IWMC 2024

Z-Rietveld and its cooperation with other magnetic crystallography tools

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Outline

Z-Rietveld

- background of development
- project and package
- user friendly interface
- problems on magnetic structure analysis

Demonstration of magnetic structure analysis

- simple case
- commensurate structure using irreducible representation
- commensurate and incommensurate structure using magnetic (super)space group

future and summary

Background

Since neutron powder diffraction at MLF, J-PARC was expected to

1) cover $S(Q)$ and SANS as well as Powder Diffraction:
Q (< 0.01 Å^{-1} & > 50 Å^{-1})
→ nano structure, crystal structure, and local structure

2) have the highest intensity or the highest resolution
→ operando studies/ real time/ *in situ* studies,
tiny distortion, peak broadening, complicated structures, *etc*...

3) adopt event data recording
→ each ~10^4 detector pixels have ~10^4 time channel

long-term development of various hard & software developments were considered

Development of Z-Code project

Z-Code Project (from credits)

member

Takashi Kamiyama (CSNS), Toru Ishigaki (CROSS), Yoshihisa Ishikawa (CROSS)

Masato Hagihala (JAEA),

Development of GUI

Innoface Inc.

algorism and program

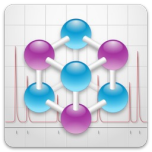
Ryoko Oishi-Tomiyasu (Kyushu Univ.), Satoshi Tamura(VIC)

former member

Masao Yonemura, Ryoko Oishi-Tomiyasu, Miao Ping, Junrong Zhang

Shanghyun Lee, Akinori Hoshikawa, Takashi Saito, Shuki Torii, Ryoji Kiyanagi,

Takahiro Morishima



Z-Rietveld software

Rietveld analysis for

- NPD for both TOF and angle-dispersive
- XRD data for both laboratory and synchrotron radiation
- Analysis of multiple histogram data
- Multi-points analyses

