



HFIR HB-2C WAND²

Rietveld Refinement of Constant Wavelength Neutron Diffraction Data (WAND²) Using GSAS-II

MagStr 2026, Duke University July 20-24

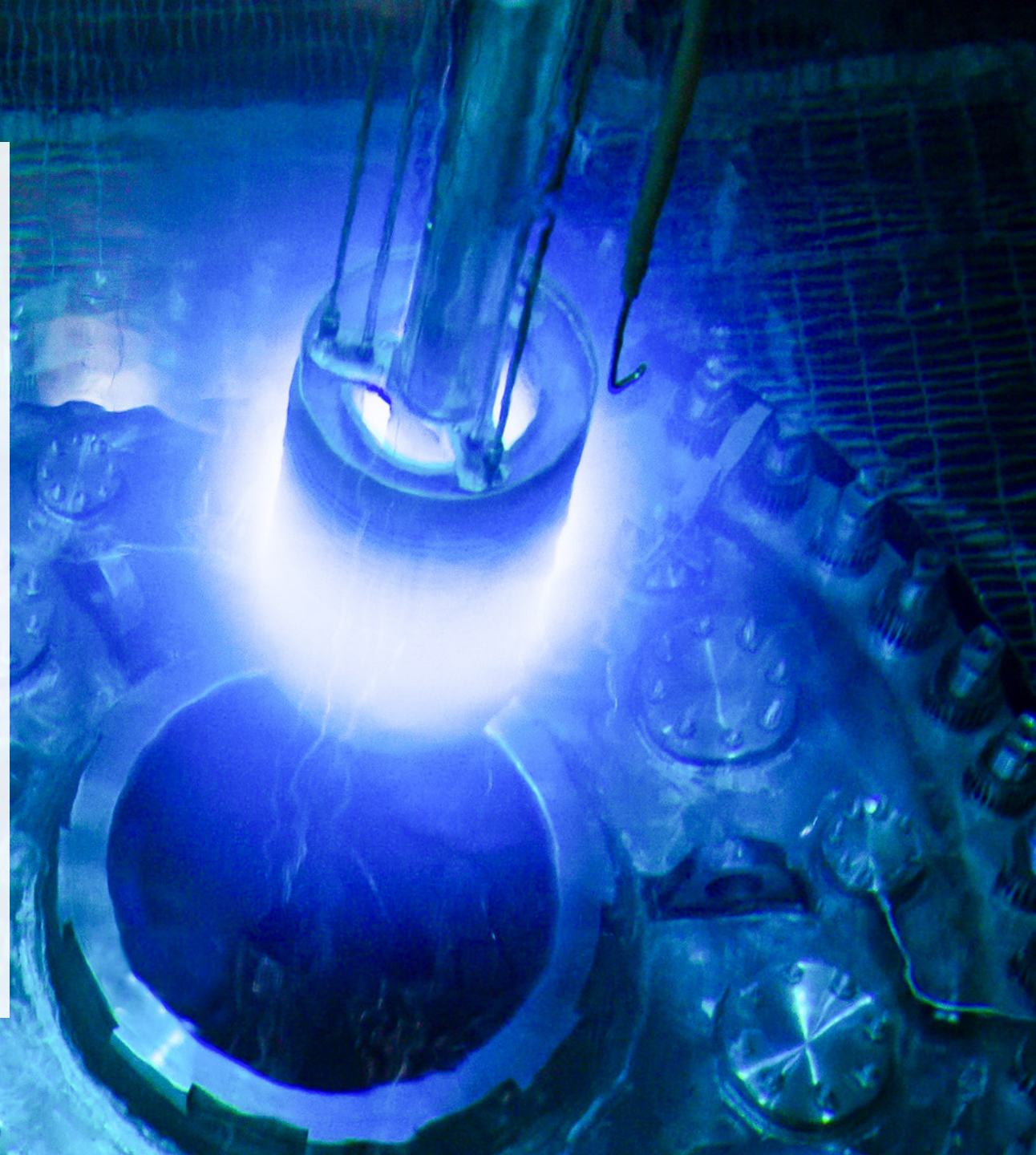
Si Athena Chen

Neutron Diffraction Scientist
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U.S. DEPARTMENT OF
ENERGY

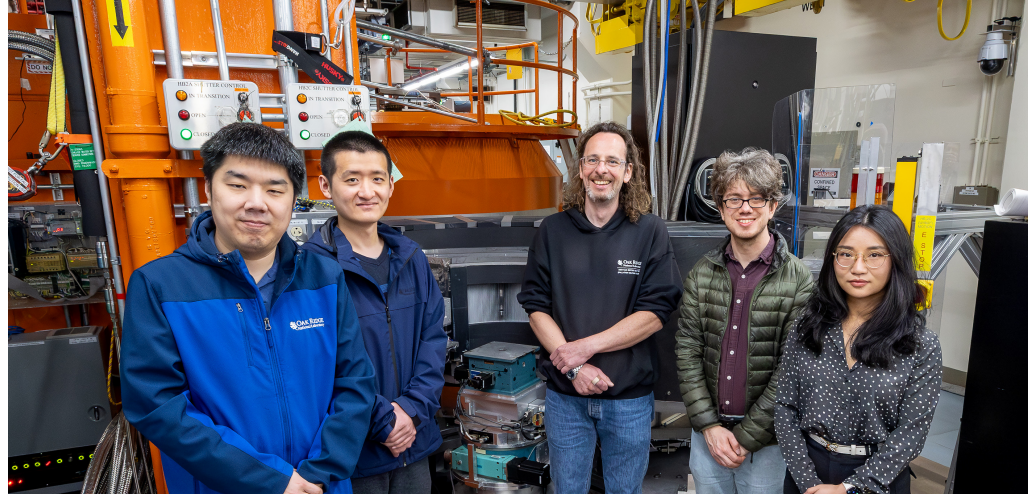
ORNL IS MANAGED BY UT-BATTELLE LLC
FOR THE US DEPARTMENT OF ENERGY



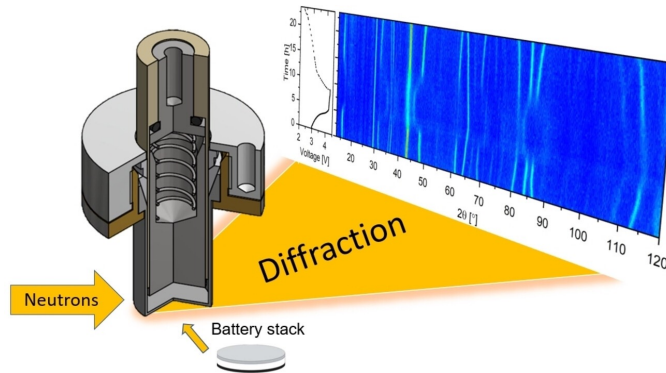
HB-2C WAND²

Versatile, high-flux, fast read-out neutron single-crystal/powder diffractometer.

Team members:
Matthias Frontzek (IS/POC)
Si Athena Chen (IS)
Xiao Hu (CIS/IS)
Joe Paddison (CIS)
Jie Xing (SA)



Fast Powder Diffraction

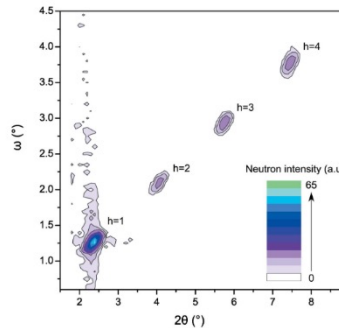


WAND² collects data in Event-mode; Measurement time of **seconds** is sufficient for refinement, **milliseconds** to track changes for time resolved, *operando* measurements.

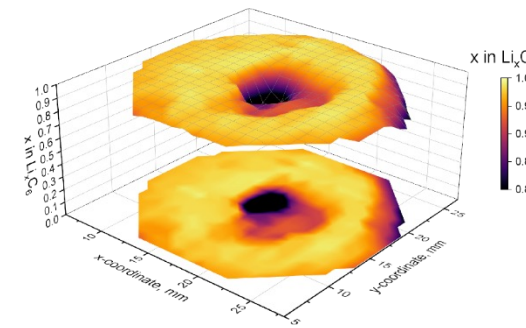


μg single crystals can be measured on WAND²

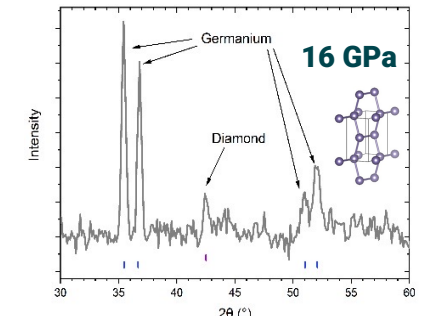
Versatile Sample Environments and Diverse Science



Sunflower lecithin

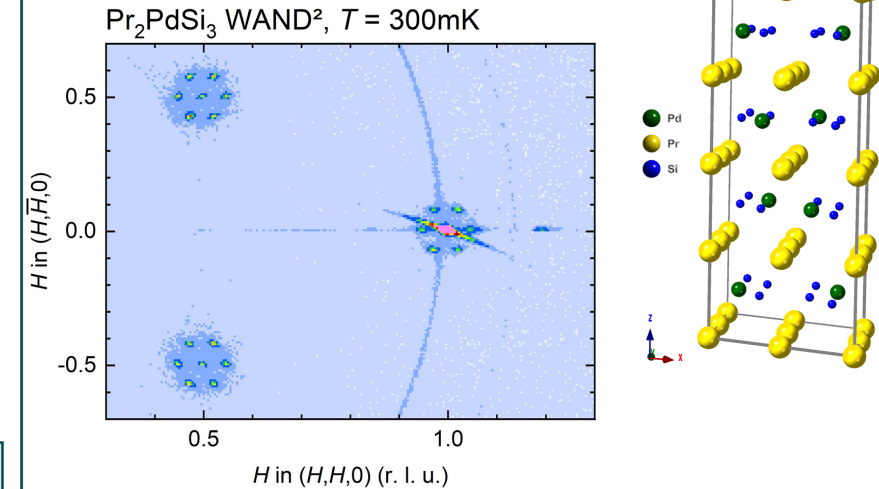


Li distribution in graphite anode



Ge phase diagram-16 GPa

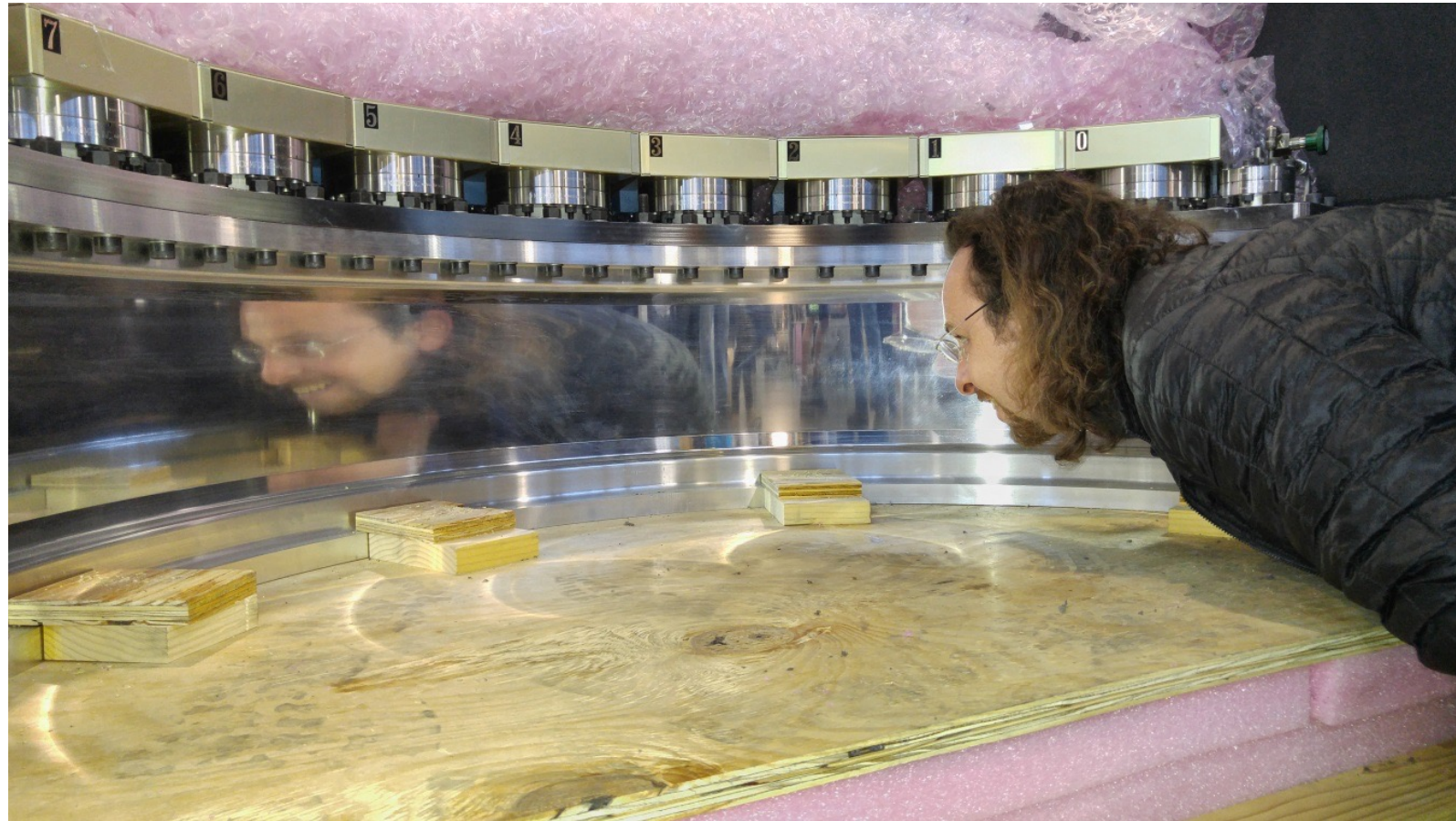
Low Background High Flux Single Crystal Diffraction



Pr₂PdSi₃ single crystal showing multiple k Skyrmion structure with $k \sim (1/20, 1/20, 0)$

WAND², Since May 2018

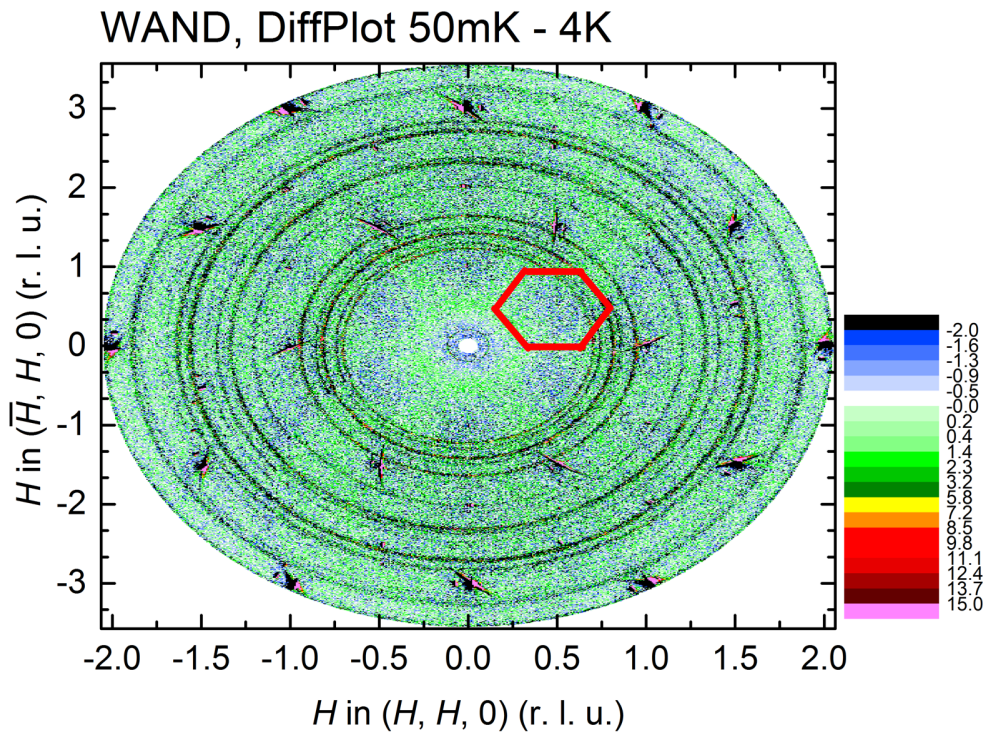
- New detector shielding
 - low background
- New radial oscillating collimator
- New detector electronics
 - Event mode - Time resolved and Stroboscopic measurements
 - Reduced data acquisition time
- New MANTID based data analyzation and visualization
- Updated instrument control software EPICS based
 - Same GUI as SNS instruments



Dr. Matthias Frontzek
(Point of Contact of WAND²)

Single crystal measurements on HB-2C WAND²

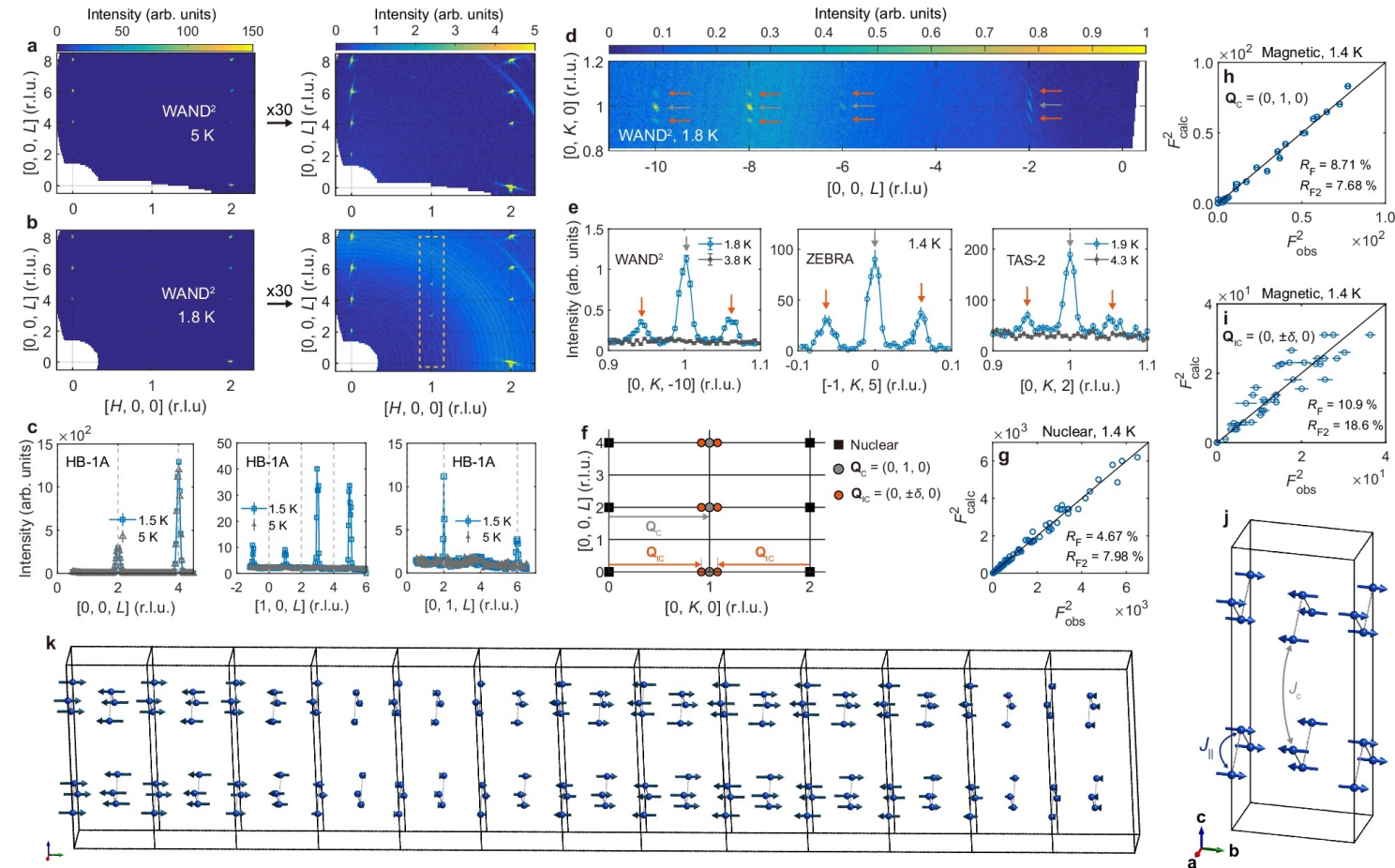
Diffuse Scattering



Shen et al. (2016) Nature

<https://doi.org/10.1038/nature20614>

k-vector, Order Parameter, Structural Refinement

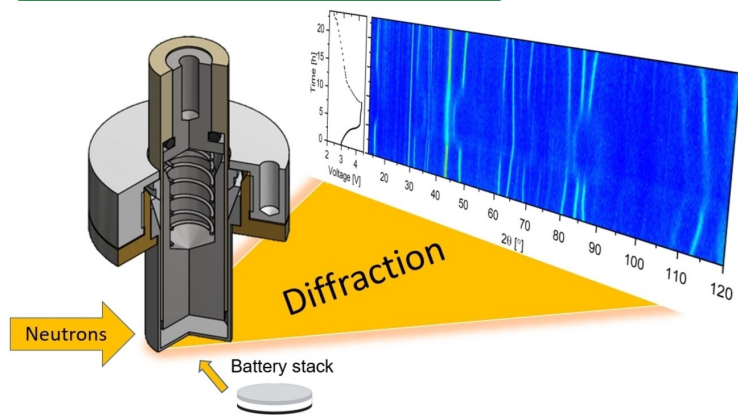


Park et al. (2025) Nature Communications

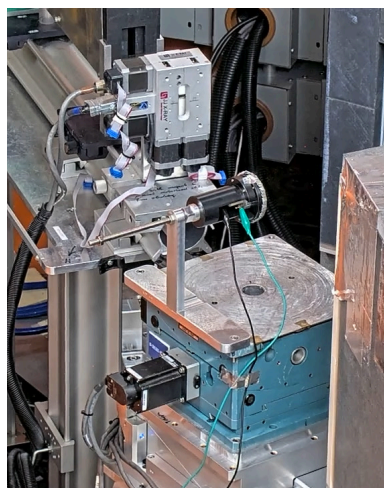
<https://doi.org/10.1038/s41467-025-59460-4>

