

Single Crystal Diffraction

Feng Ye

Neutron Scattering Division

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U.S. DEPARTMENT OF
ENERGY

My career path to neutron scattering

UC, Santa Cruz

Center for neutron
scattering

Neutron Scattering
Sciences Division

Quantum Condensed
Matter Division

Neutron Scattering
Division

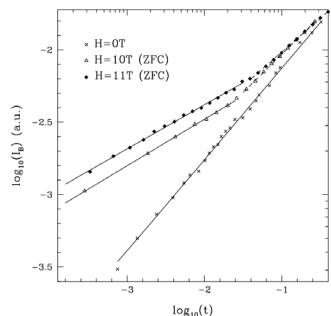
1999-2003
Physics Department Graduate student

2003-2008
Triple axis spectrometer Postdoc fellow

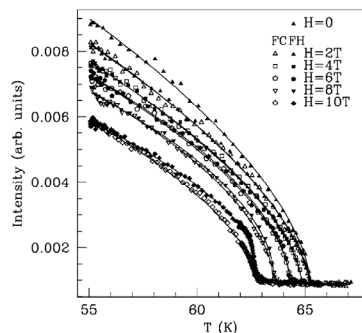
2008-2011
Single Crystal
Neutron Diffraction Instrument Scientist for Elastic diffuse scattering

2011-2017
Structure of Matter Corelli

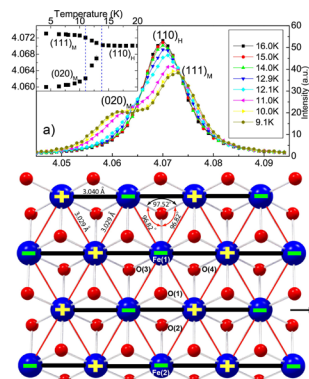
2018-Current
Single Crystal Diffraction



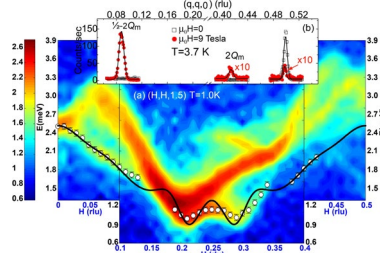
Ye *et al.*, Phys. Rev. Lett. (2002).



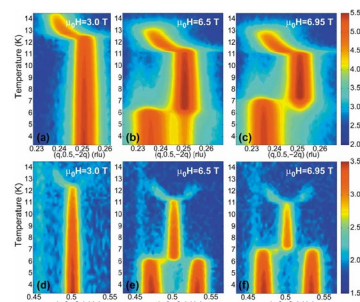
Ye *et al.*, Phys. Rev. B (2006).



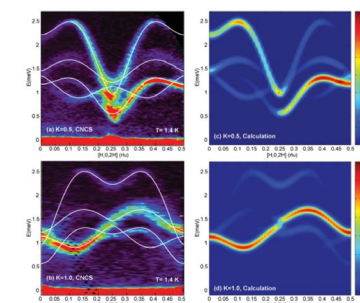
Ye *et al.*, Phys. Rev. B (2006).



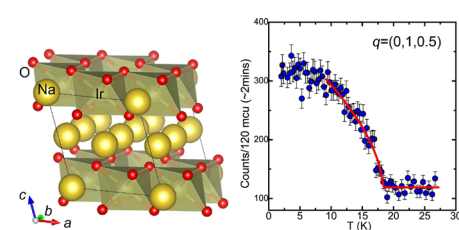
Ye *et al.*, Phys. Rev. Lett. (2007).



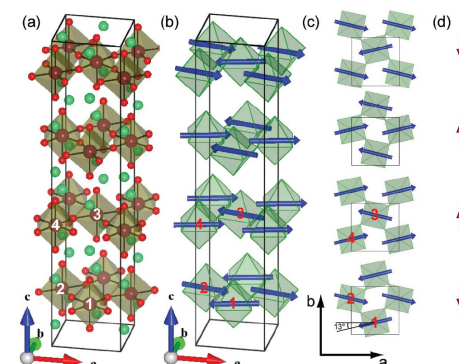
Ye *et al.*, Phys. Rev. B (2008).



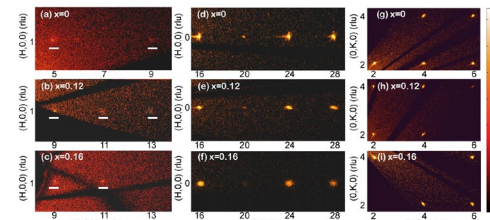
Ye *et al.*, Phys. Rev. B (2011).