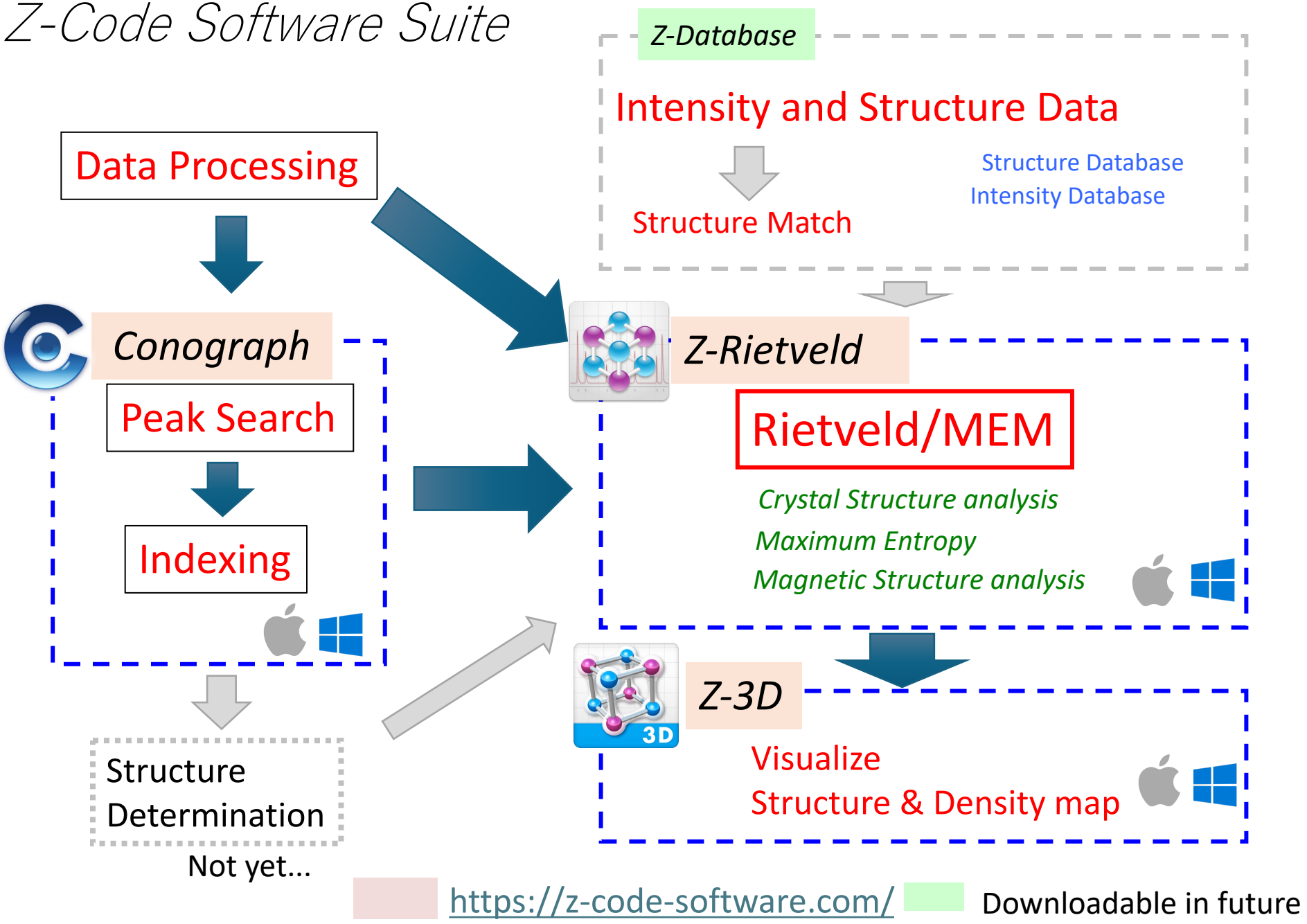
User friendly functions

- GUI based program
- Japanese/Korean/Chinese OS as well as English OS

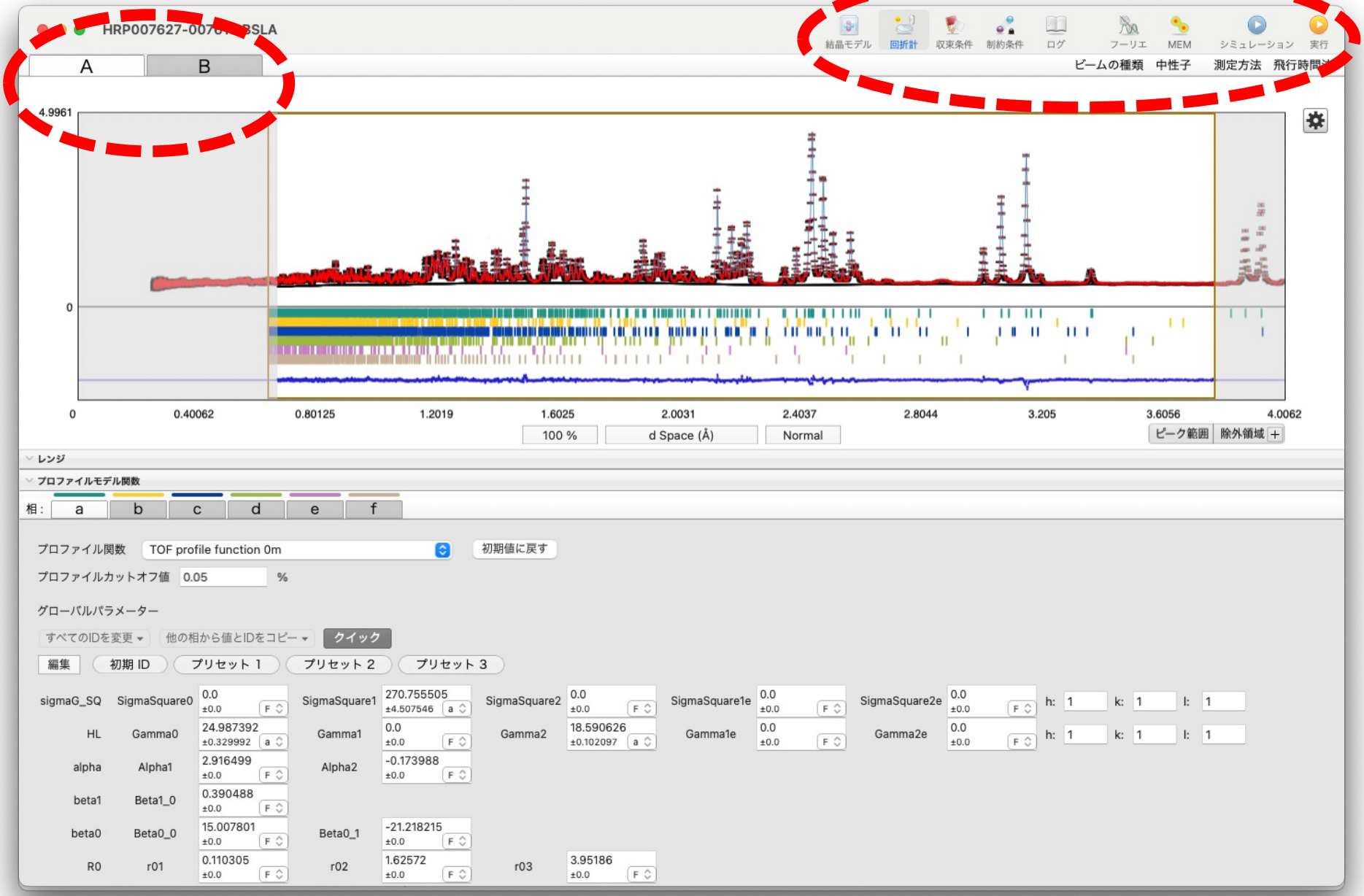
Advanced functions

- Inequality constraints available
- New global optimization using Sequential Quadratic Programming (conventional Levenberg-Marquardt Algorithm is also available)
- Pawley method, and joint Pawley and Rietveld analysis
- MEM and Fourier analysis

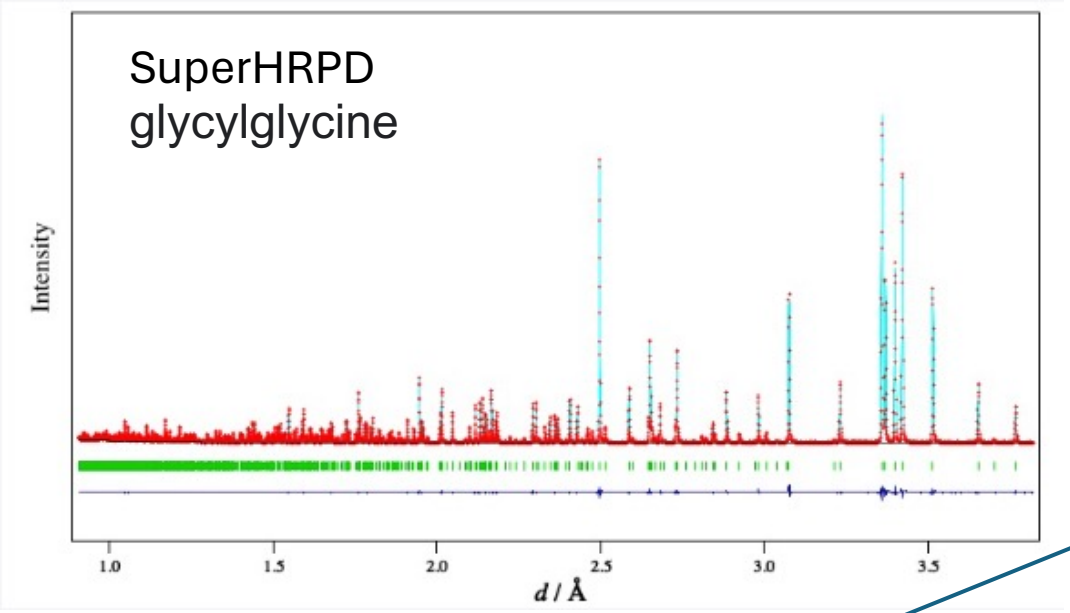
Z-Code Software Suite



Z-Rietveld user friendly interface



Z-Rietveld Advanced functions 1



Pawley method

high degree of freedom

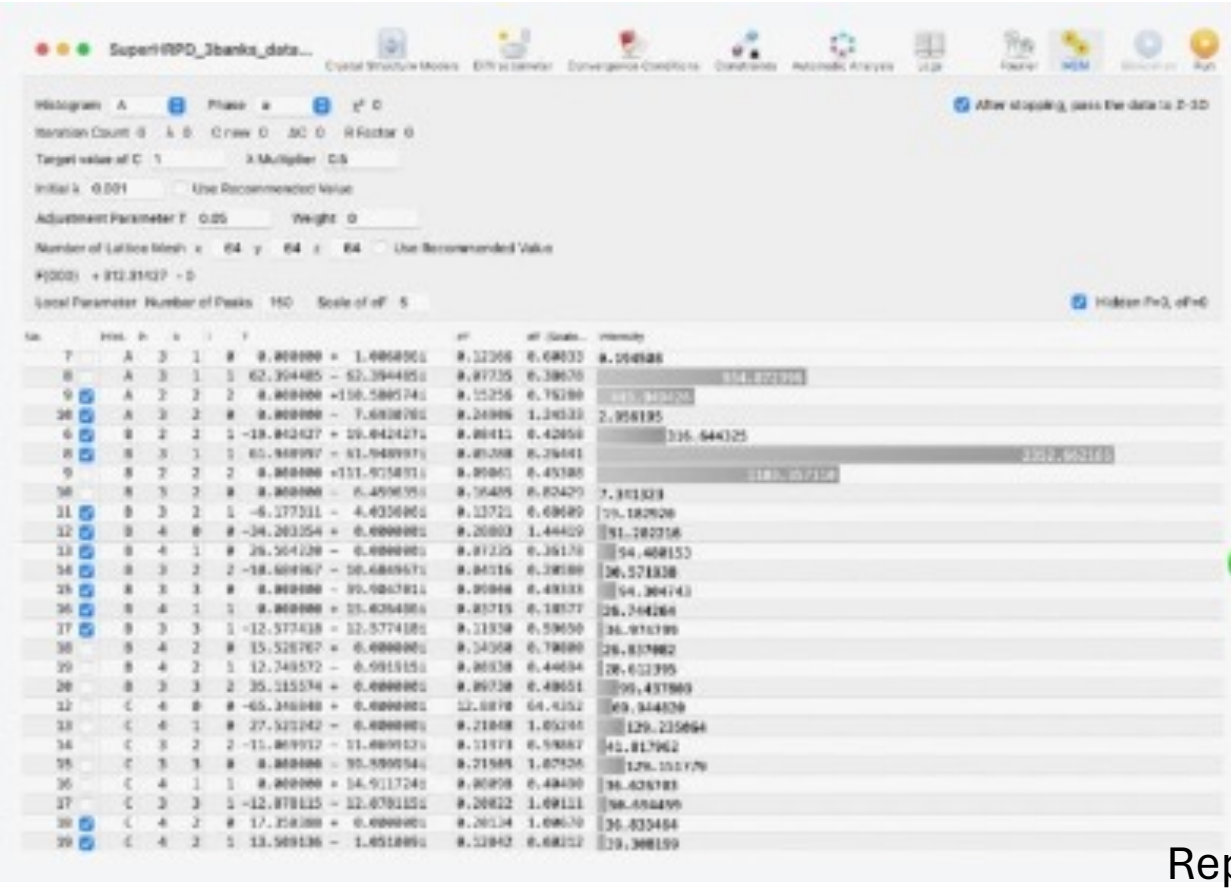
combination of
sort and limited range function
is very useful