Powder diffraction on WAND²

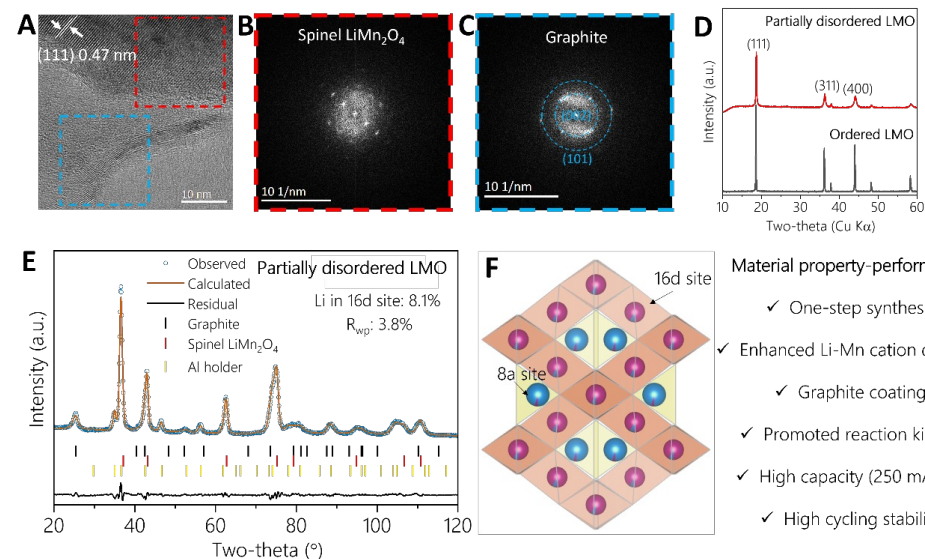
Battery Cycling



Sorensen et al. (2022), Chem. Methods

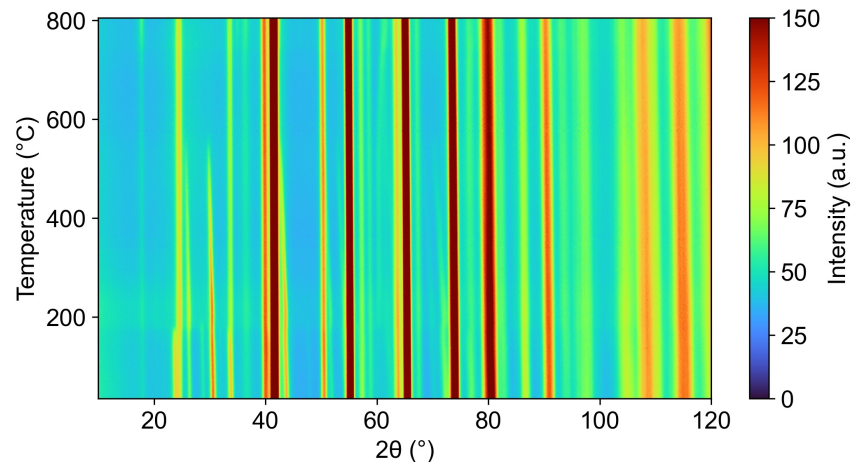


Energy Storage Materials

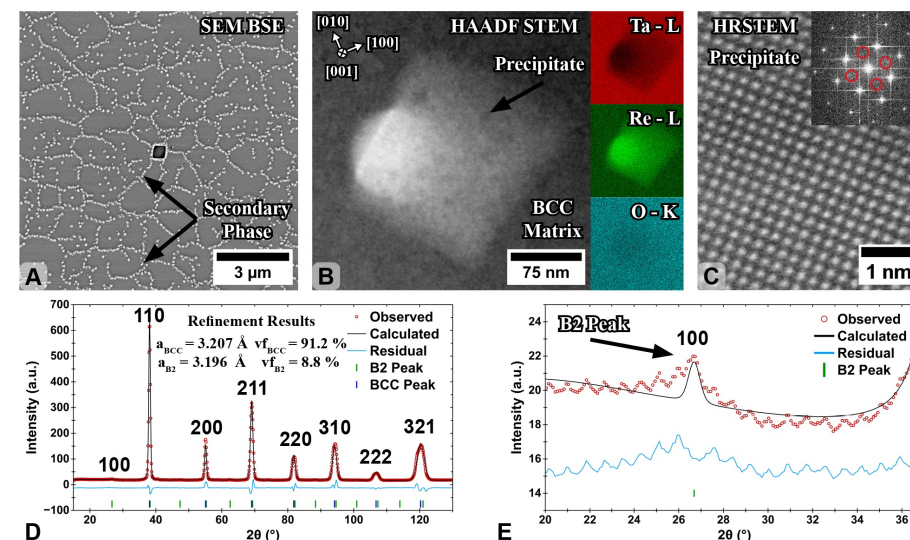


Xia et al., (2025) Advanced Materials

Critical Element Recovery (Li, Ni)



Superalloy



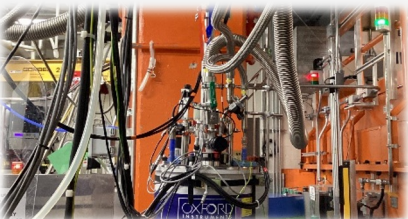
Crossman et al. (2025), Acta Materialia

Thermodynamic

- High Temperature (to **1500°C**)



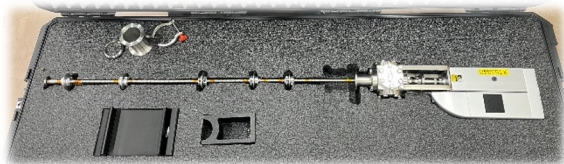
- Low Temperature (to 50mK)



- Magnetic Field (to 6T)



- Pressure (to 20GPa)



In-Operando

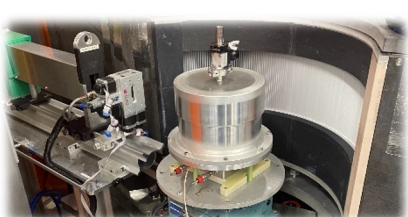
- Battery Charging / Discharging



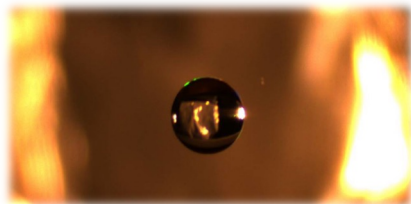
- Laser pump-probe



- Humidity/T control



- Levitator



Versatility and Support

- Compatible with various sample environments
- Support teams from instrument teams, sample environments, CIS, DAC, etc.



- X-ray labs
- Bio-labs
- High pressure labs
- Chemical labs
- Deuteration labs

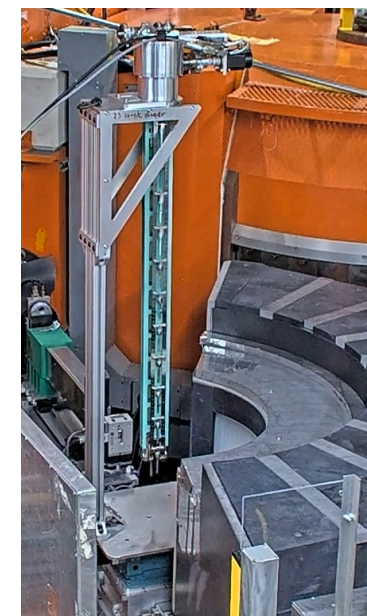


Commissioned in 2025

- Z-stage



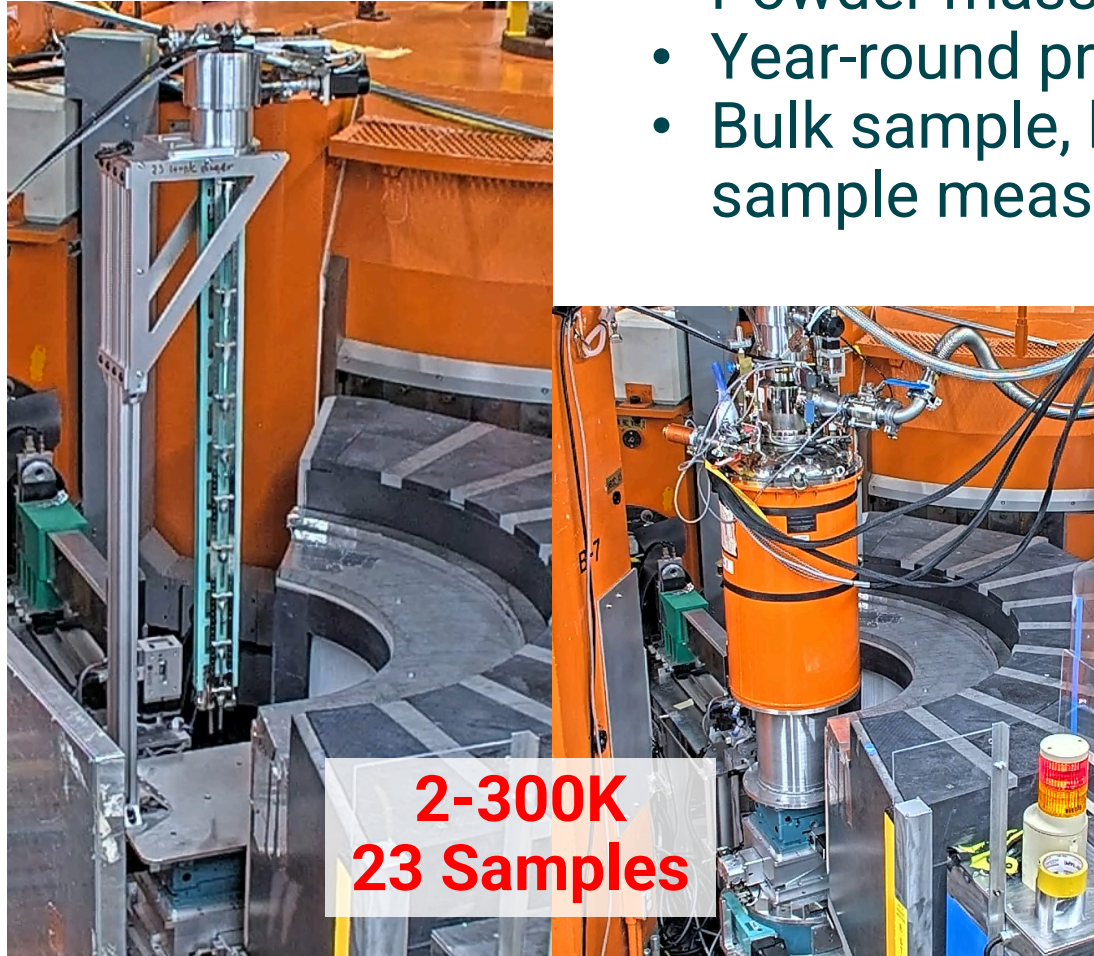
- Automation:
Automated sample changer
• 23 samples
• 2-300K,
• Mail-in program



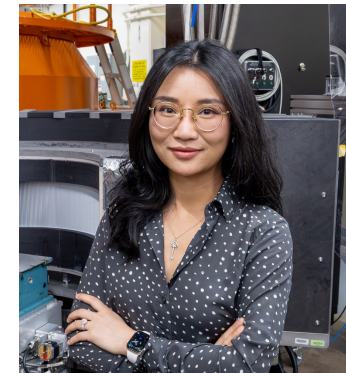
HB-2C WAND² Mail-in Program

Belt-driven
automated sample
changer

- Fast powder diffraction
- Order parameter measurement
- Powder mass: 2g (ideal); lower detection limit: 50 mg
- Year-round proposal submission
- Bulk sample, biological, geological, engineering sample measurements



Contact:

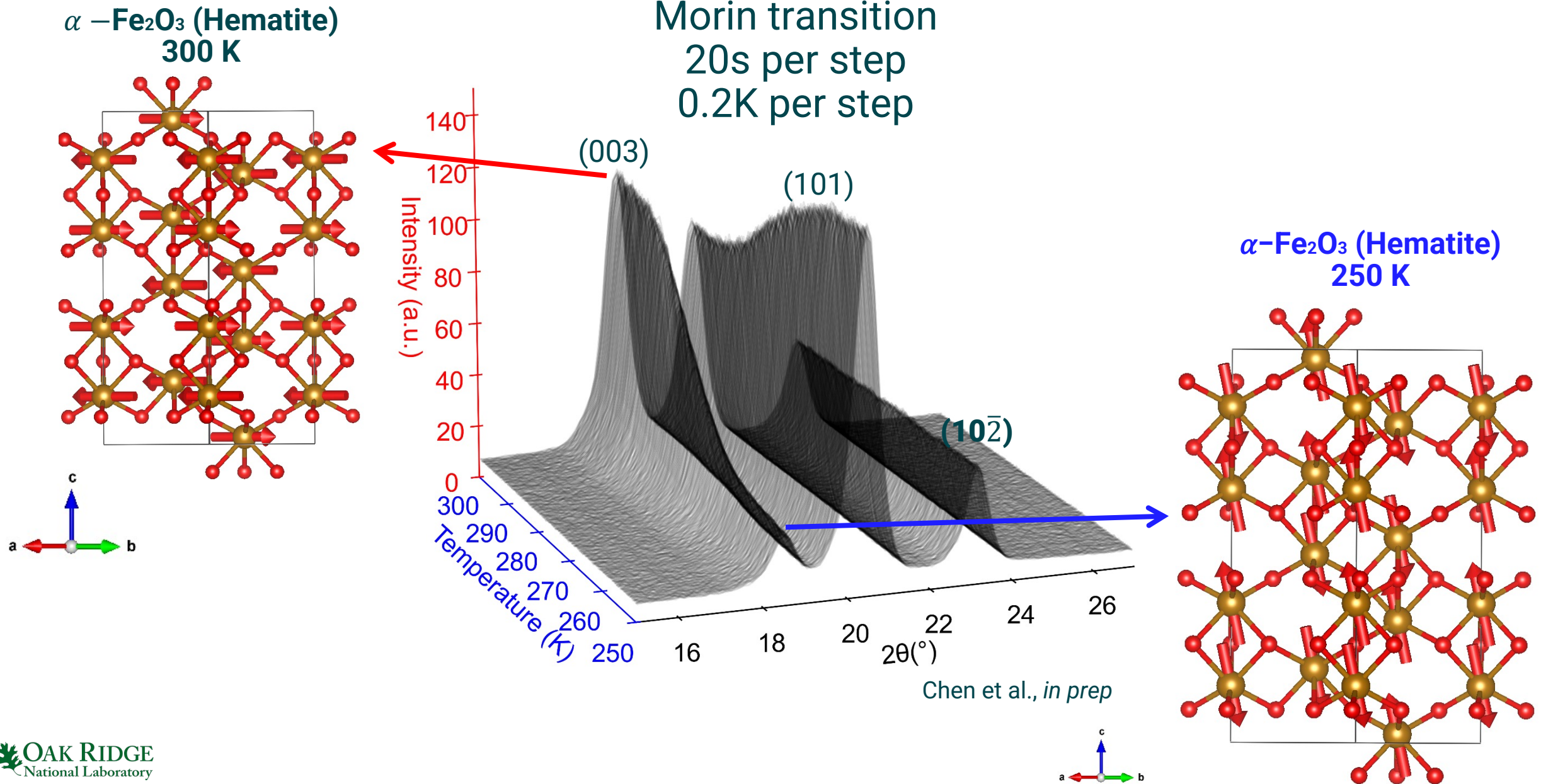


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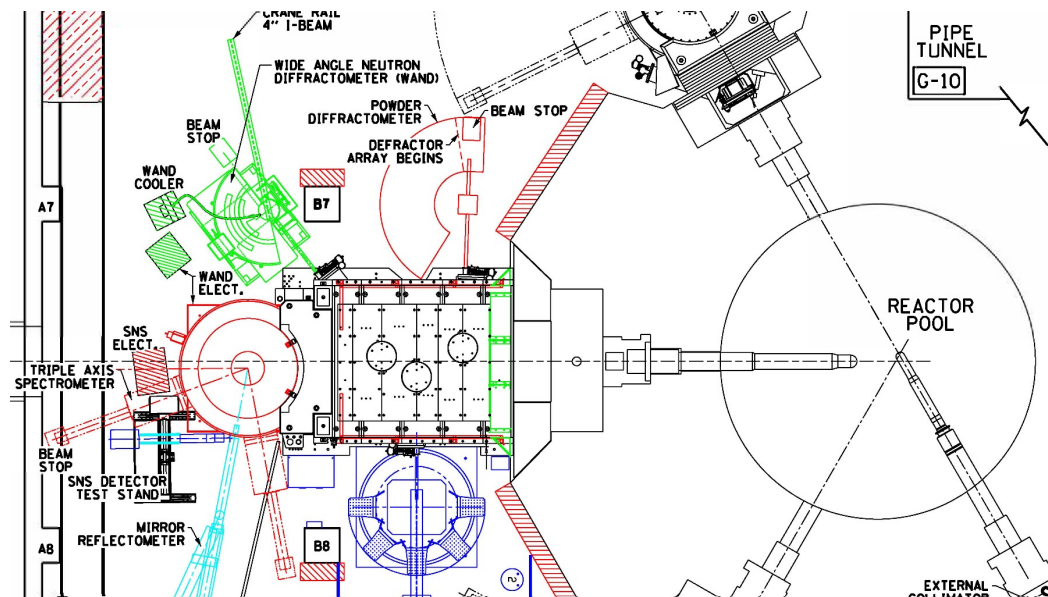
Operando Neutron Diffraction on WAND² – Event Filtering Mode



Exercise steps

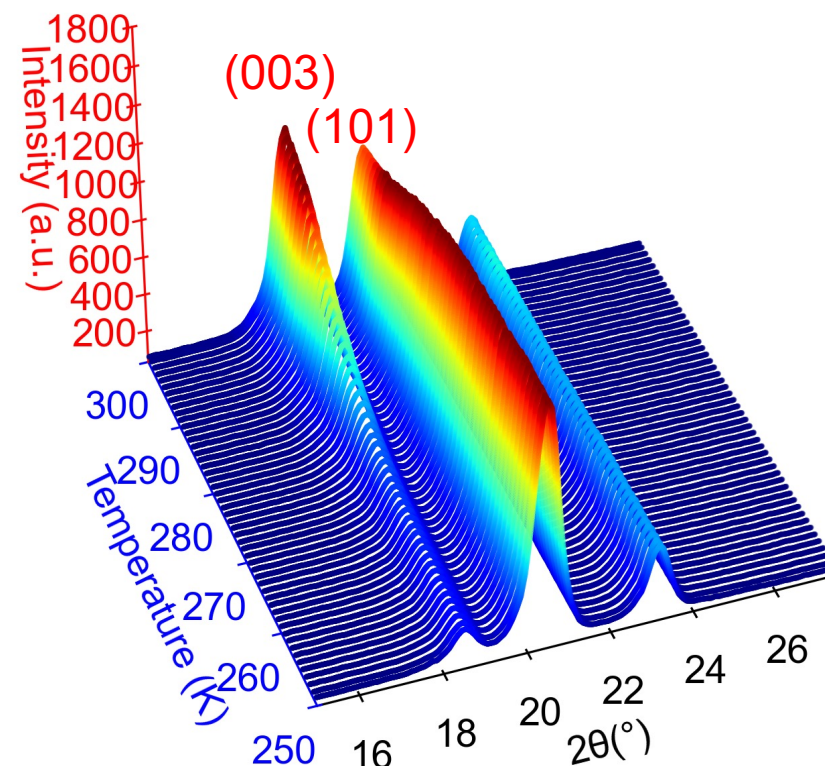
General workflow:

1. Identify magnetic peaks
2. Refine the nuclear structure ($T > T_N$)
3. Refine the nuclear + magnetic structure ($T < T_N$)
4. Publish the magnetic structure and refinement plots