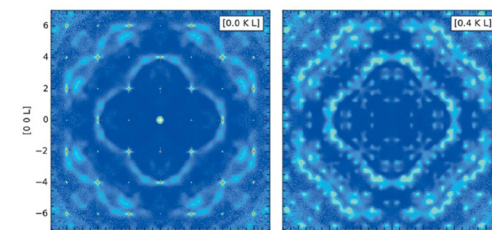
Ye *et al.*, Phys. Rev. B (2011).



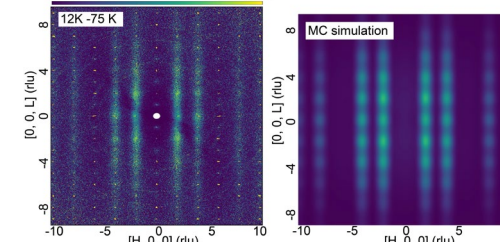
Ye *et al.*, Phys. Rev. B (2013).



Ye *et al.*, Phys. Rev. B (2015).



Ye *et al.*, J. App. Cryst. (2018).



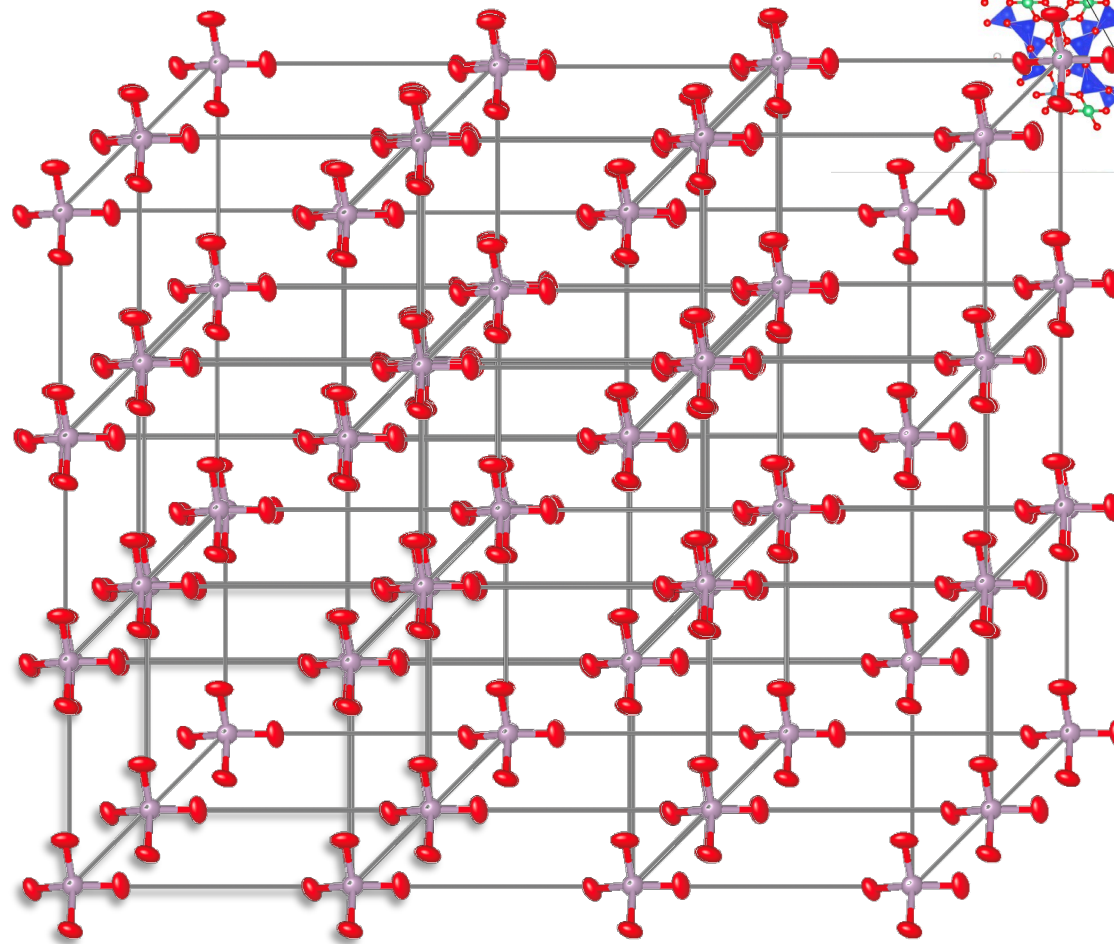
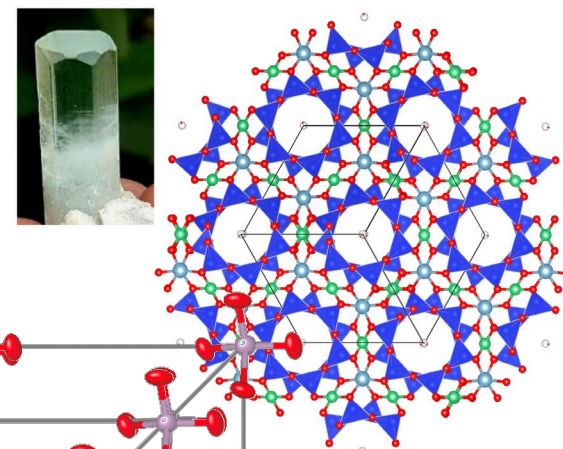
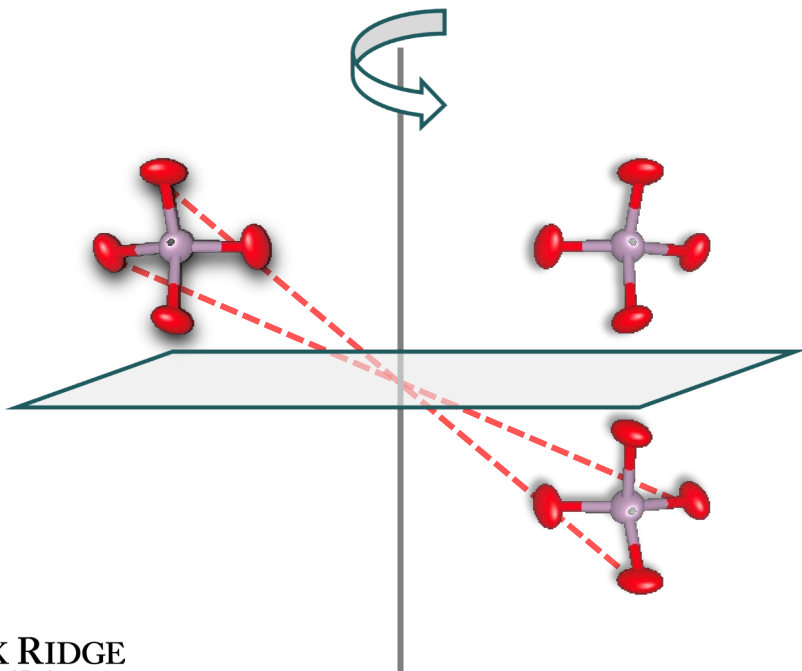
Ye *et al.*, Phys. Rev. B (2021).