ローカルパラメーター　Line　～　フィルターを解除　すべて選択解除

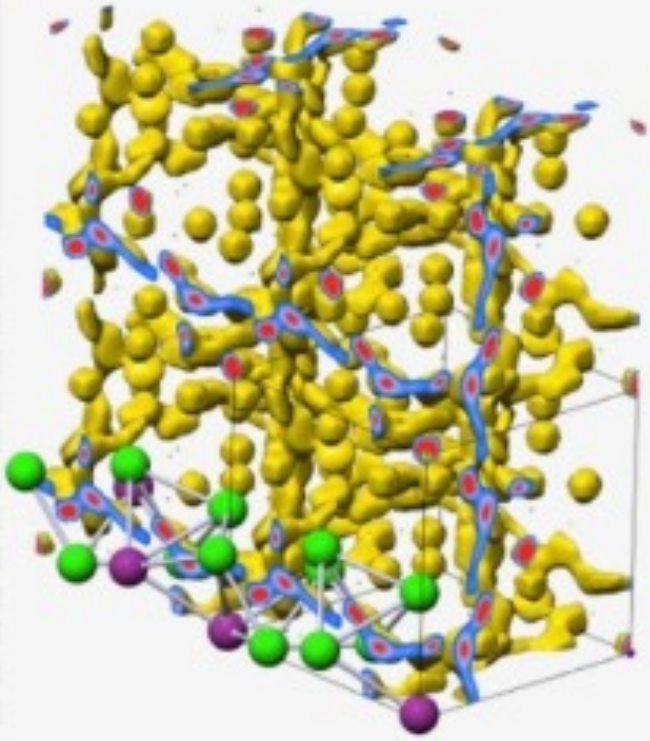
Line	No.	h	k	l	Peak Position	d	Intensity	sigmaG_SQ	HL	alpha	beta1	beta0	R0
1	1	2	1	0	186486.1452... ±0.087073 D	3.913753	27.15 ±0 V	2147.4 ±19.5 D	5.0963 ±0.4864 D	0.4767 ±0 D	0.4557 ±0 D	2.3561 ±0 D	0.104 ±0 D
2	2	1	0	2	179587.0852... ±0.104423 D	3.768958	440.47 ±3.23 V	1979.1 ±15.8 D	5.5648 ±0.4171 D	0.4671 ±0 D	0.4557 ±0 D	2.4128 ±0 D	0.104 ±0 D
3	3	1	2	1	176416.5725... ±0.059156 D	3.702417	104.17 ±2.2 V	1904.5 ±14.3 D	5.7608 ±0.3874 D	0.4629 ±0 D	0.4557 ±0 D	2.4403 ±0 D	0.1039 ±0 D
4	4	2	0	-2	174100.618781 ±0.087197 D	3.653811	852.64 ±3.79 V	1851.1 ±13.3 D	5.8963 ±0.3665 D	0.4598 ±0 D	0.4557 ±0 D	2.4611 ±0 D	0.1039 ±0 D
5	5	1	1	2	167519.4696... ±0.080933 D	3.515689	1935.4 ±5 V	1704.2 ±10.7 D	6.2457 ±0.3115 D	0.4514 ±0 D	0.4557 ±0 D	2.5231 ±0 D	0.1038 ±0 D
6	6	2	1	-2	163039.95206	3.421676	3626.2	1608.3	6.4536	0.4458	0.4557	2.5683	0.1037

Z-Rietveld Advanced functions 2

MEM analysis



visualized by Z-3D



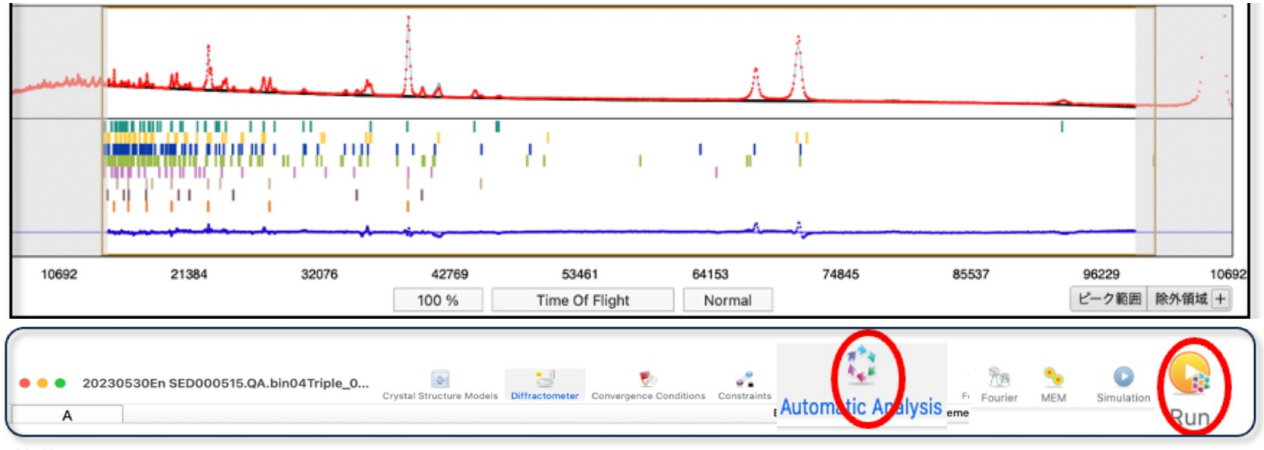
Represents the positive and negative density of the scattering length