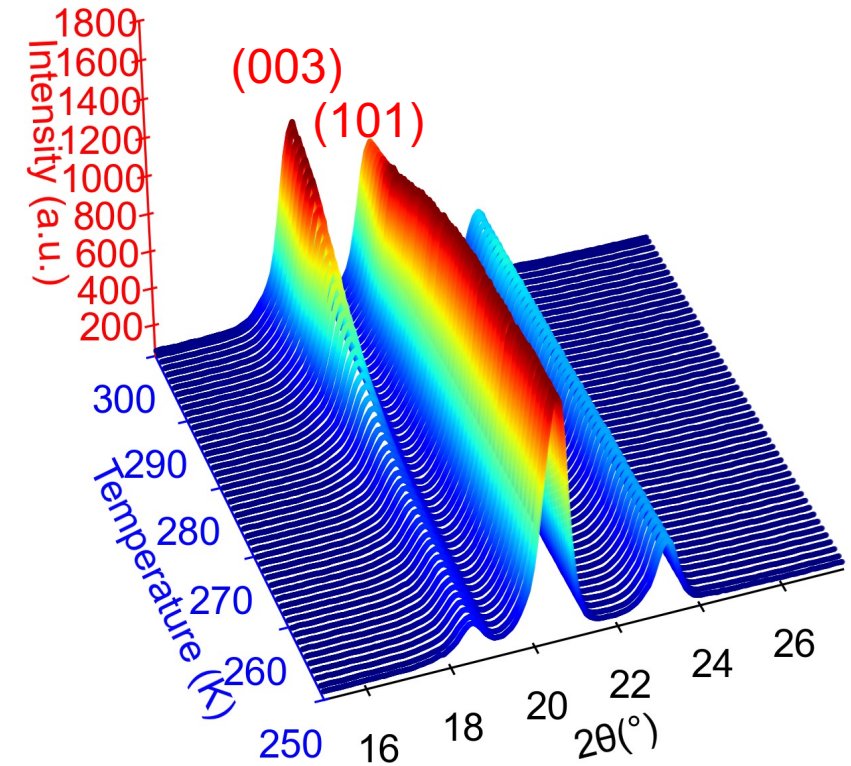
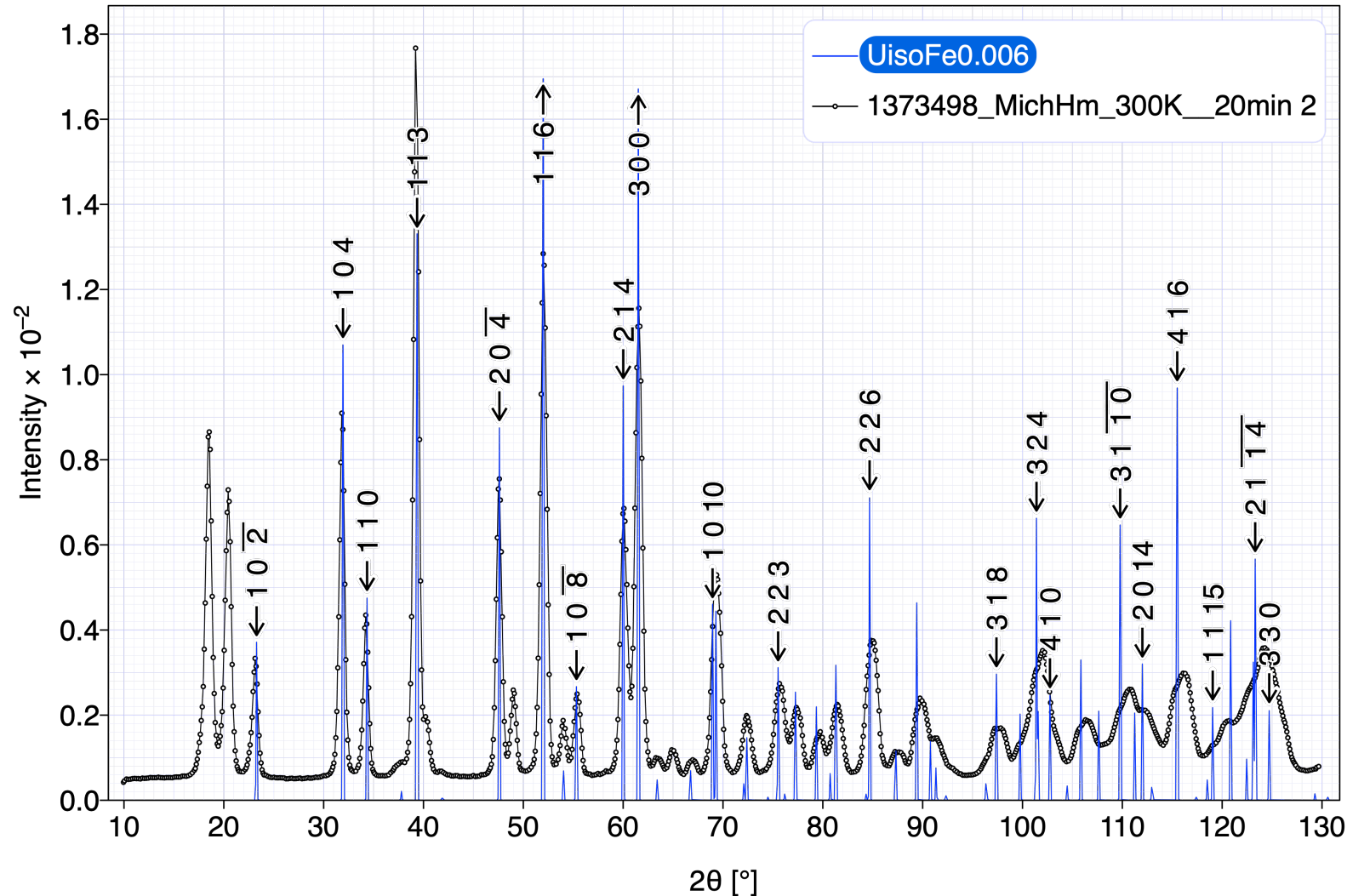


In this tutorial:

1. Identify magnetic peaks in α -Fe₂O₃ hematite
2. Refine the nuclear structure of α -Fe₂O₃ at 300 K
3. Determine the magnetic propagation vector
4. Determine the magnetic space group
5. Refine the magnetic structure of α -Fe₂O₃ at 300 K
6. Publish the magnetic structure and refinement plots



Find the magnetic scattering peak through simulation



Necessary files for GSAS-II refinement

- Cif file
- Data
- Instrument parameters

Cif file can be downloaded from:

- Inorganic Crystal Structure Database (ICSD)
- American Mineralogist Crystal Structure Database (AMCSD, free)
- Crystallography Open Database

Blake1966_Fe2O3.cif
MichHm_300K__20min.xy
WAND2_Ge113_1p486...r2024_GSASII.instprm

1373498_MichHm_300K__20min.dat

```
# MichHm_300K__20min
# Instrument: WAND^2 | HB-2C | HFIR
# Wavelength: 1.4865 angstrom
# Primary flying path length: 3.289 m
# Failed to find proposal
# Run number: 1373498
# Temperature: 300.0 K
#
```

2th deg	Y	E
9.95225	53.49085477	0.67391787
10.05210	57.78870070	0.52355085
10.15195	61.63116744	0.53699358
10.25180	63.12979102	0.49931913
10.35165	62.77206576	0.50780183
10.45150	62.19767417	0.46110276
10.55135	62.59417845	0.45824979
10.65120	62.86870590	0.43982001
10.75105	63.46219753	0.41303554
10.85090	64.32490732	0.41246651
10.95075	65.17395036	0.39762166
11.05060	65.06123658	0.39976929
11.15045	64.05267020	0.38635122
11.25031	64.44293151	0.38272644
11.35016	64.57341446	0.38105822
11.45001	64.51073411	0.37285323
11.54986	64.48512636	0.36700382
11.64971	63.60803215	0.35829754
11.74956	65.46742501	0.35943042

WAND2_Ge113_1p486A_Cycle505_Mar2024_GSASII.instprm

```
#GSAS-II instrument parameter file; do not add/delete items!
Type:PNC
Lam:1.488584398008619
Zero:0.03961975115277752
Polariz.:0.0
U:4503.723479971857
V:-2893.1329916567033
W:976.5365572120386
X:11.997956908812998
Y:0.0
Z:0.0
SH/L:0.0005
Azimuth:0.0
Source:
Bank:1.0
```

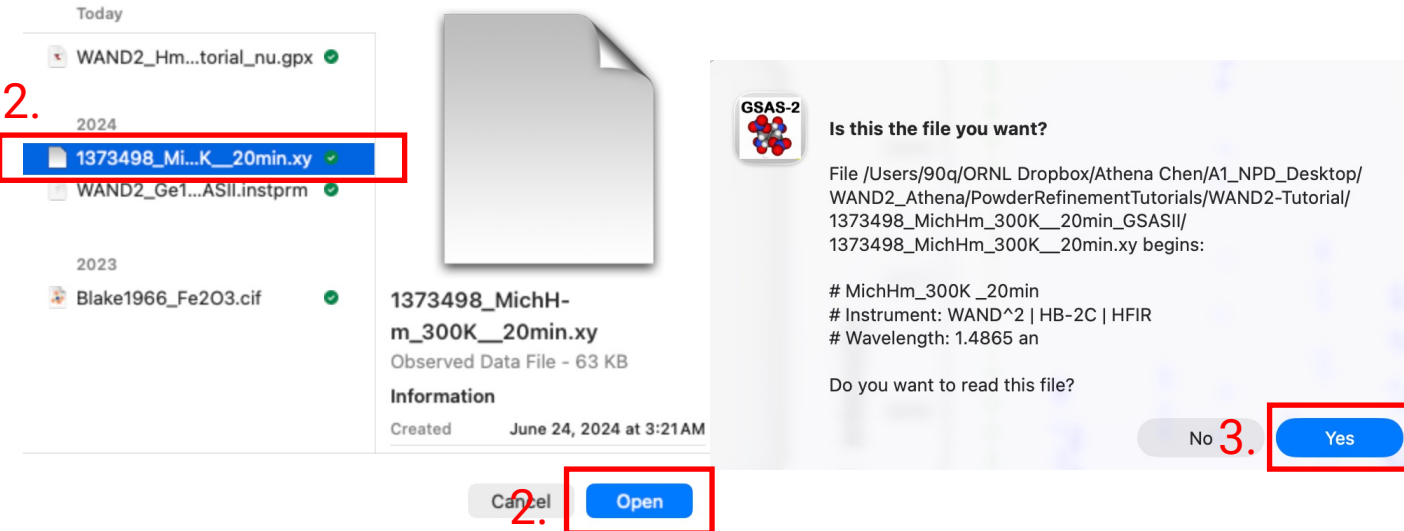
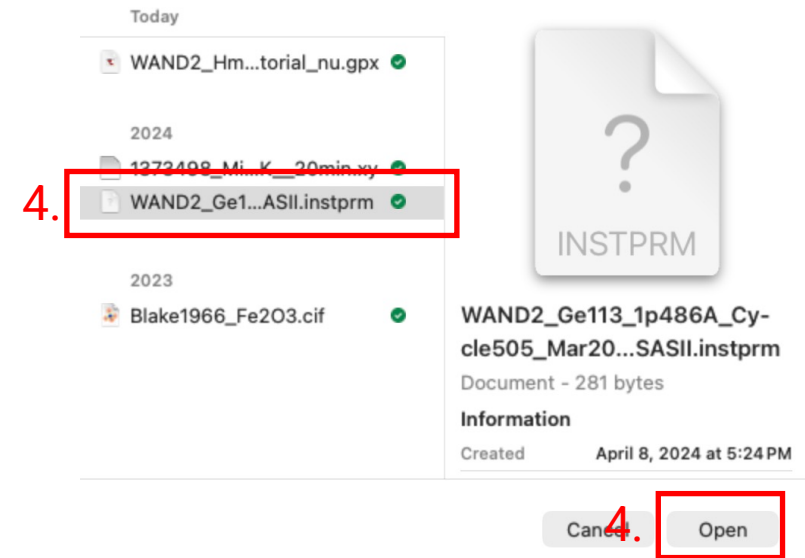
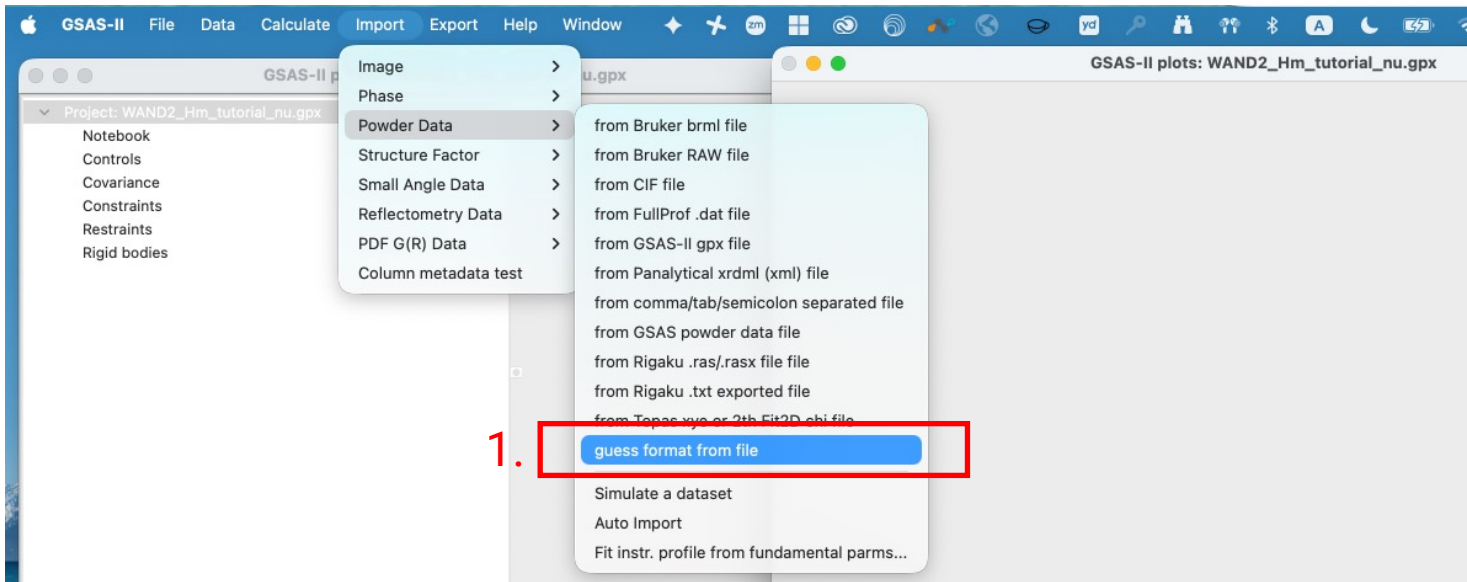
From Si calibration

Gaussian: $\sigma^2 = U \tan^2\theta + V \tan\theta + W + \frac{P}{\cos^2\theta}$

FWHM = $\sigma * (8 \ln 2)^{0.5}$

Lorentzian: FWHM = $X / \cos\theta + Y \tan\theta + Z$

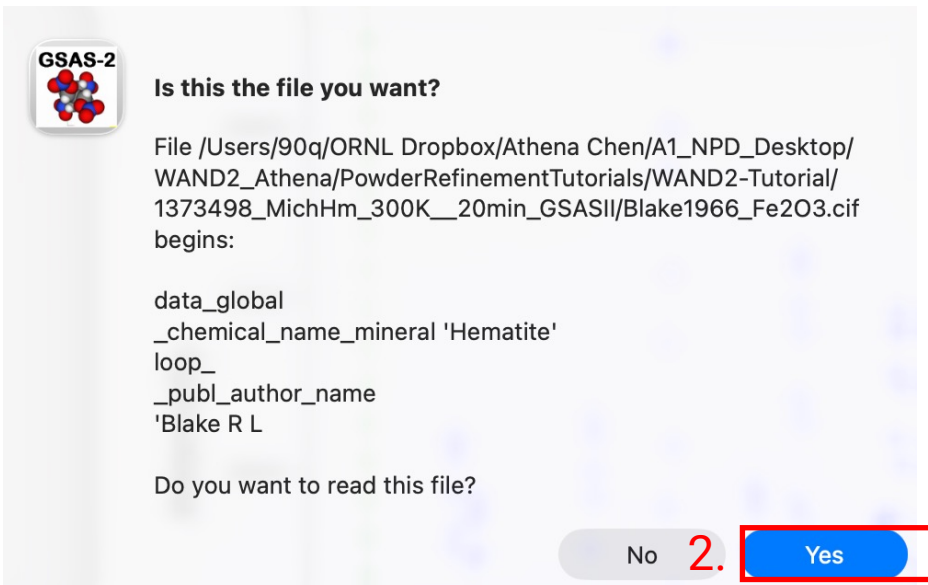
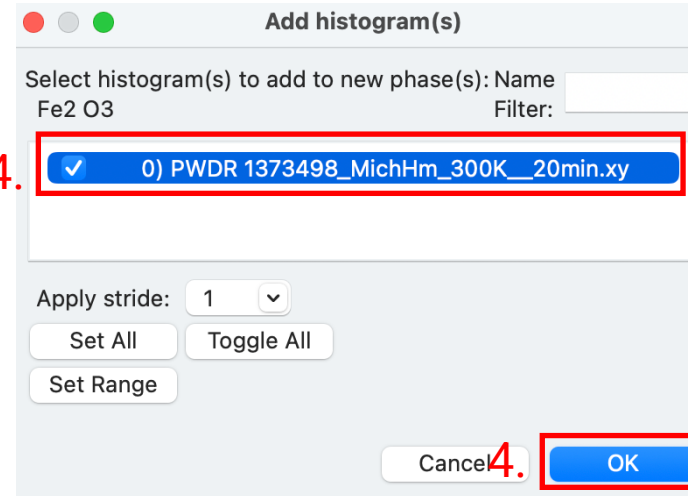
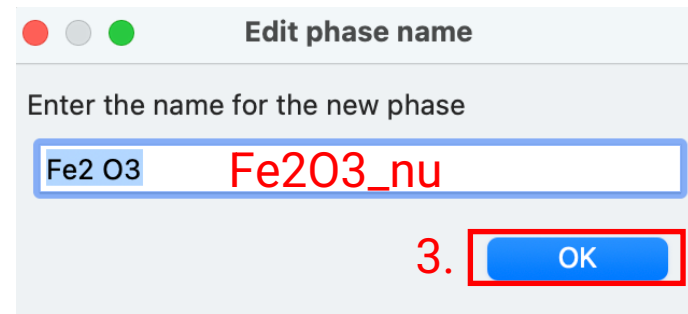
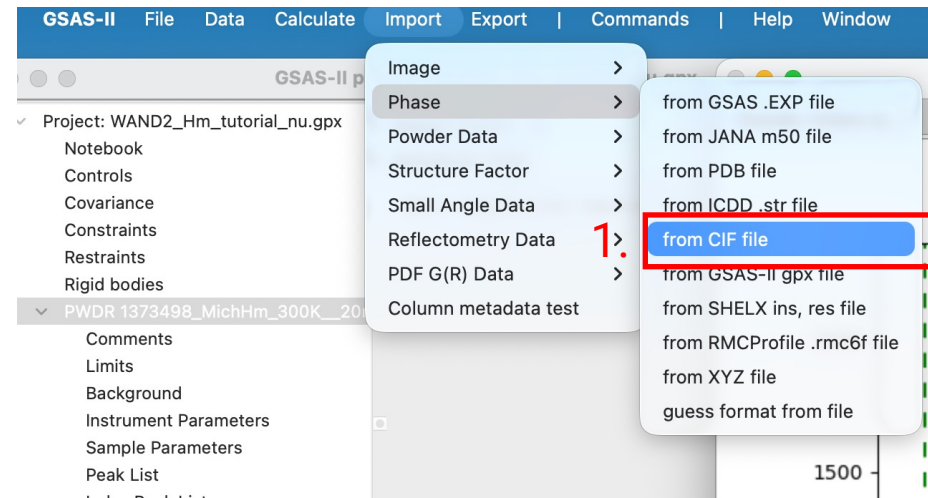
Import data and WAND² instrument parameters



Some helpful troubleshoot tips:

- Check your data file format (try .dat or .xy)
- Delete headers

Import cif file to indicate phases

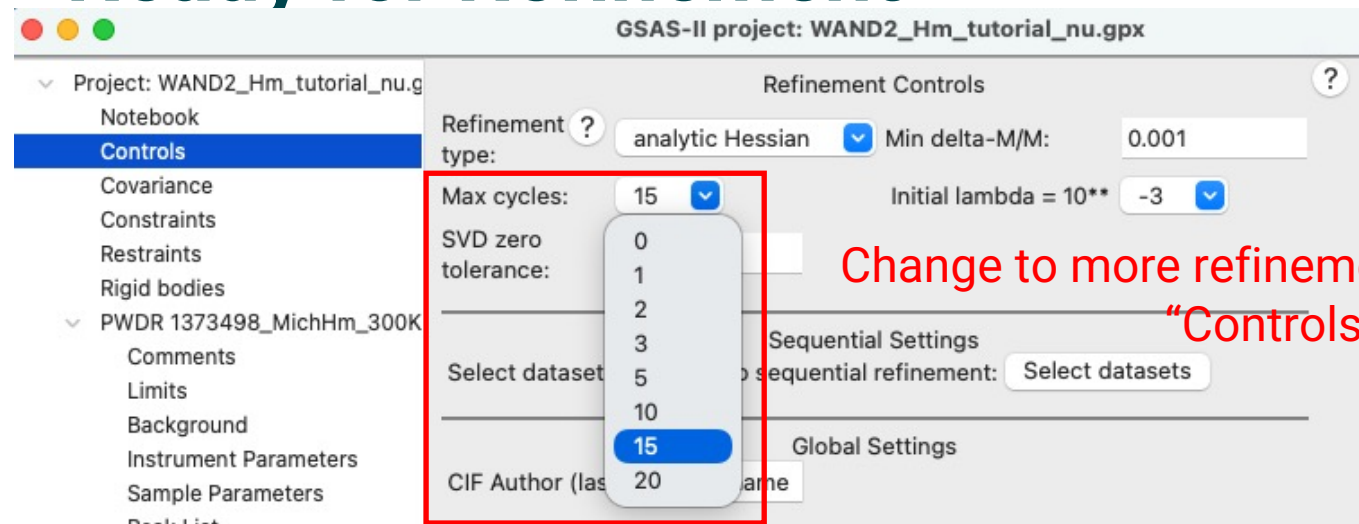


Tips:

