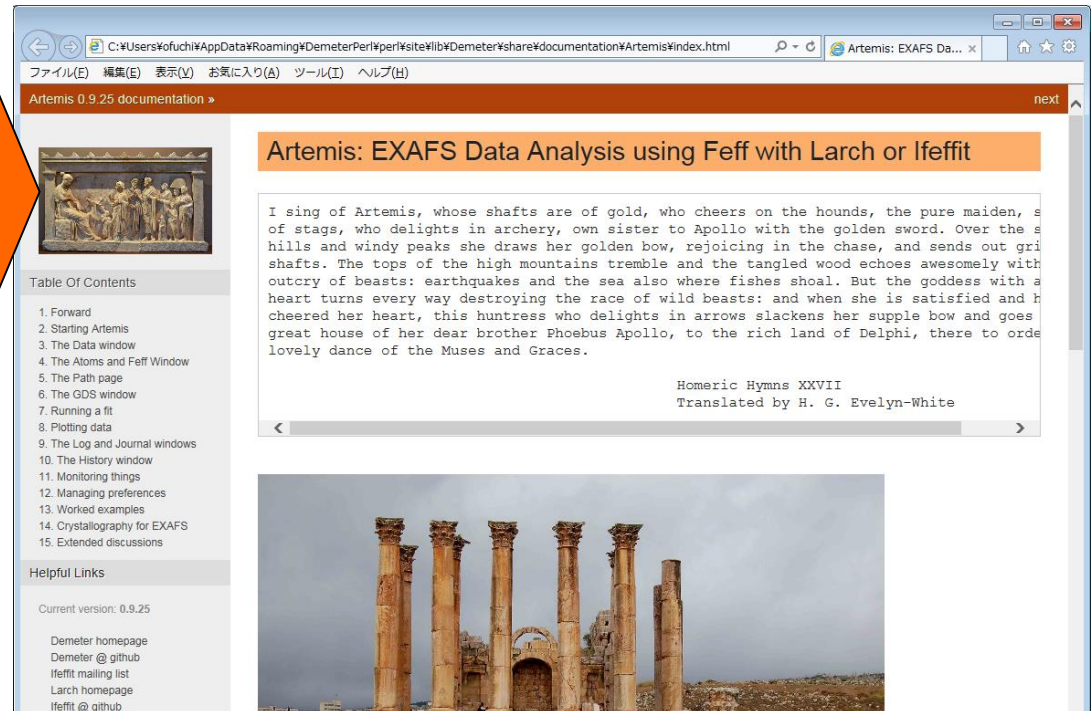
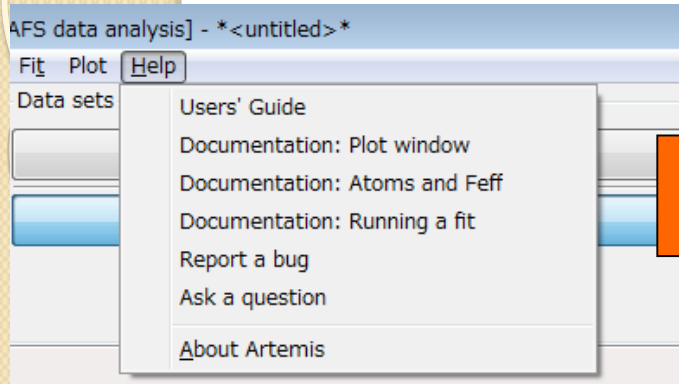
guess parameters:

enot	=	6.52933613	# +/-	4.61178939	[0]
delr	=	0.00526280	# +/-	0.03464803	[0]
ss	=	0.00426398	# +/-	0.00214664	[0.00300]
delr2	=	0.07558349	# +/-	0.01580759	[0]
ss2	=	0.00587195	# +/-	0.00173998	[0.00300]
delr3	=	0.06709850	# +/-	0.45434628	[0]
ss3	=	0.02003908	# +/-	0.04215019	[0.00300]
delr4	=	-0.17898697	# +/-	0.09329982	[0]
ss4	=	0.01080335	# +/-	0.03990845	[0.00300]

いずれのパラメータも妥当な値



- ① パラメータ数は出来るだけ少なく
 - ・ 原子間距離の近いPathは1つにまとめる
 - ・ 場合によっては配位数を固定する
 - ・ 標準試料から S_0^2 の値を求めて未知試料に適用する
- ② 初期パラメータは出来るだけ実験値に近く
 - ・ 実験値から大きくずれていると収束しない場合がある
- ③ フィッティングにより得られたパラメータの確認
 - ・ 値が大きくずれる場合はモデルを再検討する



Html版マニュアル

<https://bruceravel.github.io/demeter/documents/Artemis/index.html>

各種参考情報

<http://xafs.org/Tutorials>

特にShelly D. Kelly 氏(Argonne Natl. Lab.) のAthenaとArtemisに関するtutorial

http://xafs.org/Tutorials?action=AttachFile&do=get&target=Basics_of_XAFS_to_chi.pdf

http://xafs.org/Tutorials?action=AttachFile&do=get&target=Basics_of_XAFS_analysis.pdf

Iffeffitのメーリングリスト (Iffeffit, Athena, Artemisの開発者から回答してもらえる)

<http://millenia.cars.aps.anl.gov/mailman/listinfo/iffeffit/>

メーリングリストのアーカイブ (過去に同様な質問がされていないかどうか確認しておく)

<http://millenia.cars.aps.anl.gov/pipermail/iffeffit/>

- Bruce Ravel XAS course 2011
(2011年にDiamond Light Sourceで行われたXAS training courseのビデオ映像)

<http://www.diamond.ac.uk/Beamlines/Spectroscopy/Techniques/XAS.html>

- XAS Education
(Ravel氏がXAS training courseで用いた各種ドキュメント)

<http://bruceravel.github.io/XAS-Education/>

- XAFS for Everyone
(Scott Calvin, CRC Press)

XAFS解析に重点を置いた参考書

解析手法や解析の手順、解析の際の注意点などが質疑応答形式で分かりやすく説明されている

<http://www.crcpress.com/product/isbn/9781439878637>