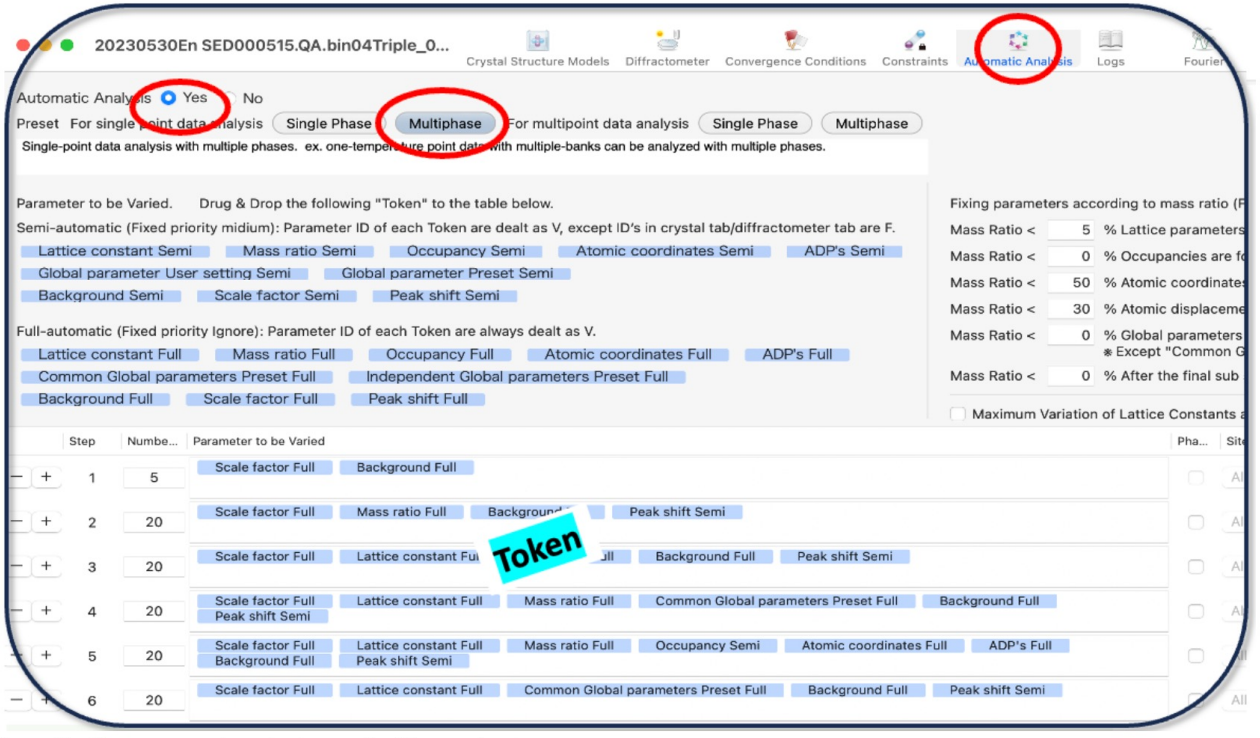
support to multi-histograms

with sorting function of Bragg reflection based on standard deviation

Z-Rietveld Advanced functions 3

Extensive automatic successive histogram analysis function





Please check if you're interested in these advanced functions.
https://z-code-software.com/new-features-of-z-rietveld-2-0-0/

Z-Rietveld for magnetic structure analysis

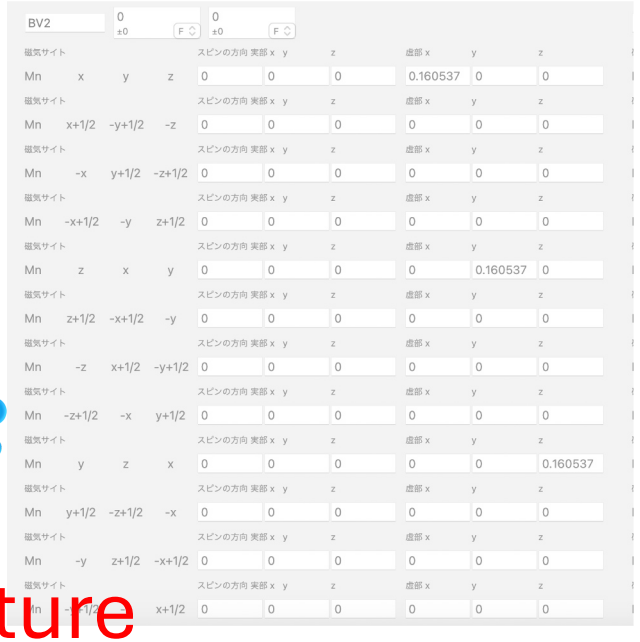
In this time, magnetic structure analysis can be carried out by Z-Rietveld,

BUT it is not user friendly at all

Under construction

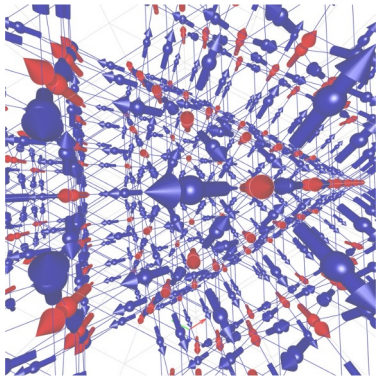
- i/o of .mcif files

- magnetic (super)space group
- irreducible representation
  input basis vectors manually💦



implement in the future

- visualization of magnetic structure
  using Z-mag program temporary

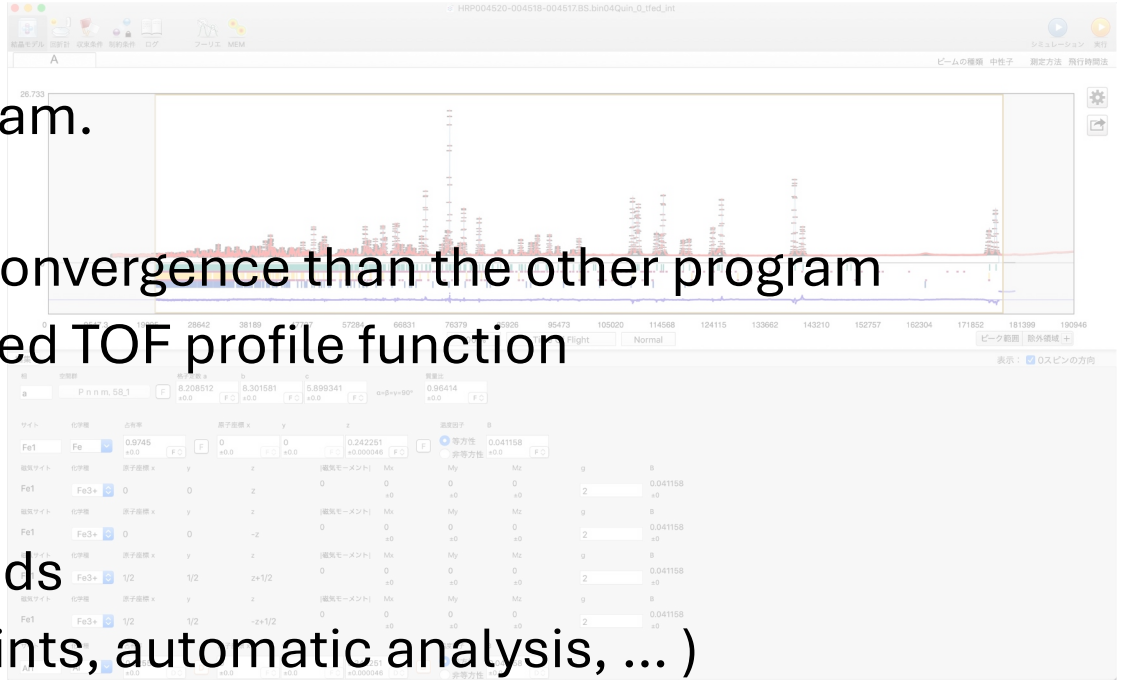


Motivation

We hope to make easier for any user
to do magnetic structure analysis.

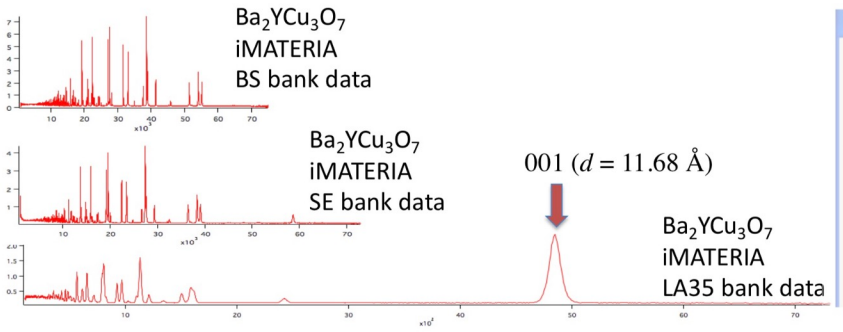
Z-Rietveld is

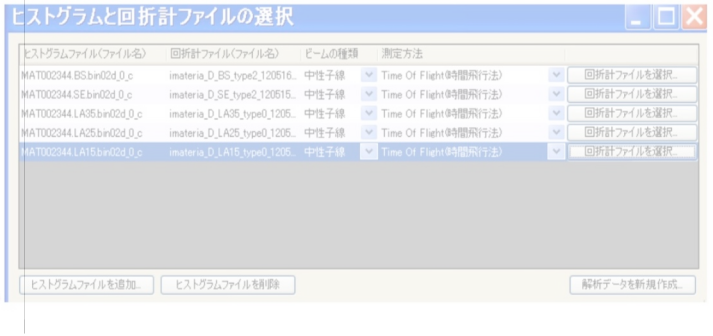
- User friendly GUI program.
- rarely divergence
  probably better convergence than the other program
- use of specially designed TOF profile function



moreover…

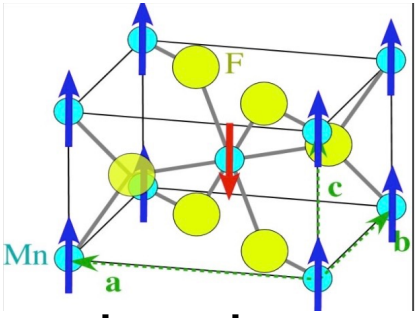
- aim to satisfy user needs
  (e.g. special constraints, automatic analysis, …)