Cif file can be downloaded from:

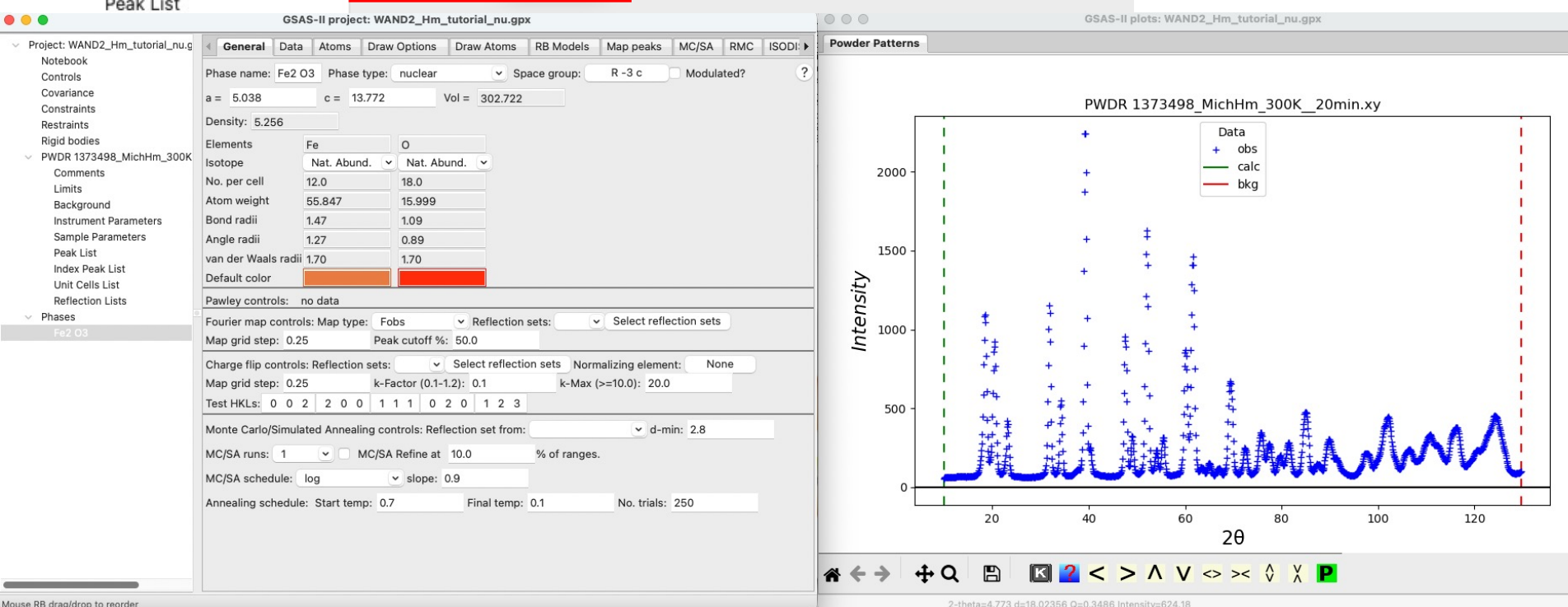
- Inorganic Crystal Structure Database (ICSD) (<https://icsd.fiz-karlsruhe.de/search/basic.xhtml>)
- American Mineralogist Crystal Structure Database (free) (<https://www.rruff.net/amcsd/>)
- Crystallography Open Database (<https://www.crystallography.net/cod/search.php>)

Ready for Refinement



General refinement logistics:

1. Background
2. Lattice parameters (Peak position)
3. Microstrain/Size (Peak width)
4. Atom positions (peak position)
5. Uiso (peak intensity ratio)
6. Occupancy (peak intensity ratio)



Background refinement

GSAS-II project: WAND2_Hm_tutorial_nu.gpx

Project: WAND2_Hm_tutorial_nu.g
Notebook
Controls
Covariance
Constraints
Restrains
Rigid bodies
PWDR 1373498_MichHm_300K
Comments
Limits
Background
Instrument Parameters
Sample Parameters
Peak List
Index Peak List
Unit Cells List
Reflection Lists

Data range to be used in fits

Original Tmin 9.9522 New: 21.7
Original Tmax 129.6728 New: 129.6728

Set the refinement limit to exclude the magnetic peaks
➤ Lower limit to 21.7

Calculate Import Export
Setup PDFs
View LS parms
Refine
Compute partials

GSAS-II project: WAND2_Hm_tutorial_nu.gpx

Project: WAND2_Hm_tutorial_nu.g
Notebook
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PWDR 1373498_MichHm_300K
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Background
Instrument Parameters
Sample Parameters
Peak List
Index Peak List
Unit Cells List
Reflection Lists
Phases
Fe2O3_nu

Background used in refinement

Background function: chebyshev-1 ☒ Refine?
Number of coeff.: 3
Background coefficients:
73.4218 3.9517 -5.1674
Debye scattering: Number of terms: 0
Peaks in background: Number of peaks: 0
Fit to fixed bkg Compute auto background Copy auto background
Fixed background histogram (for point-by-point subtraction):
☒ multiplier 1.0

GSAS-II plots: WAND2_Hm_tutorial_nu.gpx

Powder Patterns

PWDR 1373498_MichHm_300K_20min.xy cycle #1

Intensity

Phases & Data
+ obs
— calc
— bkg
| Fe2 O3

$\Delta(I)/\sigma(I)$

2 θ

2-theta=4.258 d=20.22448 Q=0.3107 Intensity=1339.62

Start to refine with three chebyshev background coefficients and check the general peak positions

Background refinement

Project: WAND2_Hm_tutorial_nu.g

Notebook

Controls

Covariance

Constraints

Restrains

Rigid bodies

PWDR 1373498_MichHm_300K

Comments

Limits

Background

Instrument Parameters

Sample Parameters

Peak List

Index Peak List

Unit Cells List

Reflection Lists

Phases

Fe2O3_nu

Histogram Type: PNC Bank: 1

Name (default)	Value	Refine?
Azimuth:	0.00	
Lam (Å): (1.488584)	1.488584	☐
Zero (0.0396):	0.0	☒
U (4503.723):	4503.723	☐
V (-2893.133):	-2893.133	☐
W (976.537):	976.537	☐
X (11.998):	11.998	☐
Y (0.000):	0.0	☐
Z (0.000):	0.0	☐
SH/L (0.00050):	0.0005	☐

Toggle "Zero" offset and refine

GSAS-2

Refinement results, $R_w = 19.379$

Detailed results are in /Users/90q/ORNL Dropbox/Athena Chen/A1_NPD_Desktop/WAND2_Athena/PowderRefinementTutorials/WAND2-Tutorial/1373498_MichHm_300K_20min_GSASII/WAND2_Hm_tutorial_nu.lst

Final Reduced χ^2 : 3671.334 (before ref: 3671.332)

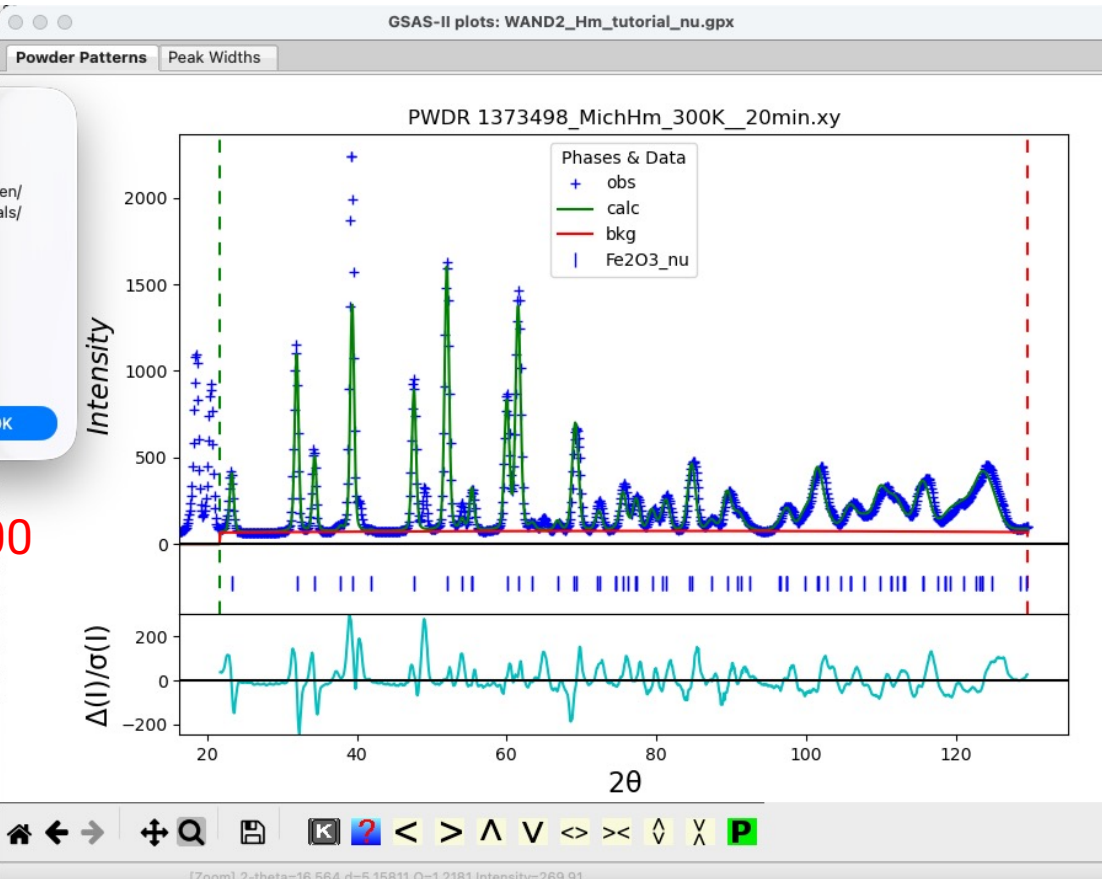
Max shift/sigma=0.000

Load new result?

Cancel

OK

Until Max shift/sigma=0.00



Refine Background

GSAS-II project: WAND2_Hm_tutorial_nu.gpx

Project: WAND2_Hm_tutorial_nu.g

- Notebook
- Controls
- Covariance
- Constraints
- Restraints
- Rigid bodies
- PWDR 1373498_MichHm_300K
 - Comments
 - Limits
 - Background
 - Instrument Parameters
 - Sample Parameters
 - Peak List
 - Index Peak List
 - Unit Cells List
 - Reflection Lists
- Phases
 - Fe2O3_nu

Background used in refinement

Background function: chebyshev-1 ☒ Refine?

Number of coeff.: 6

Background coefficients:

71.6281	1.0762	-4.0118	0.0	0.0
0.0				

Debye scattering: Number of terms: 0

Peaks in background: Number of peaks: 0

Fit to fixed bkg Compute auto background Copy auto background

Fixed background histogram (for point-by-point subtraction):
multiplier 1.0

Add more coefficients

GSAS-2

Refinement results, $R_w = 19.262$

Detailed results are in /Users/90q/ORNL Dropbox/Athena Chen/A1_NPD_Desktop/WAND2_Athena/PowderRefinementTutorials/WAND2-Tutorial/1373498_MichHm_300K__20min_GSASII/WAND2_Hm_tutorial_nu.lst

Final Reduced χ^2 : 3637.532 (before ref: 3681.590)

Max shift/sigma=3.141

Load new result?

Cancel OK

Refine

Project: WAND2_Hm_tutorial_nu.g

Background used in refinement

Background function: chebyshev-1 ☒ Refine?

Number of coeff.: 6

Background coefficients:

71.2164	2.4027	-2.6322	5.085	3.1816
1.5264				

Debye scattering: Number of terms: 0

Peaks in background: Number of peaks: 0

Fit to fixed bkg Compute auto background Copy auto background

Fixed background histogram (for point-by-point subtraction):
☒ multiplier 1.0

GSAS-II project: WAND2_Hm_tutorial_nu.g

Project: WAND2_Hm_tutorial_nu.g

- Notebook
- Controls
- Covariance
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- Restraints
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 - Comments
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 - Index Peak List
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- Phases
 - Fe2O3_nu

Histogram Type: PNC Bank: 1

Name (default)	Value	Refine?
Azimuth:	0.00	
Lam (Å): (1.488584)	1.488584	☐
Zero (0.0396):	-0.0291	☒
U (4503.723):	4503.723	☐
V (-2893.133):	-2893.133	☐
W (976.537):	976.537	☐
X (11.998):	11.998	☐
Y (0.000):	0.0	☐
Z (0.000):	0.0	☐
SH/L (0.00050):	0.0005	☐

Tip: The number of background coefficients depends on the dataset and the selected background function. Because the data used in this tutorial have a relatively flat background, six coefficients are sufficient. For typical WAND² data, six to nine coefficients are generally good enough.

Refine lattice parameters

GSAS-II project: WAND2_Hm_tutorial_nu.gpx

Project: WAND2_Hm_tutorial_nu.gpx

- ▼ Notebook
- Controls
- Covariance
- Constraints
- Restraints
- Rigid bodies
- ▼ PWDR 1373498_MichHm_300K
- Comments
- Limits
- Background
- Instrument Parameters
- Sample Parameters
- Peak List
- Index Peak List
- Unit Cells List
- Reflection Lists
- ▼ Phases
- Fe2O3_nu

General Data Atoms Draw Options Draw Atoms RB Models Map peaks

Phase name: Fe2O3_nu Phase type: nuclear Space group: R -3 c

☒ Refine unit cell: a = 5.038 c = 13.772 Vol = 302.722

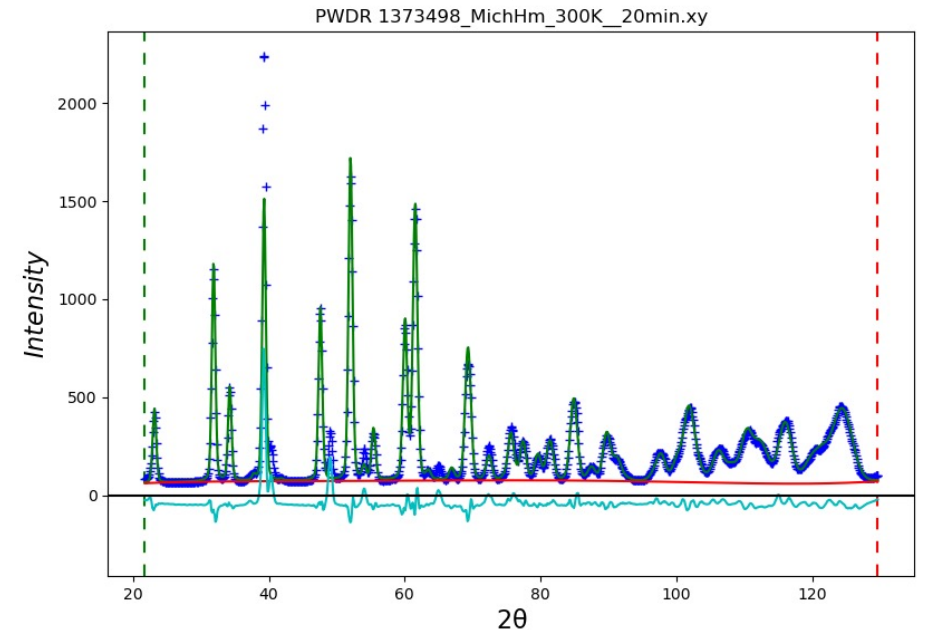
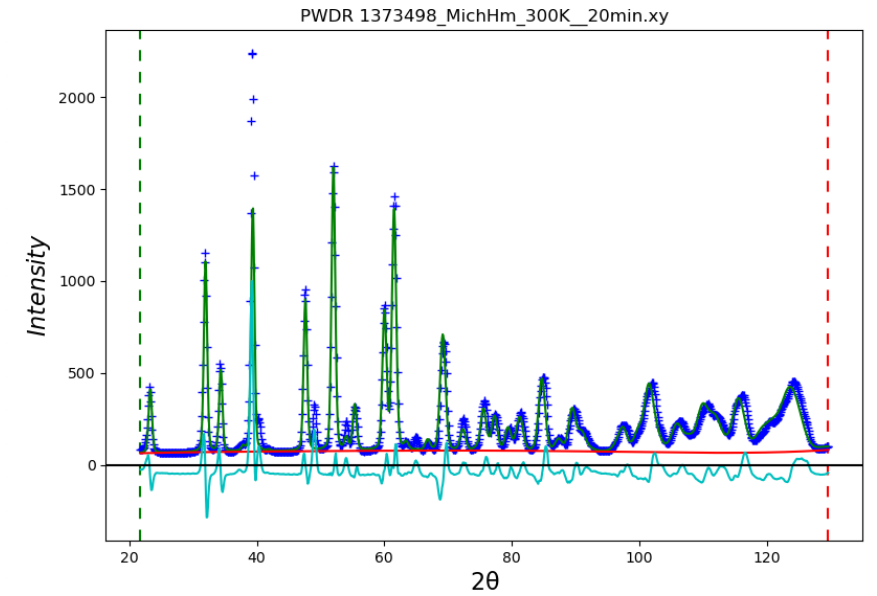
Density: 5.256

Elements	Fe	O
Isotope	Nat. Abund.	Nat. Abund.
No. per cell	12.0	18.0
Atom weight	55.847	15.999
Bond radii	1.47	1.09
Angle radii	1.27	0.89
van der Waals radii	1.70	1.70
Default color		

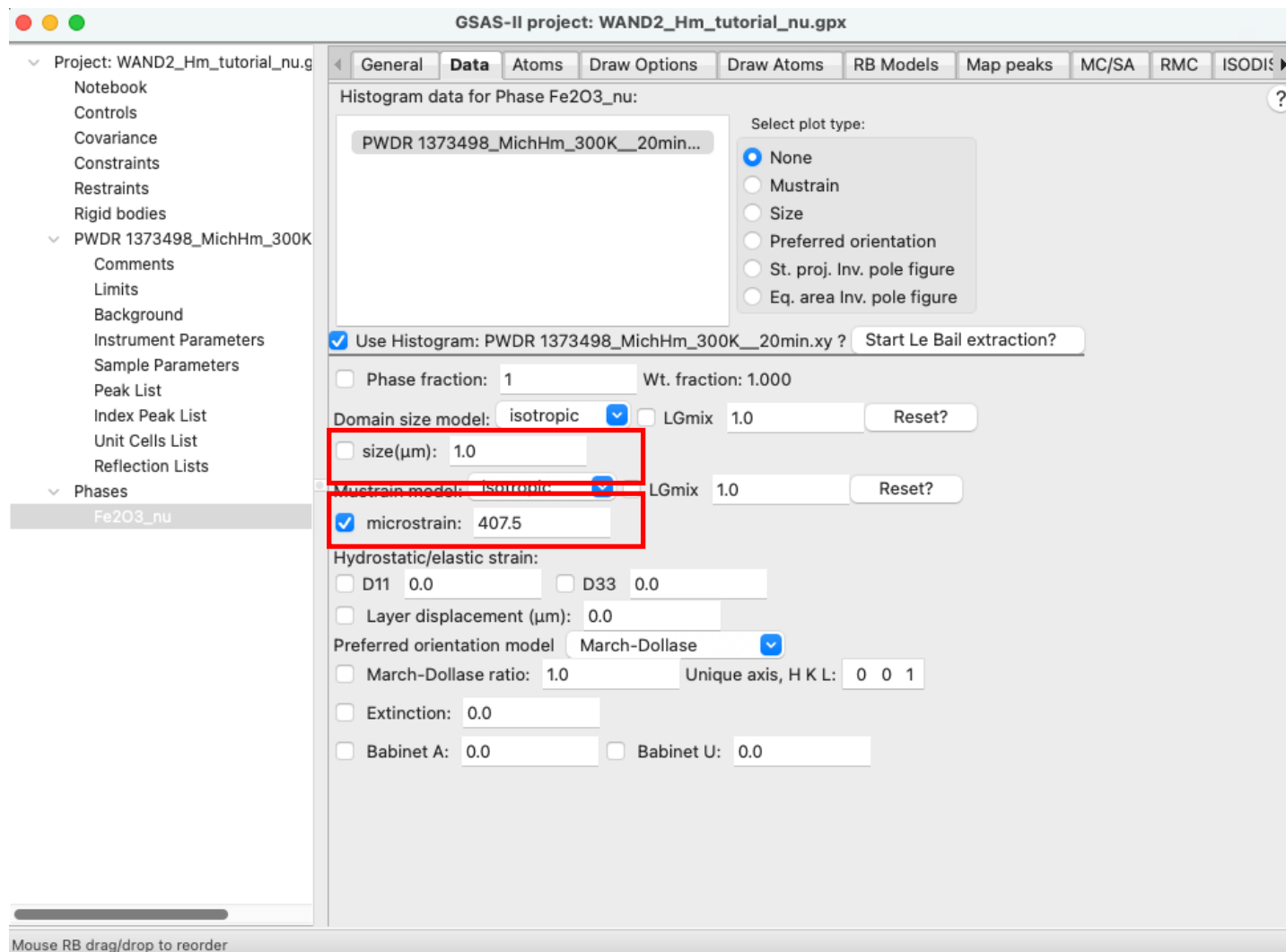
Pawley controls: Do Pawley refinement? ☐ dmin: 1.0 dmax: 3.94875 Pawley r

d-space range 0.82224 to 3.94875 Å⁻¹ (1 histograms)