Outline

- Formalism for diffraction (neutron and X-ray)
- Workflow for single crystal diffraction
- Single crystal diffractometers at HFIR and SNS
 - Overview
 - Scientific highlights

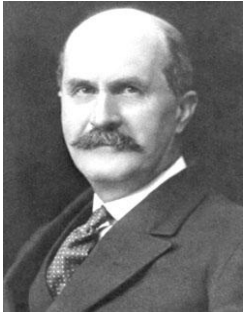
A Single Crystal

- Repeating 3-D grid of atoms / molecules
- Forming a long-range ordered structure
 - **Translation symmetry**
- Adhering to symmetry rules
 - **Rotation, Inversion, Mirror plane, ...**
 - **Glide plane, Screw axis**
- Completely fills a volume (1,2,3,4,6 fold)
➔ 7 lattice systems
- With some mis-arrangement
 - Disorder, local order, domains



- 14 Bravais lattices
- 32 point groups
- 230 space groups

Reflections from Lattice Planes

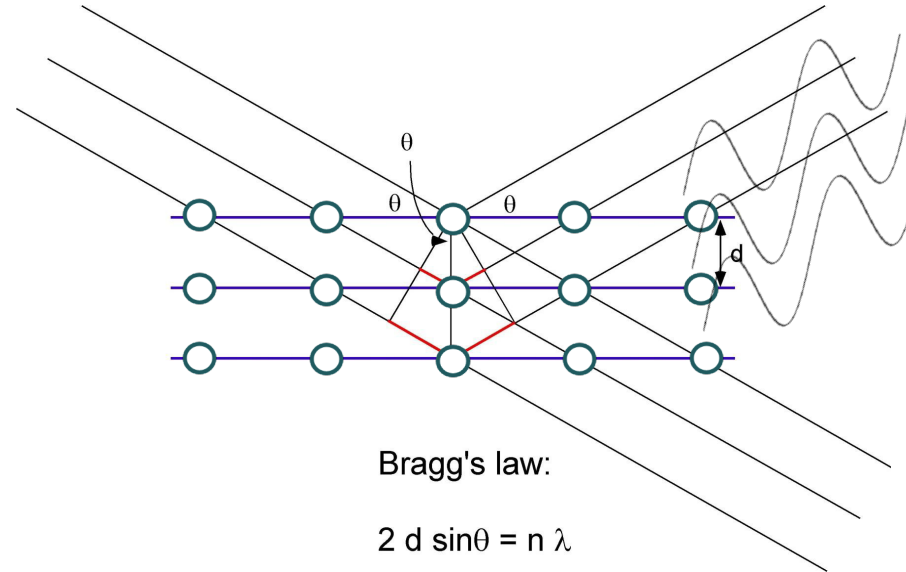


William Henry Bragg



William Lawrence Bragg

Jointly awarded the 1915 Nobel Prize in Physics

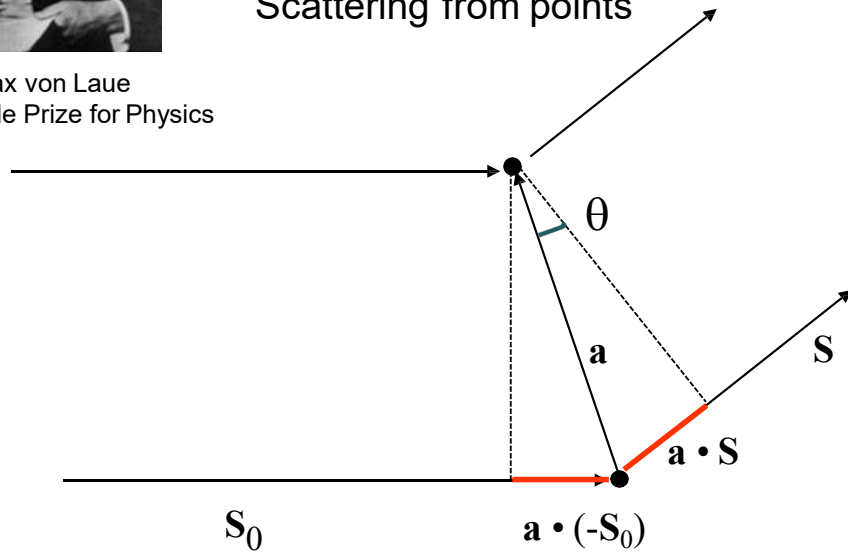


Laue Equation



Max von Laue
1914 Noble Prize for Physics

Scattering from points



$$\psi_i(\mathbf{r}) = \psi_0 e^{i\mathbf{k}_i \cdot \mathbf{r}},$$

incident plane wave

$$\mathbf{k}_i = \frac{2\pi}{\lambda} \mathbf{s}_0 \quad \mathbf{k}_f = \frac{2\pi}{\lambda} \mathbf{s}$$

$\mathbf{s}_0$, and $\mathbf{s}$ are unit vectors

$$\Delta\phi = (\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{R} = -\mathbf{Q} \cdot \mathbf{R}$$

phase difference

$$\mathbf{R} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c},$$

$\mathbf{R}$: lattice vector

$$\mathbf{Q} \cdot \mathbf{R} = u(\mathbf{Q} \cdot \mathbf{a}) + v(\mathbf{Q} \cdot \mathbf{b}) + w(\mathbf{Q} \cdot \mathbf{c}) \text{ integer multiple of } 2\pi$$

$$\mathbf{Q} \cdot \mathbf{a} = 2\pi h,$$

$$\mathbf{Q} \cdot \mathbf{b} = 2\pi k,$$

$$\mathbf{Q} \cdot \mathbf{c} = 2\pi l,$$

Laue Equation in reciprocal-space form

$$\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i = \frac{2\pi}{\lambda} (\mathbf{s} - \mathbf{s}_0)$$