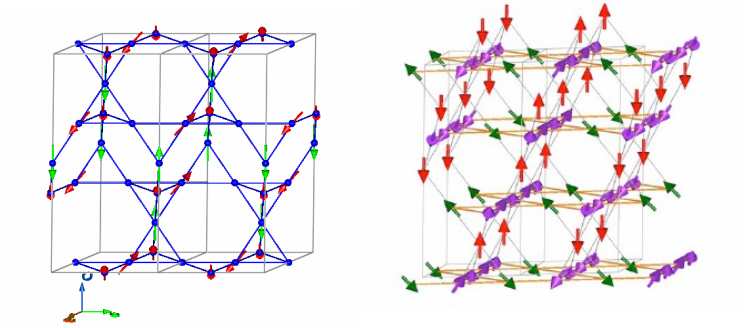


Example of magnetic structure analysis using current version

- MnF_2 antiferromagnetic

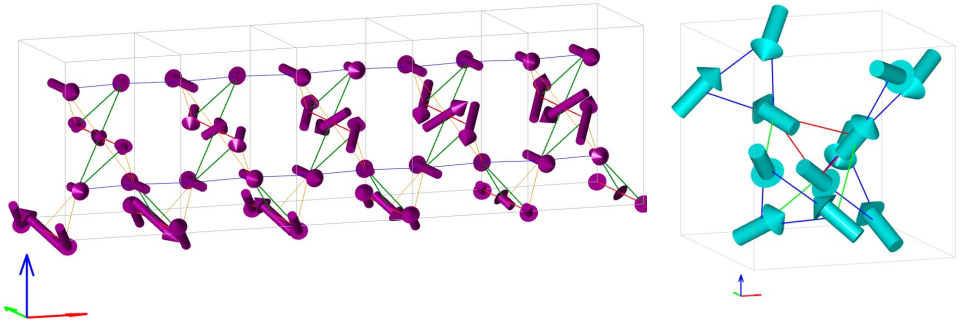


- $Co_2(OD)_3Br$ commensurate structure with multi-***q***

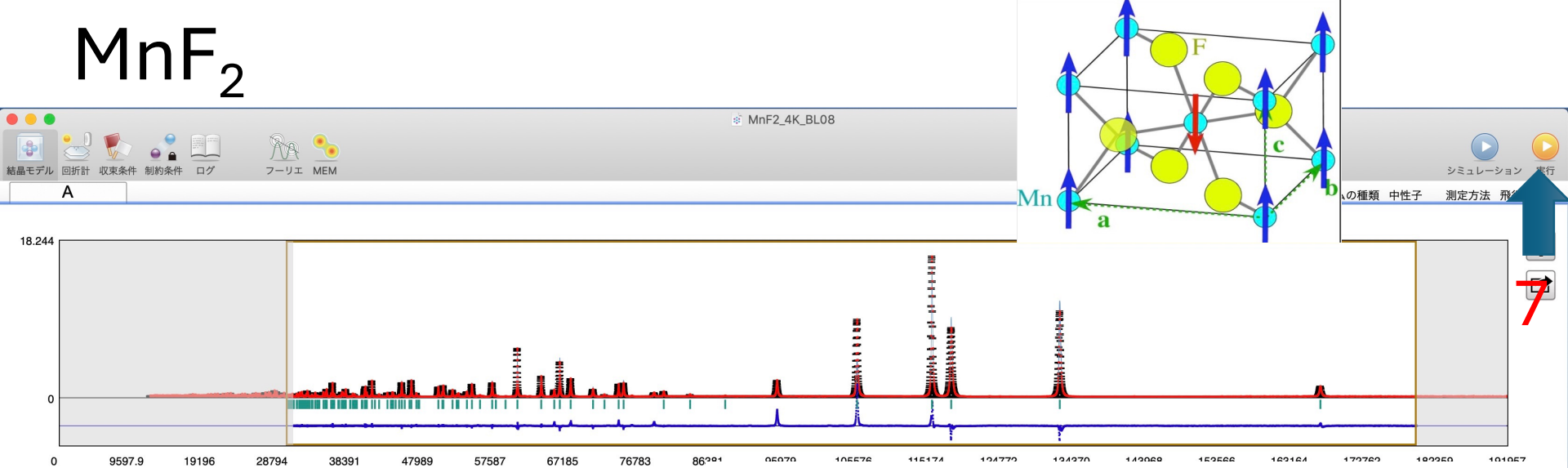


- incommensurate structure (multi-q)