Fourier map controls: Map type: Fobs Reflection sets: ☒ Select refle

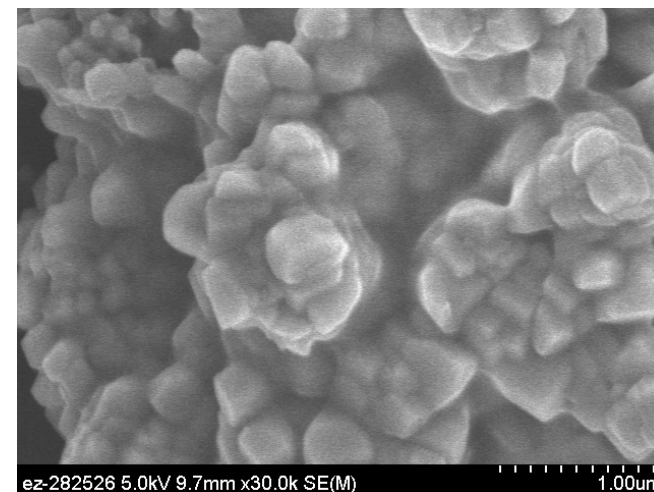


Refine Microstrain/Size



Tips:

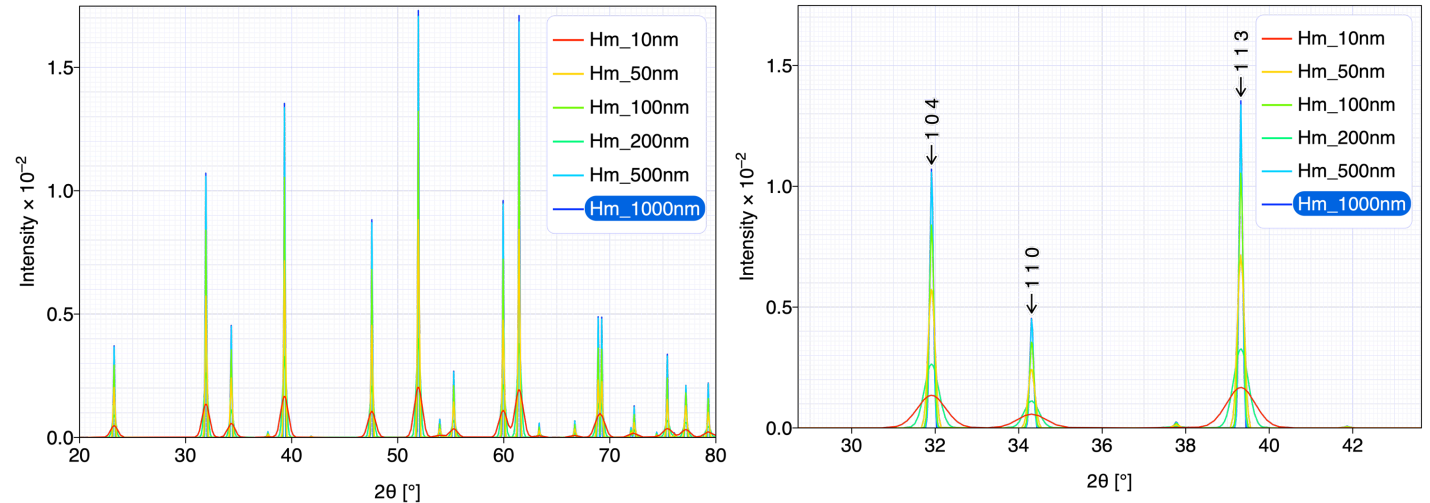
1. Domain size and microstrain can be both refined using high-resolution neutron or X-ray diffraction data.
2. WAND² currently has medium resolution that limits the accuracy of size + microstrain refinement. The refined crystallite size should be validated using complementary methods, such as electron microscopy.
3. The refined microstrain value should always remain positive. If it becomes negative during refinement, reset it.



Definition of Size and Microstrain in GSAS-II

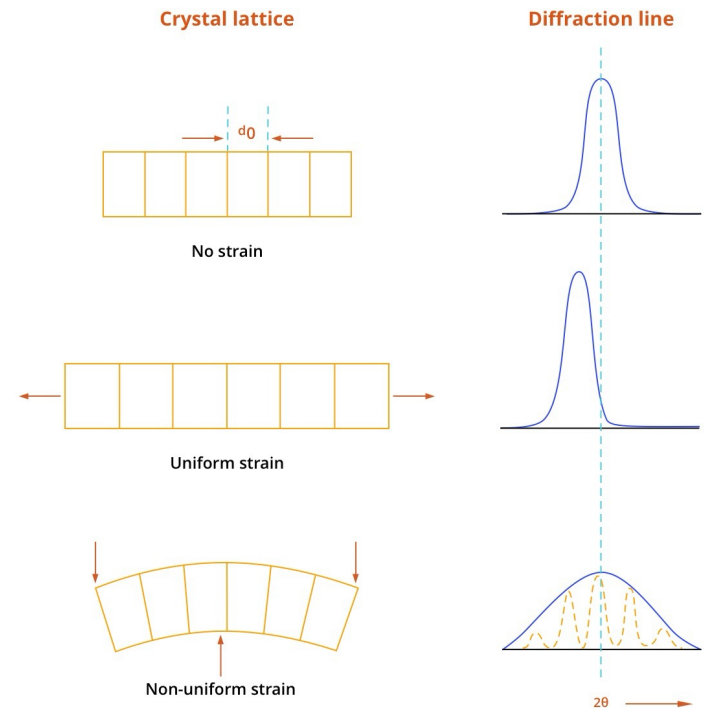
Size (in microns)

- Isotropic (single value)
- Axial (two values and an axis)
- Ellipsoidal (6 values -- like U_{ij})



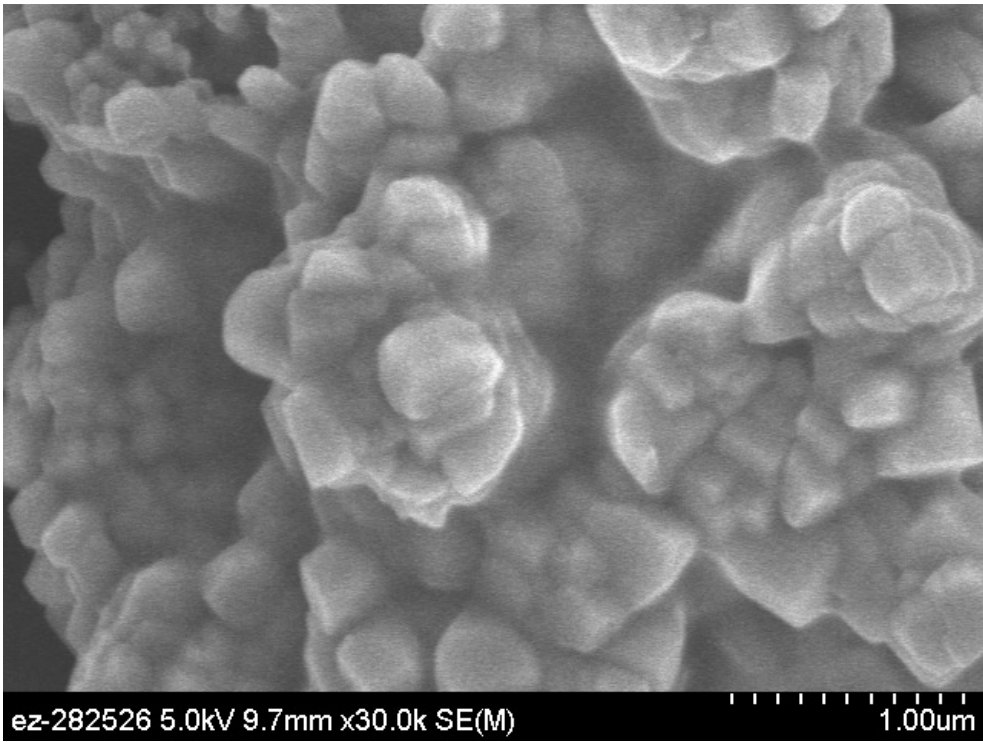
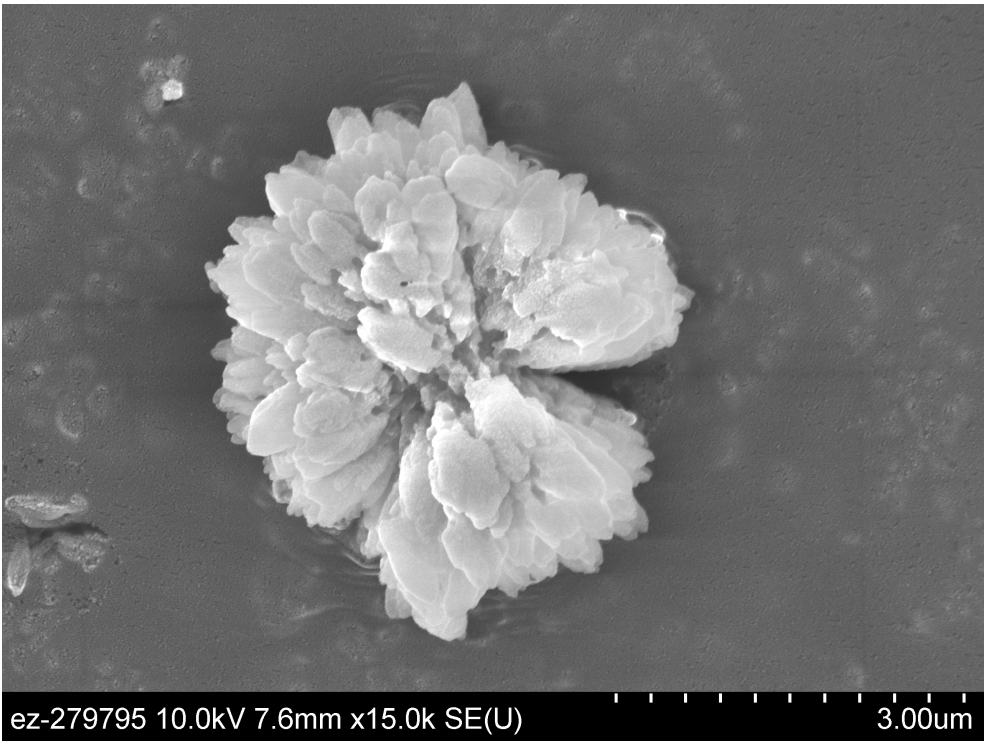
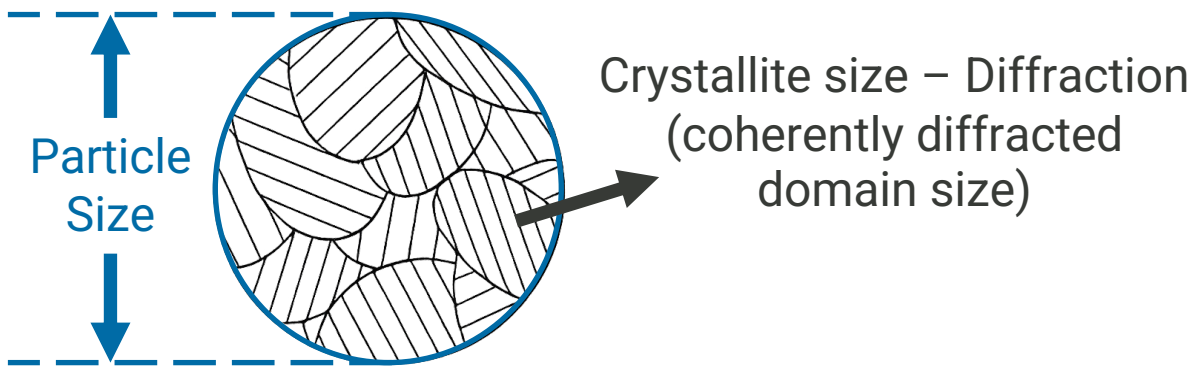
Microstrain ($\Delta Q/Q \times 10^6$)

- Isotropic (single value)
- Axial (two values and an axis)
- General (Stephens model; # of terms depend on Laue class)



LGmix is amount of Lorentzian vs. Gaussian (usually 1 is best)

Crystallite size versus particle size



Atomic Displacement Parameters

GSAS-II project: WAND2_Hm_tutorial_nu.gpx

Project: WAND2_Hm_tutorial_nu.gpx

- ▼ Notebook
- Controls
- Covariance
- Constraints
- Restraints
- Rigid bodies
- ▼ PWDR 1373498_MichHm_300K
 - Comments
 - Limits
 - Background
 - Instrument Parameters
 - Sample Parameters
 - Peak List
 - Index Peak List
 - Unit Cells List
 - Reflection Lists
- ▼ Phases
 - Fe2O3_nu

General Data **Atoms** Draw Options Draw Atoms RB Models Map peaks MC/SA RMC ISODIS

Atom parameters list for Fe2O3_nu:

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso	U11
0	Fe	Fe		0.00000	0.00000	0.35530	1.0000	3	12	A		0.00
1	O	O		0.30590	0.00000	0.25000	1.0000	2(100)	18	A		0.00

We use isotropic mode here because the limited Q range doesn't support anisotropic modeling in the current dataset. Anisotropic mode would work for high-resolution, larger Q range data.

Thermal Motion

Select

Isotropic

Anisotropic

Cancel OK

General Data **Atoms** Draw Options Draw Atoms RB Models Map peaks MC/SA RMC ISODIS

Atom parameters list for Fe2O3_nu:

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso	U11
0	Fe	Fe	X	0.00000	0.00000	0.35528	1.0000	3	12	I	0.00608	
1	O	O	X	0.30504	0.00000	0.25000	1.0000	2(100)	18	I	0.00633	

General Data **Atoms** Draw Options Draw Atoms RB Models Map peaks MC/SA RMC ISODIS

Atom parameters list for Fe2O3_nu:

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso	U11
0	Fe	Fe	XU	0.00000	0.00000	0.35532	1.0000	3	12	I	0.00783	
1	O	O	XU	0.30461	0.00000	0.25000	1.0000	2(100)	18	I	0.00516	

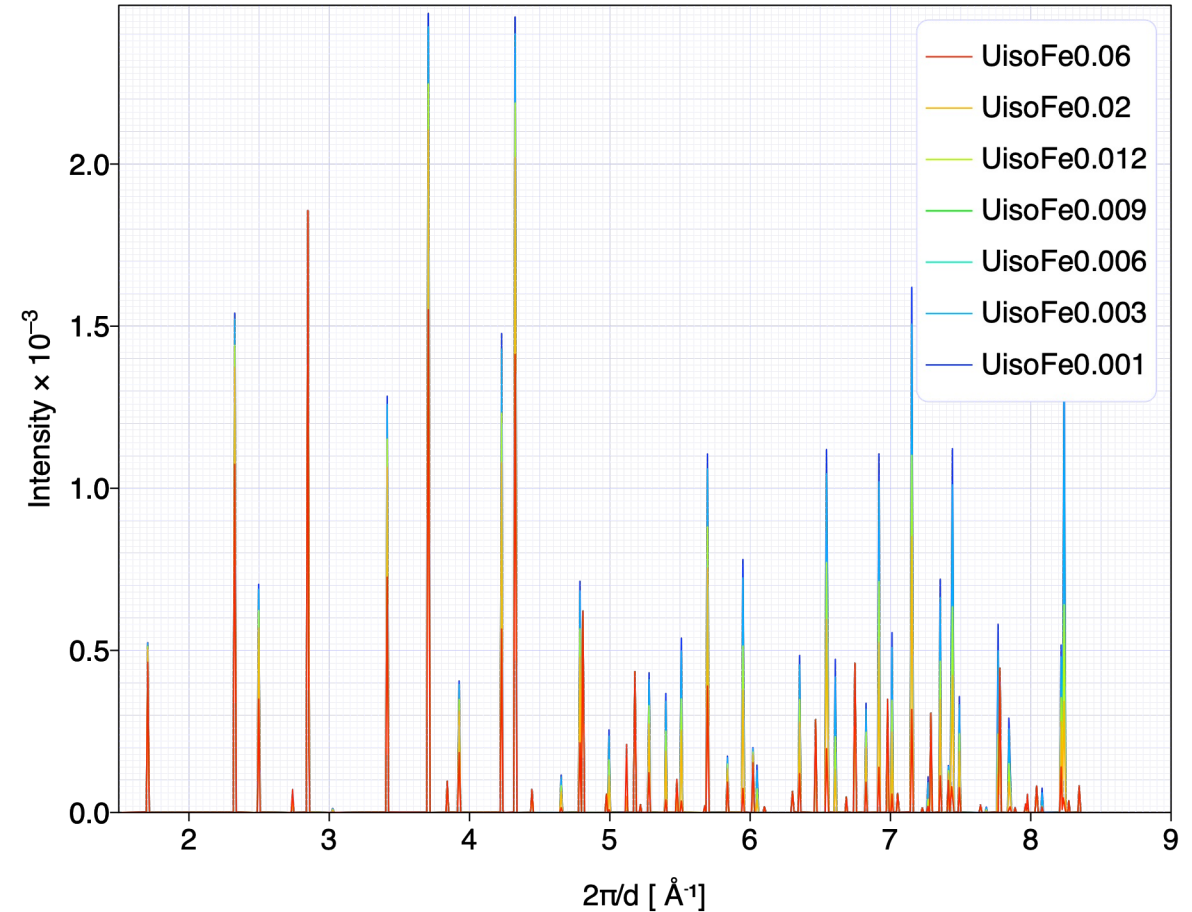
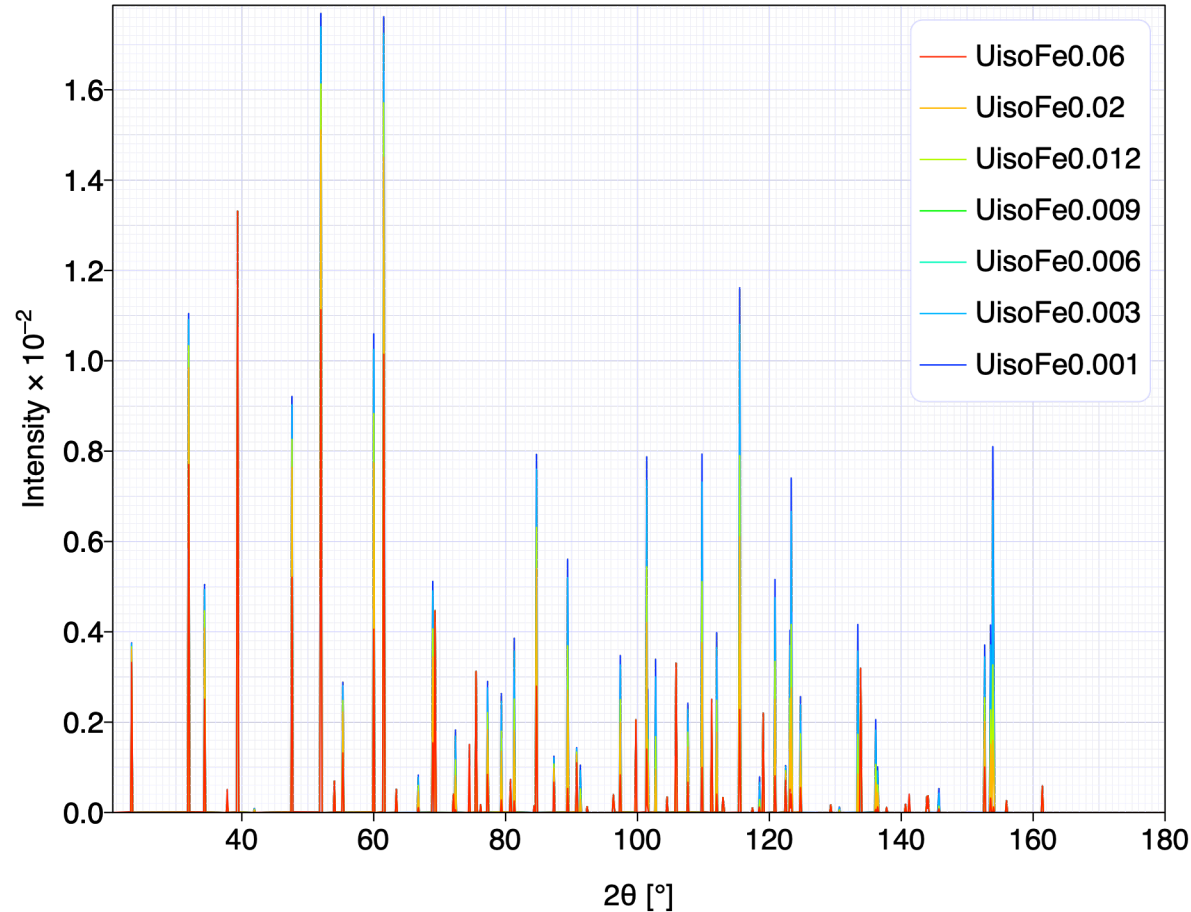
Tips:

Neutrons are more sensitive to the thermal vibrations of atoms than X-rays. The value of *Uiso* should always be positive. If it becomes negative after refinement, reset it to a reasonable positive value, as *Uiso* impacts the relative intensities of diffraction peaks.

Atomic Displacement Parameters

Fullprof GSAS-II

$$B_{iso} = 8\pi^2 U_{iso}$$



Simulated constant wavelength neutron diffraction data
using WAND² wavelength (1.486Å)

<https://addie.ornl.gov/scatteringinspector>

Powder diffraction simulation on WAND²: <https://addie.ornl.gov/hfirestimate>

Add the magnetic structure

At this point, the nuclear structure refinement is complete. The next step is to add the magnetic structure. For users who are new to refinement, it is recommended to turn off parameters such as atomic positions, *Uiso* microstrain/crystallite size, and unit-cell parameters before introducing the magnetic structure. This generally helps improve refinement stability.

Find the magnetic structure in the database

 ORNL Today

 Calendar

 Scholar

 Drive

 ORNL

 WAND2

 ResearchRelated

 Dropbox

 Documents/Data/ (...)

 Conference

 Profile



IUCr 2026
CALGARY, CANADA
AUGUST 11-18

Bilbao Crystallographic Server
in forthcoming schools and workshops

News:

- New program: SPGENPOS**
06/2026: General positions of the spin point groups
- New Article**
04/2026: Elcoro *et al.*
"Automatic calculation of symmetry-adapted tensors under spin-group symmetry: STENSOR, a new tool of the Bilbao Crystallographic Server". *J. Appl. Cryst.* (2026) **59**, 640-647
- MORPHIC EFFECTS updates**
04/2026: The magnetic-field option is now available.
- New Article**
06/2025: Etxebarria *et al.*
"Crystal tensor properties of magnetic materials with and without spin-orbit coupling. Application of spin point groups as approximate symmetries.". *Acta Cryst.* (2025) **A81**, 317-338
- New program: MINSUP for plane groups**
06/2025: Minimal supergroups of plane groups

[Contact us](#)[About us](#)[Publications](#)[How to cite the server](#)

Space-group symmetry

Magnetic Symmetry and Applications

Magnetic groups

MGENPOS
General Positions of Magnetic Space Groups

MWYCKPOS
Wyckoff Positions of Magnetic Space Groups

MKVEC
The k-vector types and Brillouin zones of Magnetic Space Groups

IDENTIFY MAGNETIC GROUP
Identification of a Magnetic Space Group from a set of generators in an arbitrary setting

BNS2OG
Transformation of symmetry operations between BNS and OG settings

mCIF2PCR
Transformation from mCIF to PCR format (FullProf).

MPOINT
Magnetic Point Group Tables

MAGNEXT
Extinction Rules of Magnetic Space Groups

MAXMAGN
Maximal magnetic space groups for a given space group and a propagation vector

MAGMODELIZE
Magnetic structure models for any given magnetic symmetry

STRCONVERT
Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)

k-SUBGROUPSMAG
Magnetic subgroups consistent with some given propagation vector(s) or a supercell

MAGNDATA
A collection of magnetic structures with portable cif-type files

MVISUALIZE
3D Visualization of magnetic structures with Jmol

MTENSOR
Symmetry-adapted form of crystal tensors in magnetic phases

MAGNETIC REP.
Decomposition of the magnetic representation into irreps

Get_mirreps
Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

Spin groups

SPGENPOS 
General positions of spin point groups

STENSOR 
Symmetry-adapted form of crystal tensors under spin point groups

CollinearSpinGroups 
Operations of Nontrivial Collinear Spin Space Groups

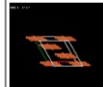
[View Full Database](#)

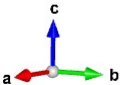
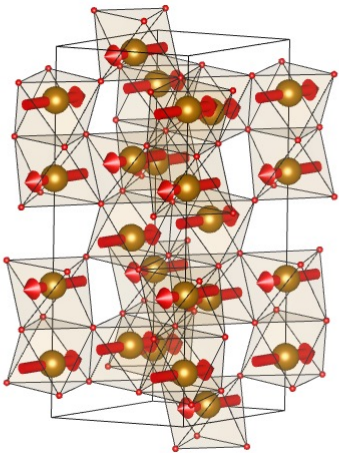
Element search (separate with space or comma): ☒ AND ☐ OR

Enter the label of the structure:

[Advanced Search](#)

To submit any published structure click [HERE](#)

0	0.65 Fe ₂ O ₃ .alpha		0,0,0	R-3c (167) (standard)	(a,b,c;0,0,0)	C2'/c' (15.89) (1/3a+2/3b+2/3c,-a,-1/3a-2/3b+1/3c;0,1/2,0)	2'/m' (5.5.16)	A.H. Hill, F. Jiao, P.G. Bruce, A. Harrison, W. Kockelmann and C. Ritter, <i>Chemistry of Materials</i> (2008) 20 4891-4899. DOI: 10.1021/cm800009s
11	0.66 Fe ₂ O ₃ .alpha		0,0,0	R-3c (167) (standard)	(a,b,c;0,0,0)	P-1 (2.4) (a,b,2/3a+1/3b+1/3c;0,0,0)	-1.1 (2.1.3)	A.H. Hill, F. Jiao, P.G. Bruce, A. Harrison, W. Kockelmann and C. Ritter, <i>Chemistry of Materials</i> (2008) 20 4891-4899. DOI: 10.1021/cm800009s

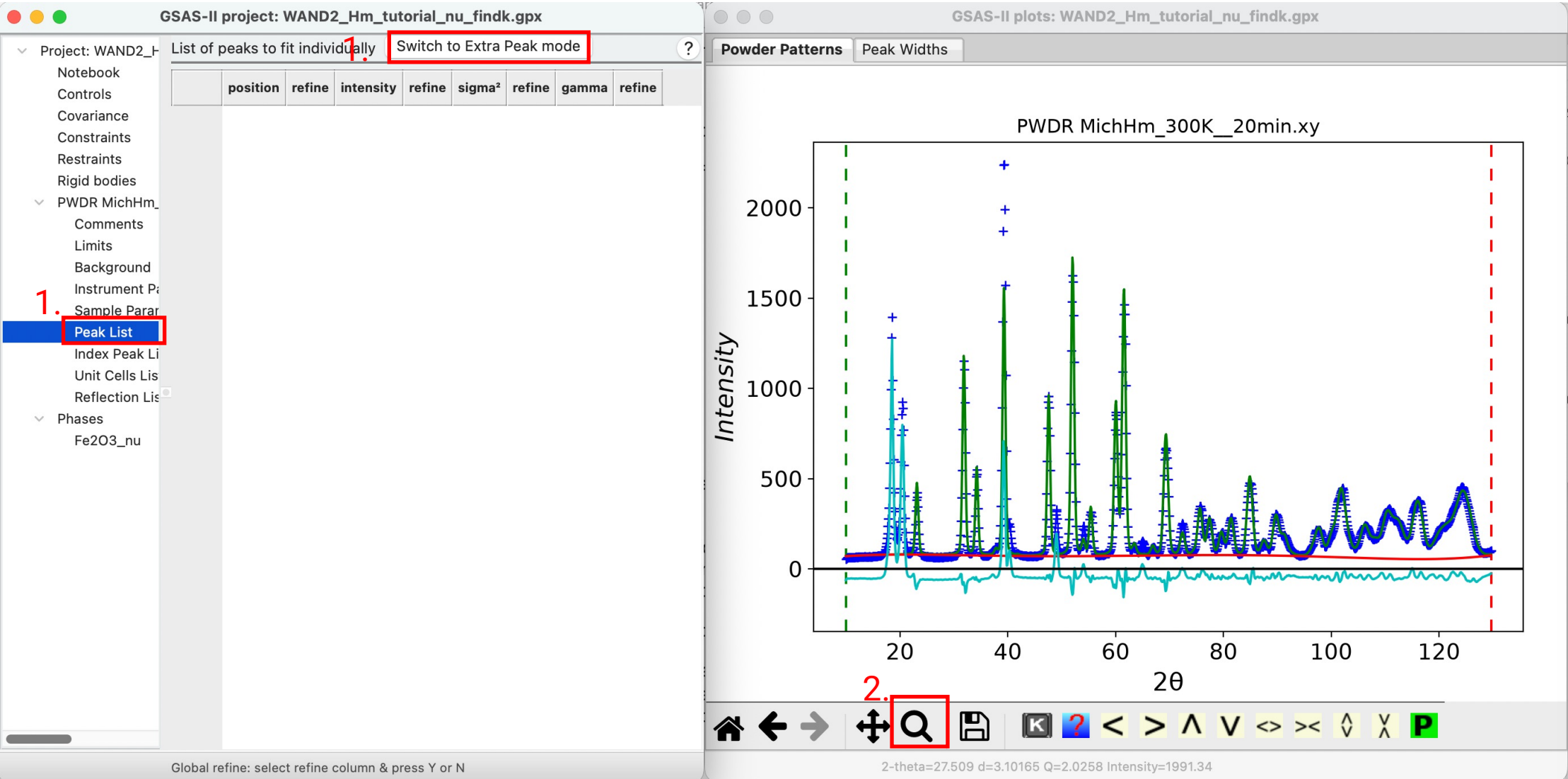


Parent space group (paramagnetic phase): [R-3c \(#167\)](#)
Propagation vector: k1 (0, 0, 0)

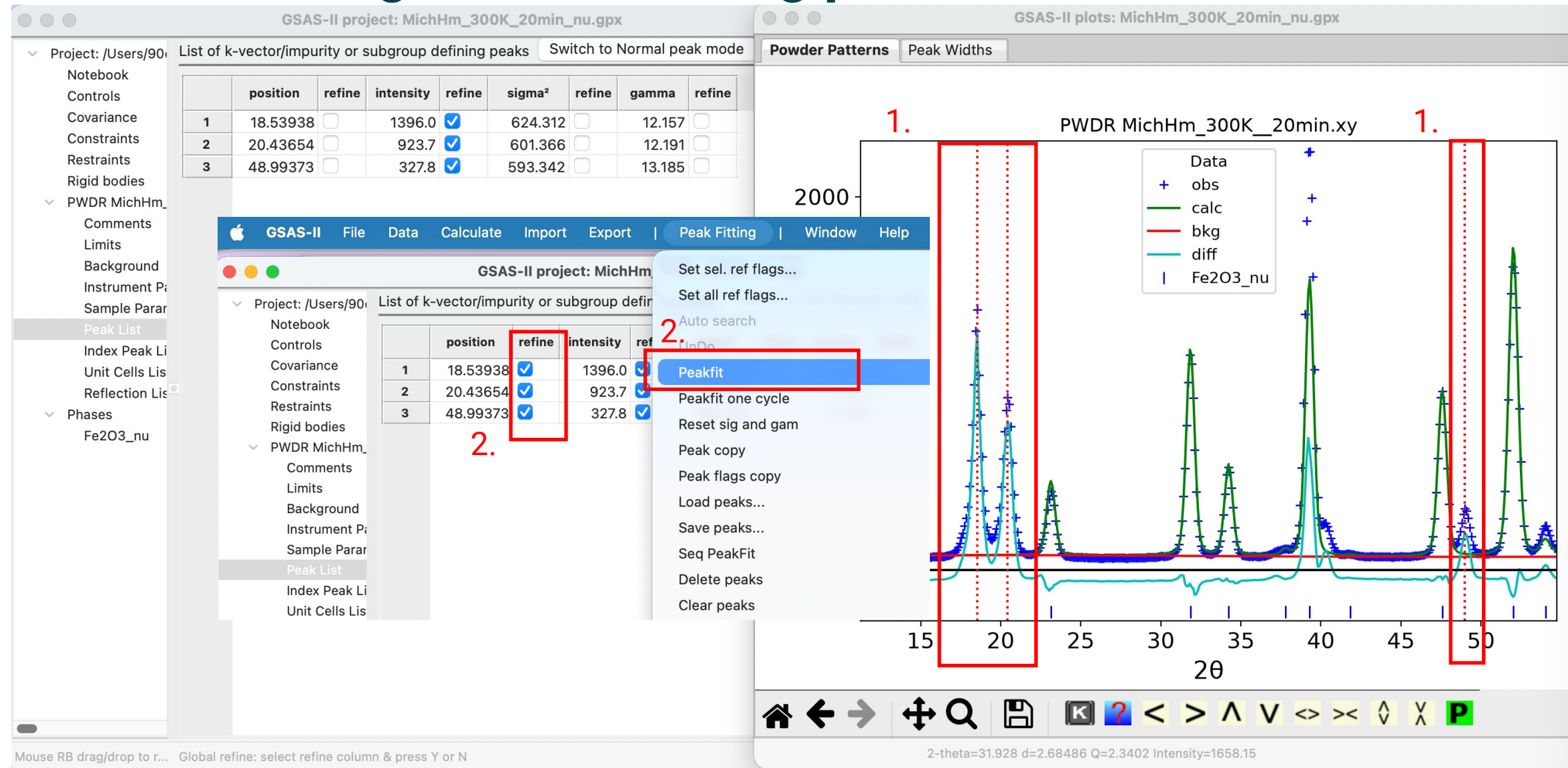
Experiment Temperature: 300 K

BNS Magnetic Space Group: C2'/c' (#15.89) (non-standard)

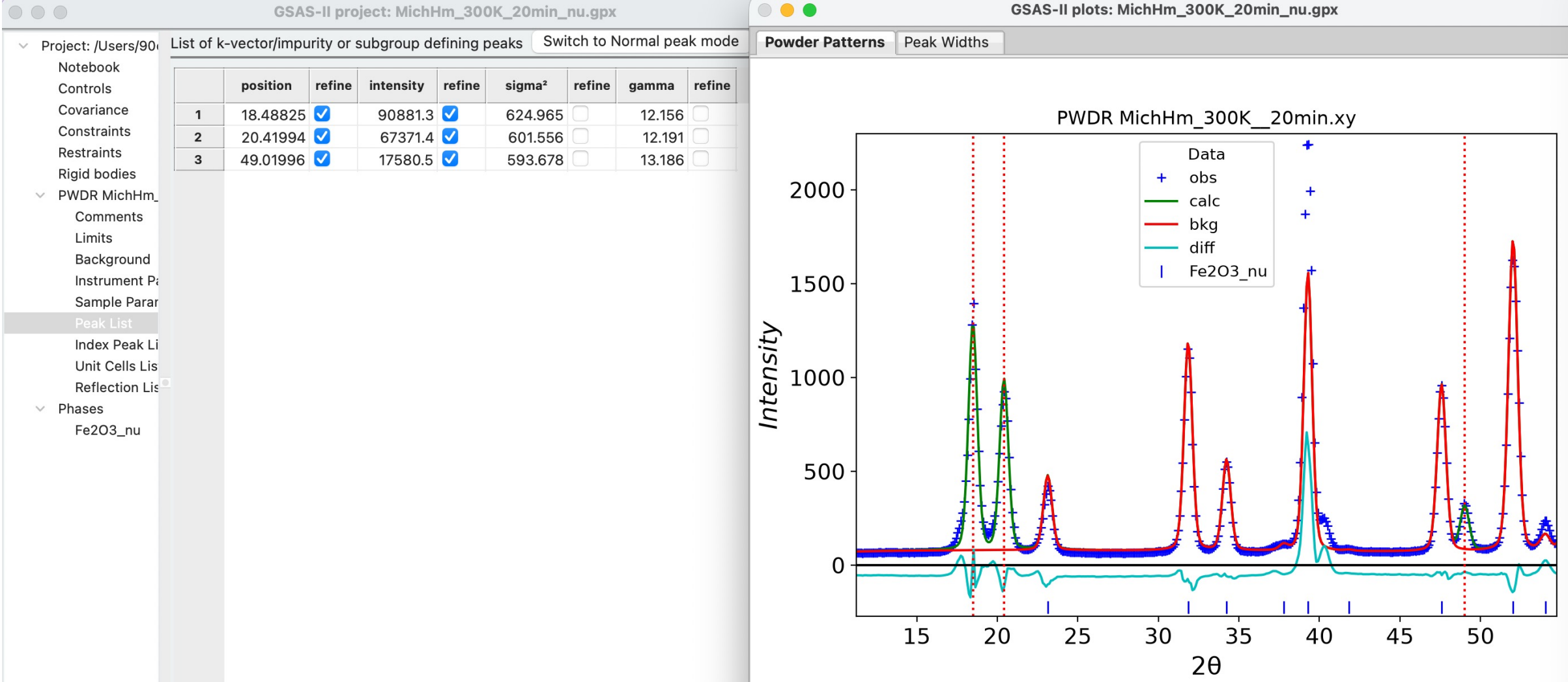
Identify magnetic scattering peaks



Add and fit magnetic scattering peaks



Search k-vector



Determine the magnetic propagation vector

GSAS-II project: MichHm_300K_20min_nu.gpx

1. **Unit Cells List**

2. **Indexing tools** ☒ Search for k-vector

k-Vector Search Mode

kx step 0.01 ky step 0.01 kz step 0.01 Number of processors 8

Search tolerance 0.0 Search option HighSymPts

3. **Start Search**

Unit Cell & Symmetry Settings for Reflection Display

Bravais lattice P1 Space group P1 Try all? ☐ Modulated? ☐

a = 1.0 b = 1.0 c = 1.0

$\alpha = 90.0^\circ \beta = 90.0^\circ \gamma = 90.0^\circ$

cell step 0.5% Zero offset 0.0 ☐ Ref?

Vol = 1.000

show HKL from cell ☐ Show Extinct ☐ highlight None ☐ Magnetic? ☐ Make new Peak list

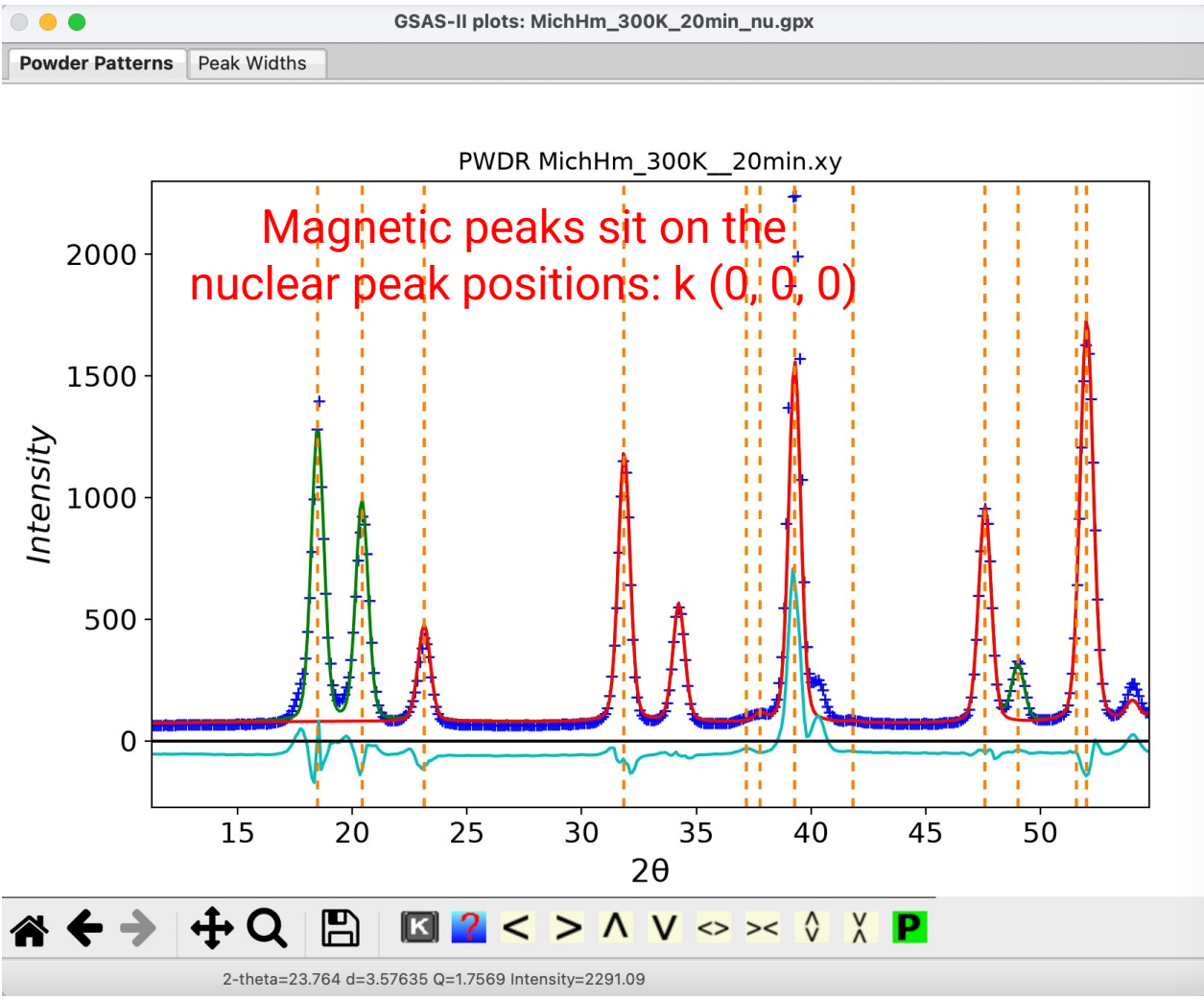
Cell Search Results

k-vector search results:

show	kx	ky	kz	Ave. $\delta d/d$	Ave. δd	Max. δd
☒	0.00000	0.00000	0.00000	0.00022	0.00094	0.00256
☐	0.50000	-0.50000	-0.50000	0.02099	0.08739	0.25313
☐	0.50000	0.00000	0.50000	0.02099	0.08739	0.25313
☐	0.00000	0.50000	-0.50000	0.02099	0.08739	0.25313
☐	0.26624	0.26624	1.50000	0.02450	0.11045	0.31220
☐	0.53249	-0.26624	1.50000	0.02450	0.11045	0.31220
☐	0.26624	0.46751	0.50000	0.02450	0.11045	0.31220
☐	0.73376	-0.46751	0.50000	0.02450	0.11045	0.31220
☐	0.00000	0.00000	1.50000	0.02462	0.10509	0.27554
☐	0.39937	-0.39937	1.50000	0.03059	0.13481	0.33664

Call ISODISTORT

Check through the k-vector!