Not shown in this slide. Sorry…



MnF_2

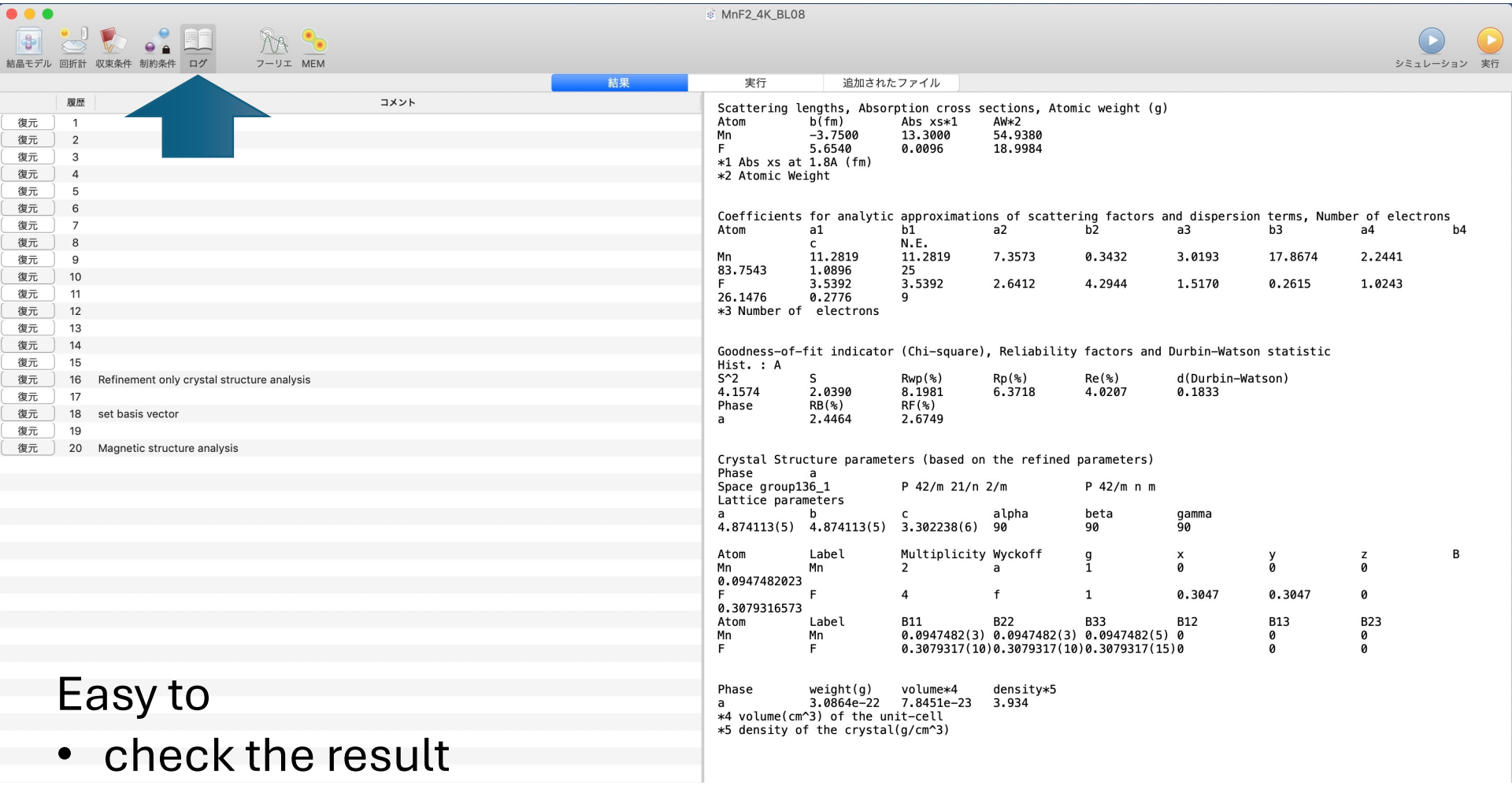


After setting the crystal structure

1. add magnetic phase (push 2 bottom)
2. choose magnetic atom (put check mark)
3. set ion for magnetic form factor

   (select in pull down menu)
4. set propagation vector
5. set basis vector(BV)
6. set coefficient of BV as variable
7. push refinement bottom

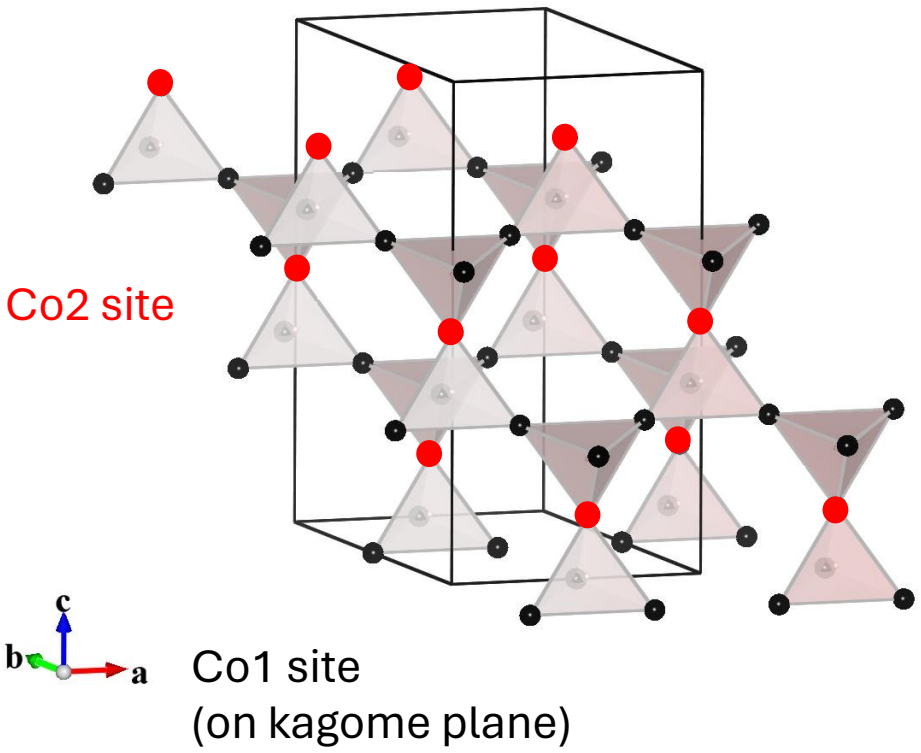
Load and save function

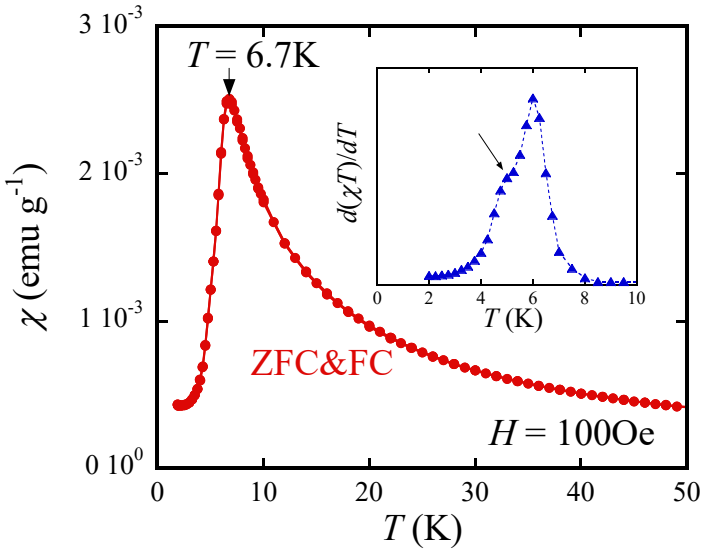


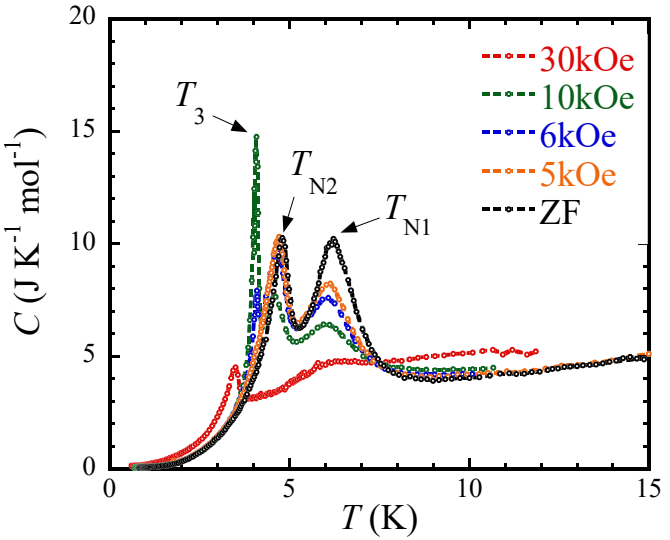
Easy to

- check the result
- go back previous result
- compare the results

$Co_2(OD)_3Br$ Space group:*R -3 m*





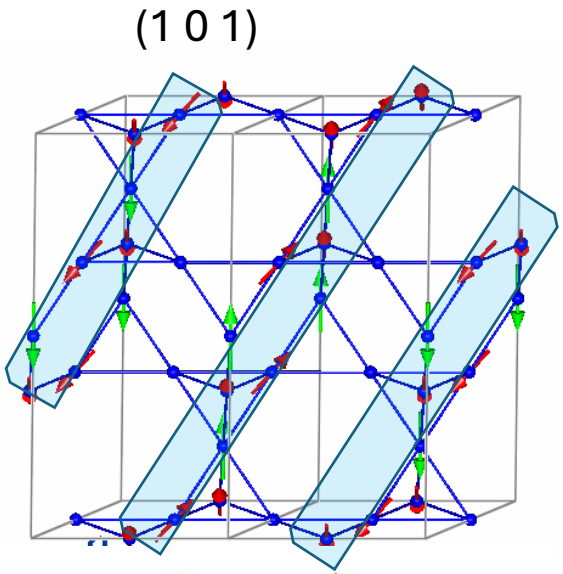


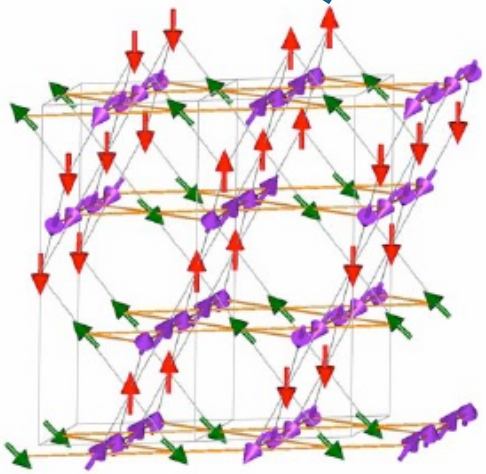
M. Hagihala, et. al., Phys. Rev. B **82**, 214424 (2010).