Delete peak lists and switch to normal peak mode

Project: /Users/9001/

GSAS-II project: MichHm_300K_20min_nu.gpx

▼ Project: /Users/9001/

▼ PWDR MichHm_300K_20min_nu.gpx

▼ Phases

Notebook

Controls

Covariance

Constraints

Restraints

Rigid bodies

Comments

Limits

Background

Instrument Parameters

Sample Parameters

Peak List

Index Peak List

Unit Cells List

Reflection List

Fe2O3_nu

List of k-vector/impurity or subgroup defining peaks

Switch to Normal peak mode

	position	refine	intensity	refine	sigma ²	refine	gamma	refine
1	18.48825	☒	90881.3	☒	624.965	☐	12.156	☐
2	20.41994	☒	67371.4	☒	601.556	☐	12.191	☐
3	49.01996	☒	17580.5	☒	593.678	☐	13.186	☐

Delete peaks

Select peaks to delete

Name

Filter:

☒ 0) 18.49

☒ 1) 20.42

☒ 2) 49.02

Apply stride: 1

Set All

Toggle All

Set Range

Cancel

OK

Global refine: select refine column & press Y or N

Generate all possible commensurate magnetic SG subgroups

1. Open File menu and select "Save project as..."

2. Select "Unit Cells List" from the Project list

3. Select "Run k-SUBGROUPMAG" from the Indexing controls

Unit cell parameters: a = 1.0, b = 1.0, c = 1.0, α = 90.0, β = 90.0, γ = 90.0, Vol = 1.000

3. Select "Run k-SUBGROUPMAG" from the Cell Index/Refine menu

Unit cell parameters: a = 5.02026, c = 13.7047, Vol = 299.1

Magnetic peaks sit on the nuclear peak positions: $k(0, 0, 0)$

4. Set k-vector 1 to 0 0 0

Options: Use whole star (checked), Filter by (dropdown), preserve axes (checked), test for mag. atoms (Fe), all have moment (checked), max unique (100)

Bilbao k-SUBGROUPSMAG

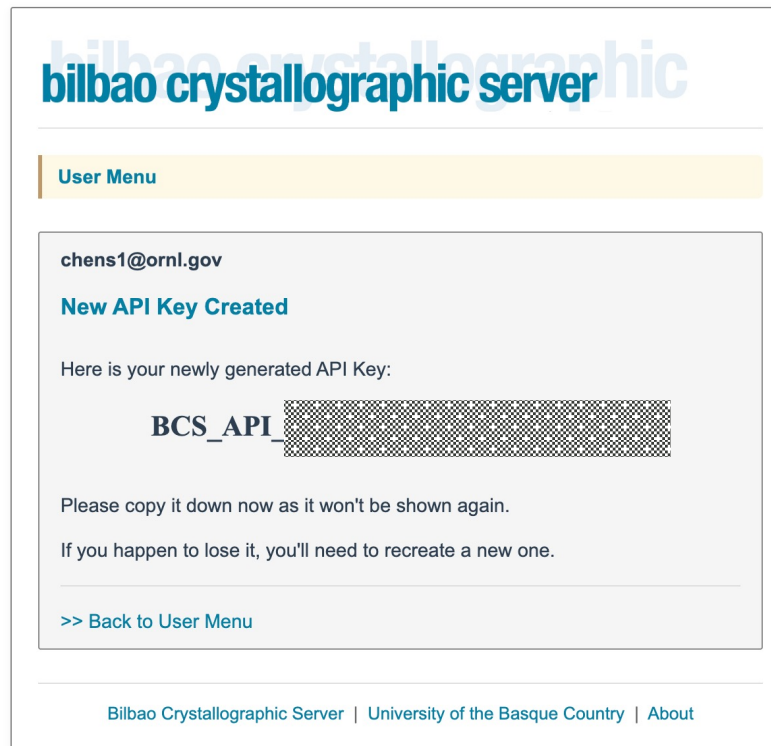
For use of k-SUBGROUPSMAG, please cite:
Symmetry-Based Computational Tools for Magnetic Crystallography, J.M. Perez-Mato, S.V. Gallego, E.S. Tasci, L. Elcoro, G. de la Flor, and M.I. Aroyo
Annu. Rev. Mater. Res. 2015. 45,217-48.
doi: <https://doi.org/10.1146/annurev-matsci-070214-021008>

OK

Troubleshoot

Update 07/15/2026

If you installed an older version of GSAS-II and are having trouble running (k)-SUBGROUPSMAG, follow this tutorial to configure GSAS-II access to the Bilbao Crystallographic Server:
<https://advancedphotonsource.github.io/GSAS-II-tutorials/RegisterBilbao/RegisterBilbao.html>



Select magnetic space group I 2'/c' for the refinement

Project: WAND2_Hm_tutorial_nu_mag

Notebook

Controls

Covariance

Constraints

Restraints

Rigid bodies

PWDR 1373498_MichHm_300K_

Comments

Limits

Background

Instrument Parameters

Sample Parameters

Peak List

Index Peak List

Unit Cells List

Reflection Lists

Phases

Fe2O3_nu

Indexing tools

Autoindexing of "Index Peak List" contents

Bravais Lattice(s) for autoindexing trials:

☐ Cubic-F
☐ Cubic-I
☐ Cubic-P
☐ Trigonal-R
☐ Trigonal/Hexagonal-P
☐ Tetragonal-I
☐ Tetragonal-P
☐ Orthorhombic-F
☐ Orthorhombic-I
☐ Orthorhombic-A
☐ Orthorhombic-B
☐ Orthorhombic-C
☐ Orthorhombic-P
☐ Monoclinic-I
☐ Monoclinic-A
☐ Monoclinic-C
☐ Monoclinic-P
☐ Triclinic

Max Nc/Nobs 4
Start Volume 25
☒ Use M20/(X20+1)?

Unit Cell & Symmetry Settings for Reflection Display

Bravais lattice R3-H
Space group R -3 c
Try all? ☐ Modulated? ☐

a = 5.02026
c = 13.7047
Vol = 299.125
cell step 0.5%
Zero offset 0.0
☐ Ref?

☐ show HKL from cell
☐ Show Extinct
highlight None
☒ Magnetic?
☐ Make new Peak list

Cell Search Results

Magnetic subgroup cells from Bilbao k-SUBGROUPSMAG for R -3 c; kvec1=(0,0,0):

	Space Gp	Try	Keep	Uniq	nConj	nSup	Trans	Vec	a
6	R3c	☐	☒	2	1	2	a,b,c	0,0,0	5.02
7	R32'	☐	☒	2	1	2	a,b,c	0,0,1/4	5.02
8	R32	☐	☒	2	1	2	a,b,c	0,0,1/4	5.02
9	R-3'	☐	☒	2	1	2	a,b,c	0,0,0	5.02
10	R-3	☐	☒	2	1	2	a,b,c	0,0,0	5.02
11	R3	☐	☒	4	1	6	a,b,c	0,0,0	5.02
12	I 2'/c'	☒	☒	1	3	1	0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c	0,1/2,0	7.3E
13	I 2/c'	☐	☒	1	3	1	0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c	0,1/2,0	7.3E
14	I 2'/c	☐	☒	1	3	1	0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c		
15	I 2/c	☐	☒	1	3	1	0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c		

Powder Patterns

PWDR 1373498_MichHm_300K_20min.xy

Intensity

2θ

Magnetic space group information

Magnetic Space Group: I 2'/c'
The lattice is centrosymmetric I-centered monoclinic
The Laue symmetry is 2/m
The magnetic lattice point group is 2'/m'
Multiplicity of a general site is 8
The unique monoclinic axis is b
The inversion center is located at 0,0,0

The equivalent positions are:

(1) X, Y, Z, (1)
(2) -X, Y, 1/2-Z, (2y)
(3) -X, -Y, -Z, (-1)
(4) X, -Y, 1/2+Z, (my)
for (1/2,1/2,1/2)+
(5) X, Y, Z, (1)
(6) -X, Y, 1/2-Z, (2y)
(7) -X, -Y, -Z, (-1)
(8) X, -Y, 1/2+Z, (my)

OAK RIDGE
National Laboratory

33

Select magnetic space group I 2'/c' for the refinement

GSAS-II project: WAND2_Hr

Project: WAND2_Hm_tutorial_nu_ma

Overall params for 'Fe2O3_nu' (type=nu)

1. **General** | Data | Atoms | Draw Op

Phase name: Fe2O3_nu Phase type:

Refine unit cell: a = 5.02026

Density: 5.319

Elements: Fe

Isotope: Nat. Abund.

No. per cell: 12.0

Atom weight: 55.847

Bond radii: 1.47

Angle radii: 1.27

van der Waals radii: 1.70

Default color: [Orange]

2. **Phases**

Fe2O3_nu

3. **Select magnetic/subgroup phase**

Fourier map

Search map

Charge flipping

4D Charge flipping

Clear map

MC/SA

Multi MC/SA

Transform

Std setting

Compare Cells

Compare polyhedra

SUBGROUPS search

Make subgroup project file(s)

Bilbao Supergroup search

ISOCIF Supergroup search

Protein quality

Test Bilbao access

Replace phase

Pawley controls: Do Pawley refinement: [] d-space range 0.8

Fourier map controls: Map type: Fobs

Map grid step: 0.25

Charge flip controls: Reflection sets:

Map grid step: 0.25 k-Factor (0.01-1.2): 0.1 k-Max (>=10.0): 20.0

Test HKLs: 0 0 2 2 0 0 1 1 1 0 2 0 1 2 3

Monte Carlo/Simulated Annealing controls: Reflection set from: PWDR 1373498_MichHm_300K_20min.xy

MC/SA runs: 1 MC/SA Refine at 10.0 % of ranges.

MC/SA schedule: log slope: 0.9

Annealing schedule: Start temp: 0.7 Final temp: 0.1 No. trials: 250

Make new magnetic phase

Select magnetic space group

(9) R-3, (a,b,c) + (0,0,0)

(10) R-3; (a,b,c) + (0,0,0)

(11) R3; (a,b,c) + (0,0,0)

3. (12) I 2'/c'; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (0,1/2,0)

(13) I 2/c; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (0,1/2,0)

(14) I 2'/c; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (0,1/2,0)

(15) I 2/c; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (0,1/2,0)

(16) I c'; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (1/5,-0)

(17) I c; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (1/5,-0)

3. Cancel OK

Magnetic atom selection

For: (12) I 2'/c'; (0.7a+1.3b+0.3c,-a,-0.3a-0.7b+0.3c) + (0,1/2,0)

Name, x, y, z, allowed moments, mag. site sym:

4. ☒ Use? Fe_0 0.60532 0.25000 0.46064 (Mx, My, Mz) 1

Yes No Delete

Save as a new gpx file

Check constrains

$$\begin{bmatrix} x_{mono} \\ y_{mono} \\ z_{mono} \end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{2} & 1 \\ 1 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 2 \end{bmatrix} \begin{bmatrix} x_{hex} \\ y_{hex} \\ z_{hex} \end{bmatrix} + \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ -\frac{1}{4} \end{bmatrix}$$

Check the constrains, Errors could happen. If you find any errors, correct them.

$$\begin{pmatrix} a_{mono} \\ b_{mono} \\ c_{mono} \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & \frac{4}{3} & \frac{1}{3} \\ -1 & 0 & 0 \\ -\frac{1}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} x_{hex} \\ y_{hex} \\ z_{hex} \end{pmatrix}$$

GSAS-II project: Fe2O3_nu-mag_12.gpx

Define/edit constraints on refined parameters

Phase Histogram/Phase Histogram Global Sym-Generated

Show Errors Show Warnings Show generated constraints Delete selected

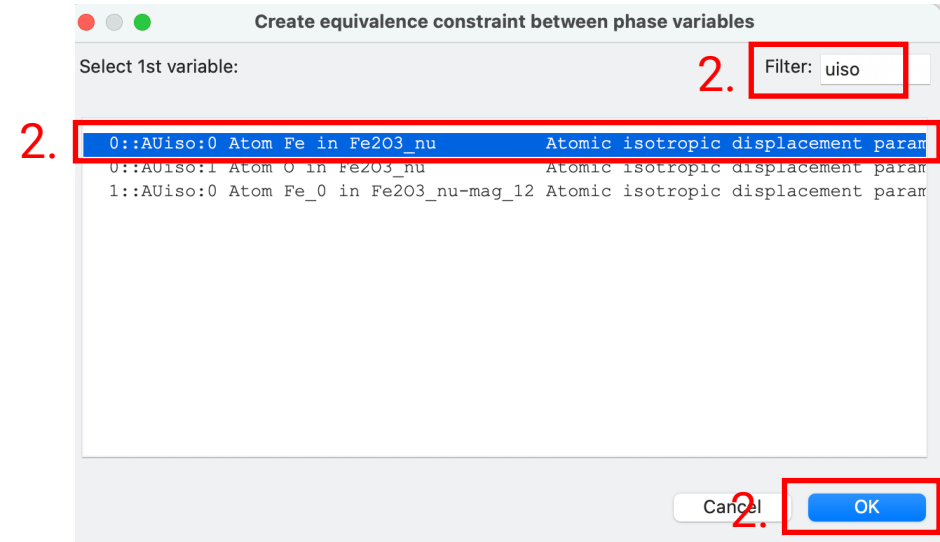
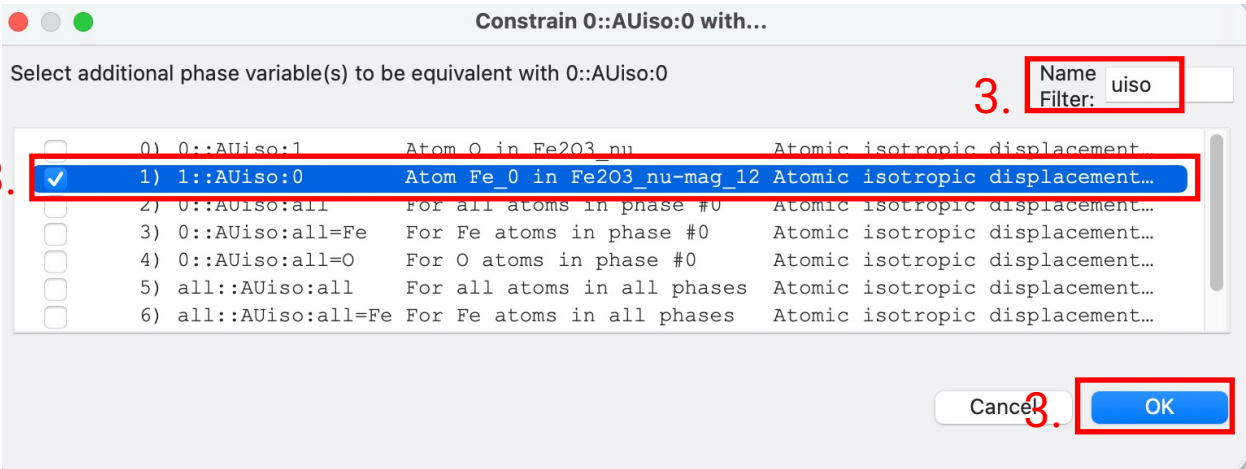
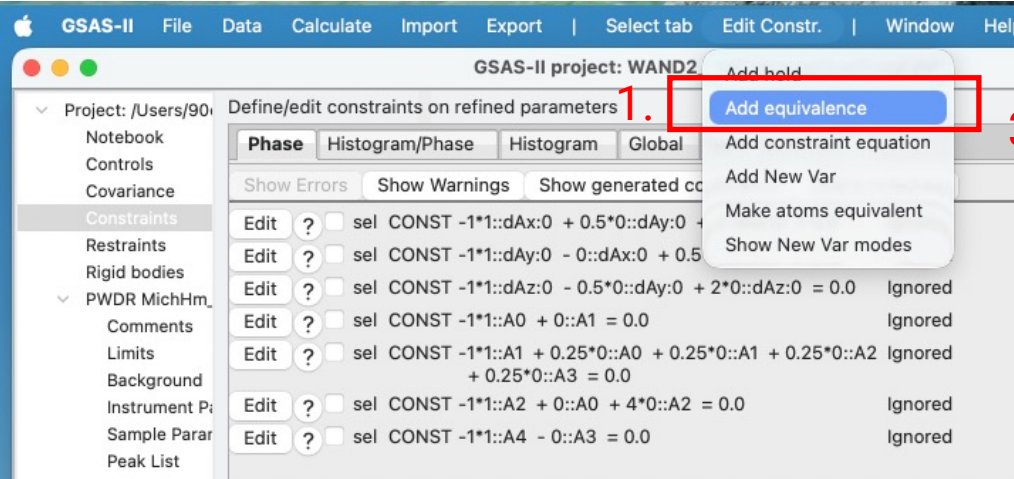
Edit	?	sel	CONST	-1*1::dAx:0 + 0.5*0::dAy:0 + 0::dAz:0 = 0.0	Ignored
Edit	?	sel	CONST	-1*1::dAy:0 - 0::dAx:0 + 0.5*0::dAy:0 = 0.0	Ignored
Edit	?	sel	CONST	-1*1::dAz:0 - 0.5*0::dAy:0 + 2*0::dAz:0 = 0.0	Ignored
Edit	?	sel	EQUIV	1::Afrac:0 = 0::dAz:0	Recast as constraint.
Edit	?	sel	EQUIV	1::AUiso:0 = 0::dAz:0	Recast as constraint.
Edit	?	sel	CONST	-1*1::A0 + 0::A1 = 0.0	Ignored
Edit	?	sel	CONST	-1*1::A1 + 0.25*0::A0 + 0.25*0::A1 + 0.25*0::A2 + 0.25*0::A3 = 0.0	Ignored
Edit	?	sel	CONST	-1*1::A2 + 0::A0 + 4*0::A2 = 0.0	Ignored
Edit	?	sel	CONST	-1*1::A4 - 0::A3 = 0.0	Ignored

Project: /Users/90q/ORNL Dropbox/At

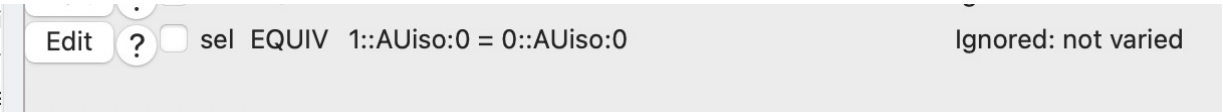
- Notebook
- Controls
- Covariance
- Constraints
- Restraints
- Rigid bodies
- PWDR 1373498_MichHm_300K_2
- Comments
- Limits
- Background
- Instrument Parameters
- Sample Parameters
- Peak List
- Index Peak List
- Unit Cells List
- Reflection Lists
- Phases
 - Fe2O3_nu
 - Fe2O3_nu-mag_12

Add constrains

Take *Uiso* as an example



Result:



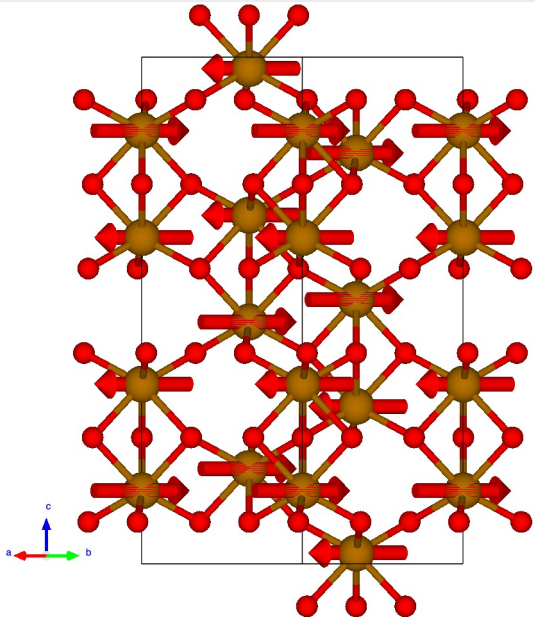
Add constrains

GSAS-II project: Fe2O3

1. Add hold

Define/edit constraints on refined parameters

Phase	Histogram/Phase	Histogram	Constraint	Status
?	sel	CONST	-1*1::dAx:0 + 0.5*0::dAz:0 = 0.0	Ignored
?	sel	CONST	-1*1::dAy:0 - 0.5*0::dAz:0 + 2*0::dAz:0 = 0.0	Ignored
?	sel	EQUIV	1::Afrac:0 = 0::dAz:0	Recast as constraint.
?	sel	EQUIV	1::AUiso:0 = 0::dAz:0	Recast as constraint.
?	sel	CONST	-1*1::A0 + 0::A1 = 0.0	Ignored
?	sel	CONST	-1*1::A1 + 0.25*0::A0 + 0.25*0::A1 + 0.25*0::A2 + 0.25*0::A3 = 0.0	Ignored
?	sel	CONST	-1*1::A2 + 0::A0 + 4*0::A2 = 0.0	Ignored
?	sel	CONST	-1*1::A4 - 0::A3 = 0.0	Ignored



2.