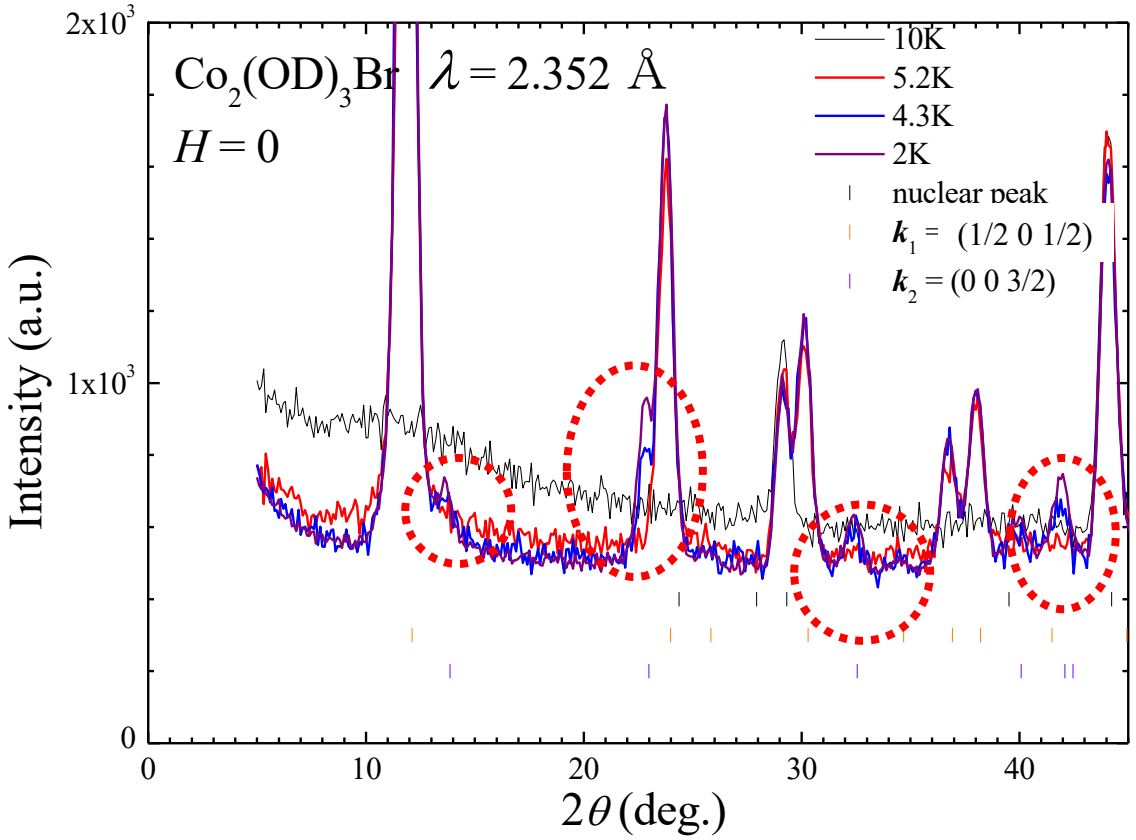
$Co_2(OH)_3Br$ is antiferromagnetic while $Co_2(OH)_3Cl$ is ferromagnetic ($\boldsymbol{k} = \mathbf{0}$)
Two successive transitions $T_{N1} = 6.2$K, $T_{N2} = 4.8$K

$Co_2(OH)_3Br$

4G:GPTAS
(JRR-3)



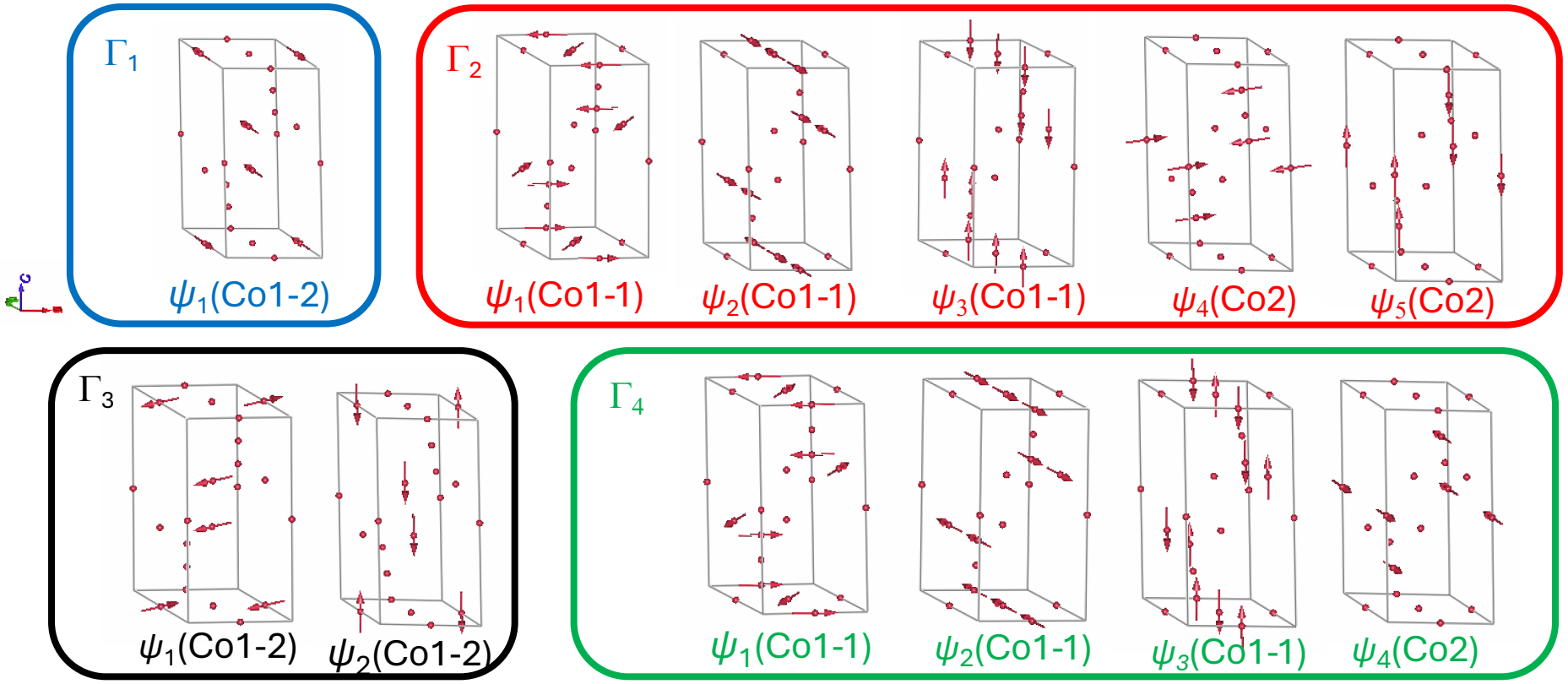




- Partial order phase with $\boldsymbol{k}_1$ =(1/2 0 1/2) at $T_{N2} < T < T_{N1}$
- All the spin order with $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ = (0 0 3/2) below T_{N2}

Irreducible Representation Analysis

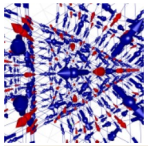
R-3m k=(1/2 0 1/2), Co1(1/2,0 ,0), Co2(0, 0, 1/2)



Unfortunately,
Basis vectors are input manually...
😭😭😭

Note that Z-Rietveld's BVs are defined as on the origin point.

Z-mag



log

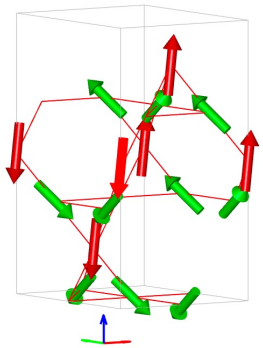
復元	50	
復元	51	
復元	52	Gamma2 fitting x^2=2.6255
復元	53	
復元	54	Gamma3 fitting x^2=3.4310
復元	55	
復元	56	Gamma2 fitting without BV4 x^2=2.6978

Finder ファイル 編集 表示 移動 ウインドウ ヘルプ

Figure 1

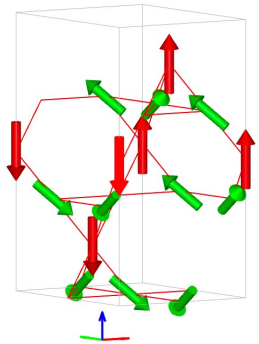
ファイル

52



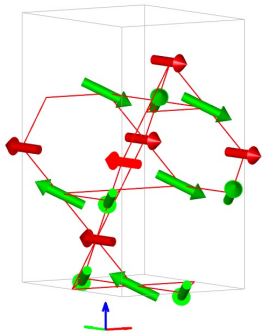
ファイル

56



ファイル

54



Input

ファイルパス:

/Users/masato/Downloads/14-23/

ファイル名:

Co2OD3Br_5p5K

相:

1

logの番号(0は最新のもの):

56

描画範囲:

0,1.2;0,1.2;0,1

磁気モーメントの長さ、太さの倍率、ヘッドの割合:

1,1,0.25

原子の倍率(0は表示しない):

0

図の番号:

3

磁気モーメント、原子の色(option):

Co1,[0,1,0];Co2,[1,0,0]

bondの描画(option):

Co1,Co1,0,4,[1,0,0],1;Co1,Co2,0,4,[1,0,0],1

Draw

Co2 (0, 1, 0.5)

m = 3.17(6)μ_B

$\boldsymbol{m}$ = (−5.4(6)x10^{-1}, −2.7(3)x10^{-1}, −3.13(6))

OK

Co2 (0, 0, 0.5)

m = 3.12(7)μ_B

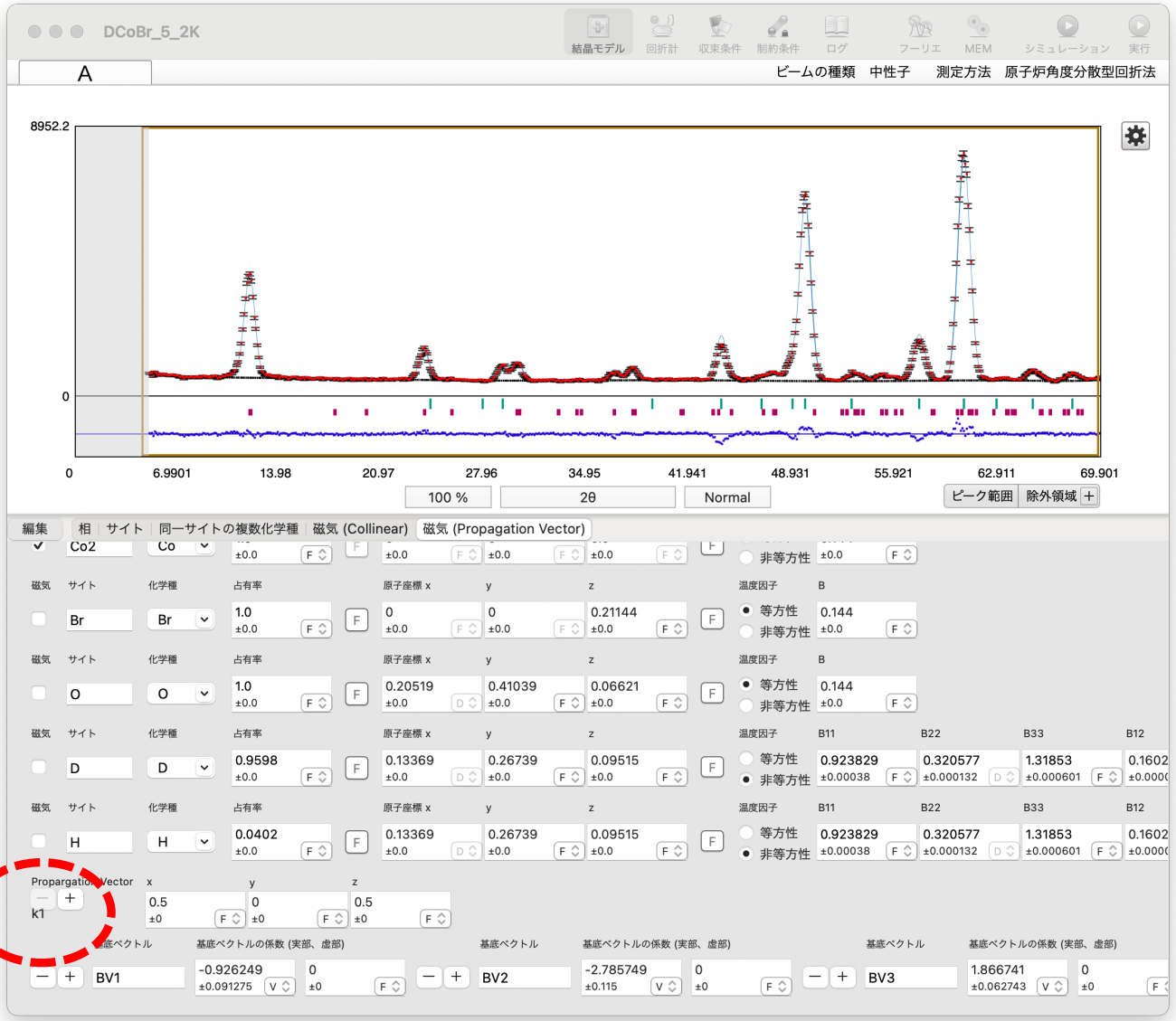
$\boldsymbol{m}$ = (0, 0, −3.12(7))

OK

スクリーンショット
2024-11...15.32.13

スクリーンショット
2024-11...16.00.06

treatment of multi-q structure



multi-q structure can be represented by additional propagation vector and basis vector.

In the future

Magnetic structure analysis

- Modification of input format
- i/o .mcif file
- Developed Semidefinite Relaxation of quadratic optimization

K. Tomiyasu et at., Scientific Report 8, 16228 (2018).

Z-Rietveld have a potential to be a powerful tool for magnetic structure analysis!

Z-Rietveld

- Rigid body analysis
- Automatic analysis system
- Simulation annealing

Summary

- Z-Code project and Z-Rietveld program
- Current state of magnetic structure analysis
  on Z-Rietveld
- Future plan of Z-Rietveld

We believe to enlarge user community of Z-Rietveld
by continuous developments and modifications!

Download software https://z-code-software.com/

Support mail pjzcode@gmail.com