Hold phase variable

Select variables to hold (Will not be varied, even if vary flag is set)

Variable	Value	Variable	Value
Phase Fe2O3_nu	0.0	Reciprocal metric tensor component 0	0.0
Phase Fe2O3_nu	0.0	Reciprocal metric tensor component 1	0.0
Phase Fe2O3_nu	0.0	Reciprocal metric tensor component 2	0.0
Phase Fe2O3_nu	0.0	Reciprocal metric tensor component 3	0.0
Phase Fe2O3_nu	0.0	Reciprocal metric tensor component 4	0.0
Phase Fe2O3_nu	0.0	Reciprocal metric tensor component 5	0.0
Atom Fe in Fe2O3_nu	0.0	Atomic isotropic displacement parameter	0.0
Atom Fe in Fe2O3_nu	0.0	Atomic site fraction parameter	0.0
Atom Fe in Fe2O3_nu	0.0	Refined change to atomic coordinate, x	0.0
Atom Fe in Fe2O3_nu	0.0	Refined change to atomic coordinate, y	0.0
Atom Fe in Fe2O3_nu	0.0	Refined change to atomic coordinate, z	0.0
Atom O in Fe2O3_nu	0.0	Atomic isotropic displacement parameter	0.0
Atom O in Fe2O3_nu	0.0	Atomic site fraction parameter	0.0
Atom O in Fe2O3_nu	0.0	Refined change to atomic coordinate, x	0.0
Atom O in Fe2O3_nu	0.0	Refined change to atomic coordinate, y	0.0
Atom O in Fe2O3_nu	0.0	Refined change to atomic coordinate, z	0.0
Phase Fe2O3_nu-mag_12	1.0	Reciprocal metric tensor component 0	0.0
Phase Fe2O3_nu-mag_12	1.0	Reciprocal metric tensor component 1	0.0
Phase Fe2O3_nu-mag_12	1.0	Reciprocal metric tensor component 2	0.0
Phase Fe2O3_nu-mag_12	1.0	Reciprocal metric tensor component 3	0.0
Phase Fe2O3_nu-mag_12	1.0	Reciprocal metric tensor component 4	0.0
Phase Fe2O3_nu-mag_12	1.0	Reciprocal metric tensor component 5	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Atomic magnetic moment parameter, x	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Atomic magnetic moment parameter, y	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Atomic magnetic moment parameter, z	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Atomic isotropic displacement parameter	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Atomic site fraction parameter	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Refined change to atomic coordinate, x	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Refined change to atomic coordinate, y	0.0
Atom Fe_0 in Fe2O3_nu-mag_12	1.0	Refined change to atomic coordinate, z	0.0

Cancel OK

Note: The magnetic moment constraints depend on the specific sample and may not be applicable to general refinements

Constraint Warning

Warning noted after adding constraint (this may be OK):

Converting equivalence to constraint: 0::dAz:0 ==> 1::Afrac:0
Independent parameter 0::dAz:0 used in constraint
Converting to "Constr"

Converting equivalence to constraint: 0::dAz:0 ==> 1::AUiso:0
Independent parameter 0::dAz:0 used in constraint
Converting to "Constr"

Unused equivalence: 0:0:Scale ==> 1:0:Scale / 1.5
Contains no varied parameters
Will ignore this equivalence

Unused equivalence: 0:0:Size;i ==> 1:0:Size;i
Contains no varied parameters
Will ignore this equivalence

Unused equivalence: 0:0:Mustrain;i ==> 1:0:Mustrain;i
Contains no varied parameters
Will ignore this equivalence

Yes No

Refine magnetic structures

Project: /Users/90q/ORNL Dropbox/At

Fe2O3_nu

Fe2O3_nu-mag_12

PWDR 1373498_MichHm_300K_2

Phases

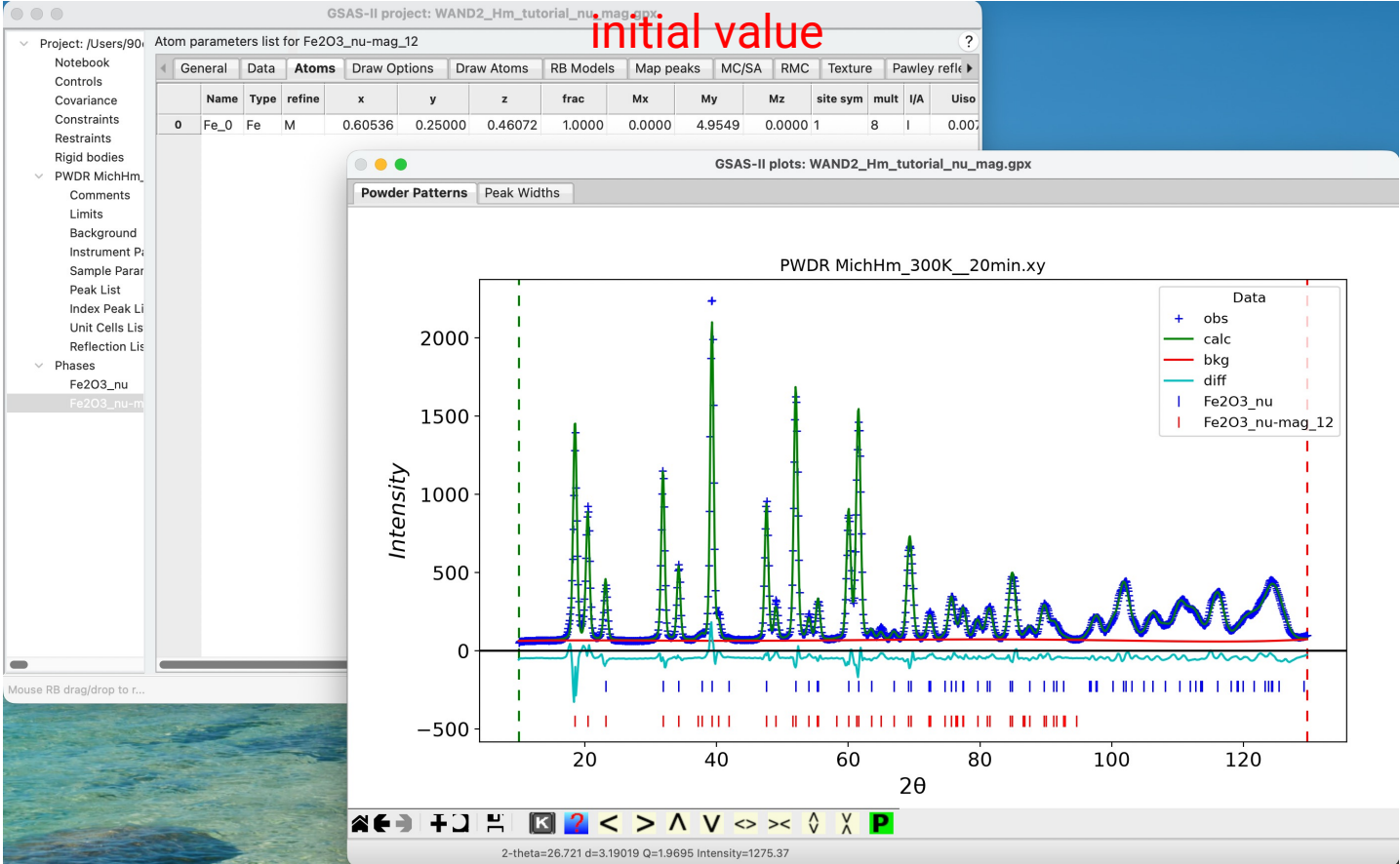
Fe2O3_nu

Fe2O3_nu-mag_12

Atom parameters list for Fe2O3_nu-mag_12

	Name	Type	refine	x	y	z	frac	Mx	My	Mz	site sym	
0	Fe_0	Fe	M	0.60532	0.25000	0.46064	1.0000	0.0000	1.0000	0.0000	1	8

Give an
initial value



Turn on other refinement parameters

GSAS-II project: WAND2_Hm_tutorial_nu_mag.gpx

Atom parameters list for Fe2O3_nu-mag_12

	Name	Type	refine	x	y	z	frac	Mx	My	Mz	site sym	mult	I/A	Uiso
0	Fe_0	Fe	MXU	0.60536	0.25000	0.46072	1.0000	0.0000	4.9549	0.0000	1	8	I	0.00

GSAS-II project: WAND2_Hm_tutorial_nu_mag.gpx

Atom parameters list for Fe2O3_nu

	Name	Type	refine	x	y	z	frac	site sym	mult	I/A	Uiso
0	Fe	Fe	XU	0.00000	0.00000	0.35536	1.0000	3	12	I	0.00711
1	O	O		0.30447	0.00000	0.25000	1.0000	2(100)	18	I	0.00390

Other refinement parameters can be gradually turned on, for example unit cell parameters, atom positions, *Uiso*, and occupancy. Be sure to check the **Constraints** page and confirm that the parameters of the two cells are properly constrained.

GSAS-II project: WAND2_Hm_tutorial_nu_mag.gpx

Histogram-specific parameters for Phase 'Fe2O3_nu'

General Data Atoms Draw Options Draw Atoms RB Models Map

PWDR MichHm_300K_20min.xy

Select plot type:

- ☒ None
- ☐ Mustrain
- ☐ Size
- ☐ Preferred orientation
- ☐ St. proj. Inv. pole figure
- ☐ Eq. area Inv. pole figure

☒ Use Histogram: PWDR MichHm_300K_20min.xy ? Histogram type: PNC Start

Phase fraction: 1 Wt. fraction: 1.000

Domain size model: isotropic ☒ LGmix 1.0 Reset?

size(μm): 1.0

Mustrain model: isotropic ☒ LGmix 1.0 Reset?

☒ microstrain: 549.2

Hydrostatic/elastic strain:

D11 0.0 D33 0.0

Layer displacement (μm): 0.0

GSAS-II project: WAND2_Hm_tutorial_nu_mag.gpx

Histogram-specific parameters for Phase 'Fe2O3_nu'

General Data Atoms Draw Options Draw Atoms RB Models Map

PWDR MichHm_300K_20min.xy

Select plot type:

- ☒ None
- ☐ Mustrain
- ☐ Size
- ☐ Preferred orientation
- ☐ St. proj. Inv. pole figure
- ☐ Eq. area Inv. pole figure

☒ Use Histogram: PWDR MichHm_300K_20min.xy ? Histogram type: PNC Start

Phase fraction: 1 Wt. fraction: 1.000

Domain size model: isotropic ☒ LGmix 1.0 Reset?

size(μm): 1.0

Mustrain model: isotropic ☒ LGmix 1.0 Reset?

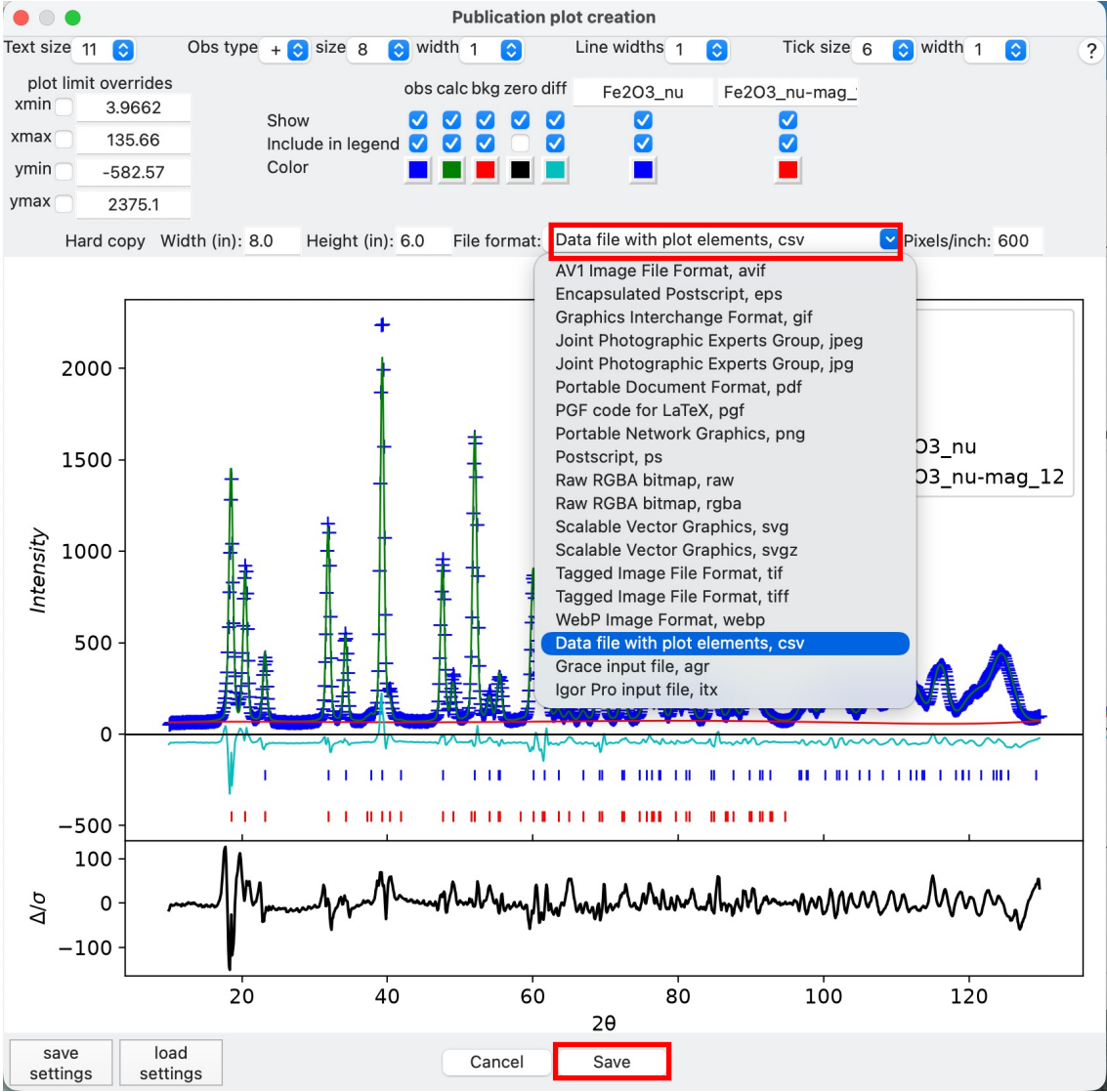
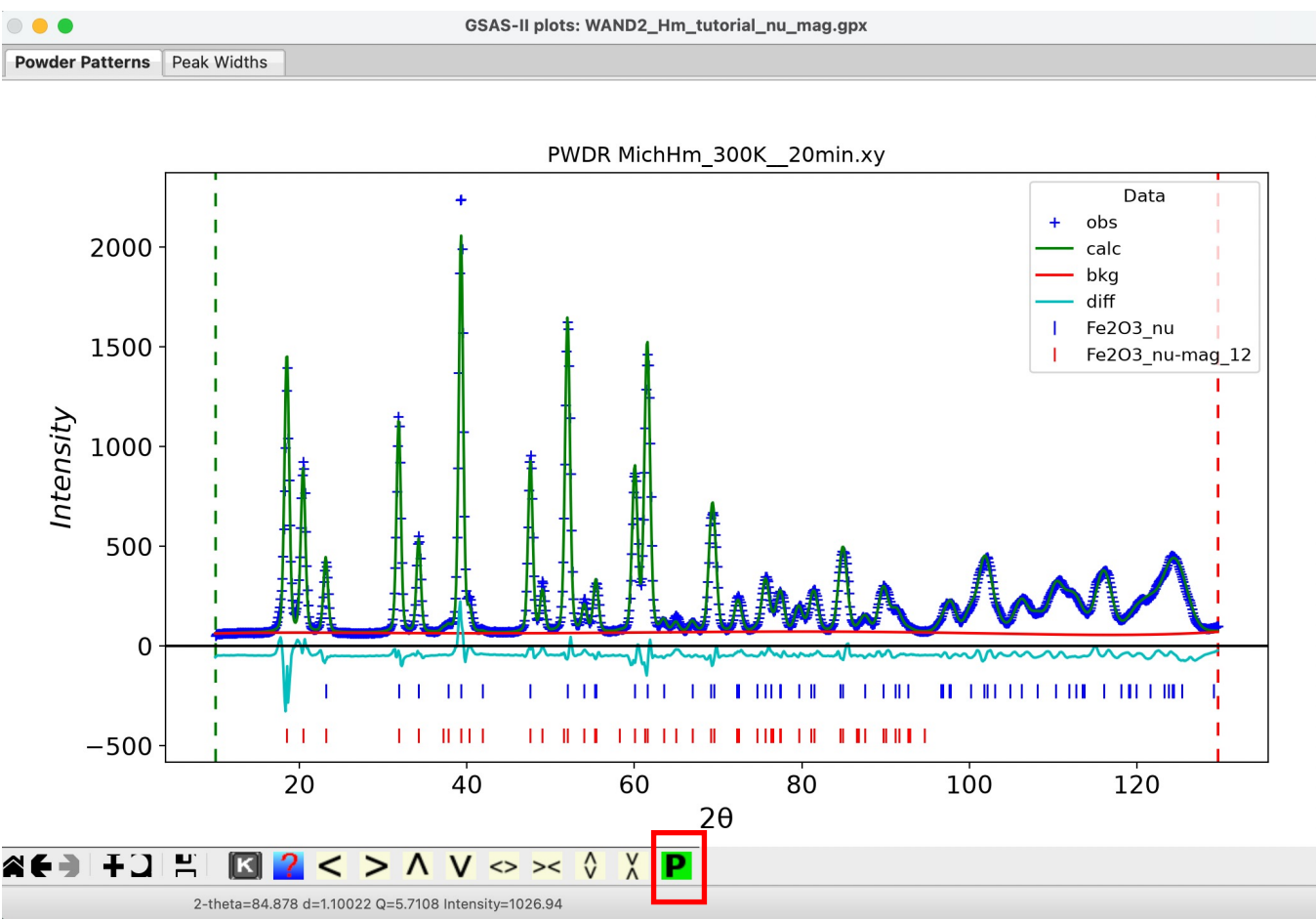
☒ microstrain: 549.2

Hydrostatic/elastic strain:

D11 0.0 D33 0.0

Layer displacement (μm): 0.0

Publish the refinement results



Visualize the magnetic structure in GSAS-II

The screenshot shows the GSAS-II software interface. The top menu bar includes Apple logo, GSAS-II, File, Data, Calculate, Import, Export, Select tab, Edit Figure, and Compute. The main window title is 'GSAS-II project: WAND2'. On the left, a tree view shows the project structure: Project: /Users/90..., Notebook, Controls, Covariance, Constraints, Restraints, Rigid bodies, PWDR MichHm..., Comments, Limits, Background, Instrument Pa..., Sample Parar..., Peak List, Index Peak Li..., Unit Cells Lis..., Reflection Lis..., Phases, Fe2O3_nu, and Fe2O3_nu-m. The 'Fe2O3_nu-m' item is highlighted with a red box and labeled '1.'. The main panel displays 'Draw Atom list for 'Fe2O3_nu-mag_12''. It has tabs for General, Data, Atoms, Draw Options, and Draw. The 'Draw' tab is selected and highlighted with a red box and labeled '2.'. Below the tabs is a table with columns: Name, Type, x, y, z. The table contains one row: Fe_0, Fe, 0.60536, 0.25000, 0.4607.

Name	Type	x	y	z
Fe_0	Fe	0.60536	0.25000	0.4607

The 'Draw' menu is open, showing options: Atom style, Atom label, Atom color, Reset atom colors, Edit atom radii, Set view point, Select from list, Add atoms, Add sphere of atoms, Transform draw atoms, Fill CN-sphere, Fill unit cell, Complete molecule, Delete atoms, Update draw atoms, Load selected atoms, and Randomized action. The 'Fill unit cell' option is highlighted with a blue bar.

GSAS-II project: WAND2_Hm_tutorial_nu_mag.gpx

Project: /Users/90/

Notebook Controls

Covariance

Constraints

Restraints

Rigid bodies

PWDR MichHm

Comments

Limits

Background

Instrument Parameters

Sample Parameters

Peak List

Index Peak List

Unit Cells List

Reflection List

Phases

Fe2O3_nu

Fe2O3_nu-m

Draw Atom list for 'Fe2O3_nu-mag_12'

	Name	Type	x	y	z	Mx	My	Mz	Sym Op	Style	Label	Color
0	Fe_0	Fe	0.60536	0.25000	0.46072	0.0000	1.0000	0.0000	1	vdW balls		
1	Fe_0	Fe	0.39464	0.25000	0.03928	-0.0000	-1.0000	-0.0000	2+1,0,0	vdW balls		
2	Fe_0	Fe	0.39464	0.75000	0.53928	0.0000	1.0000	0.0000	-1+1,1,1	vdW balls		
3	Fe_0	Fe	0.60536	0.75000	0.96072	-0.0000	-1.0000	-0.0000	-2+0,1,1	vdW balls		
4	Fe_0	Fe	0.10536	0.75000	0.96072	0.0000	1.0000	0.0000	101+-1,0,0	vdW balls		
5	Fe_0	Fe	0.89464	0.75000	0.53928	-0.0000	-1.0000	-0.0000	102+1,0,0	vdW balls		
6	Fe_0	Fe	0.89464	0.25000	0.03928	0.0000	1.0000	0.0000	-101+1,0,0	vdW balls		
7	Fe_0	Fe	0.10536	0.25000	0.46072	-0.0000	-1.0000	-0.0000	-102+-1,0,0	vdW balls		

GSAS-II plots: WAND2_Hm_tutorial_nu_mag.gpx

Powder Patterns

Peak Widths

Fe2O3_nu-mag_12

SG: C 2'/c'

Export cif file