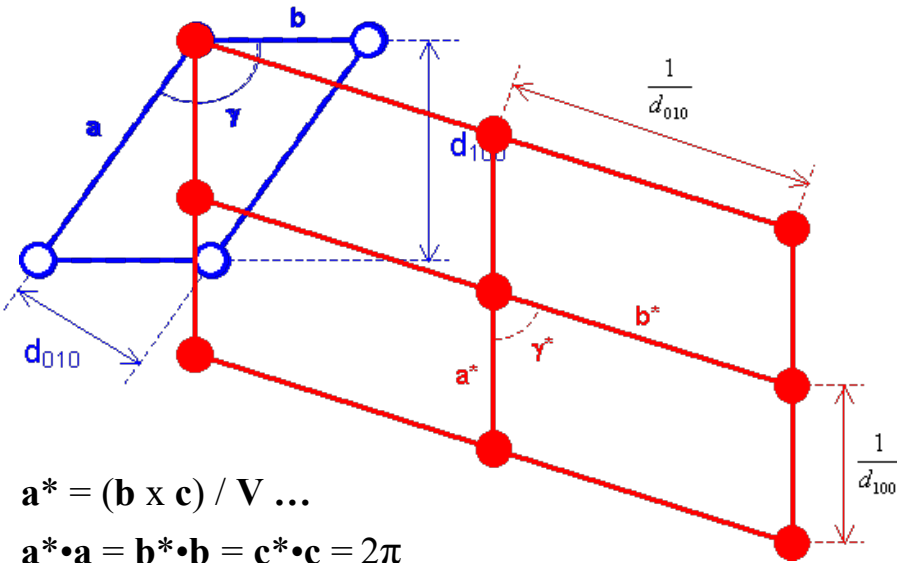
$$\mathbf{a} \cdot (\mathbf{s} - \mathbf{s}_0) = h\lambda,$$

$$\mathbf{b} \cdot (\mathbf{s} - \mathbf{s}_0) = k\lambda,$$

$$\mathbf{c} \cdot (\mathbf{s} - \mathbf{s}_0) = l\lambda.$$

Laue Equation in tradition form

Real and Reciprocal Space



$$\mathbf{a}^* = (\mathbf{b} \times \mathbf{c}) / V \dots$$

$$\mathbf{a}^* \cdot \mathbf{a} = \mathbf{b}^* \cdot \mathbf{b} = \mathbf{c}^* \cdot \mathbf{c} = 2\pi$$

$$\mathbf{a}^* \cdot \mathbf{b} = \dots = 0$$

$$\mathbf{G}_{hkl} = h \mathbf{a}^* + k \mathbf{b}^* + l \mathbf{c}^*,$$

$$\mathbf{G}_{hkl} \cdot \mathbf{a} = 2\pi h,$$

$$\mathbf{G}_{hkl} \cdot \mathbf{b} = 2\pi k,$$

$$\mathbf{G}_{hkl} \cdot \mathbf{c} = 2\pi l,$$

Laue equations:

$$\mathbf{Q} \cdot \mathbf{a} = 2\pi h,$$

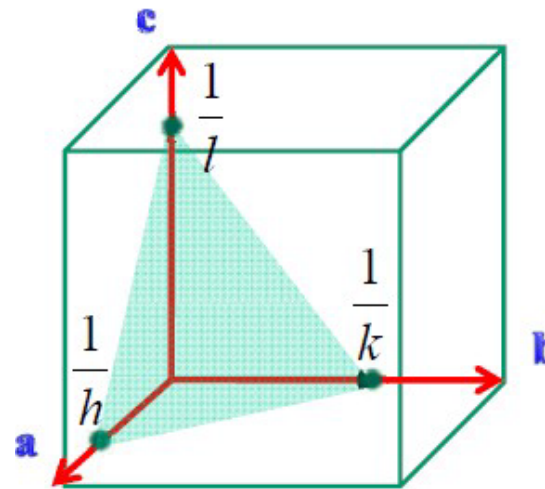
$$\mathbf{Q} \cdot \mathbf{b} = 2\pi k,$$

$$\mathbf{Q} \cdot \mathbf{c} = 2\pi l,$$

$$\mathbf{k}_f - \mathbf{k}_i = \mathbf{Q} = \mathbf{G}_{hkl}$$

$\mathbf{Q}$ is a reciprocal-lattice vector

The (hkl) plane intercepts a/h , b/k , c/l on crystallographic axes X , Y , Z , where h , k , l are relatively prime integers.

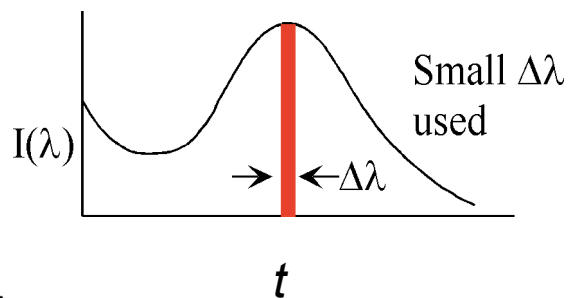
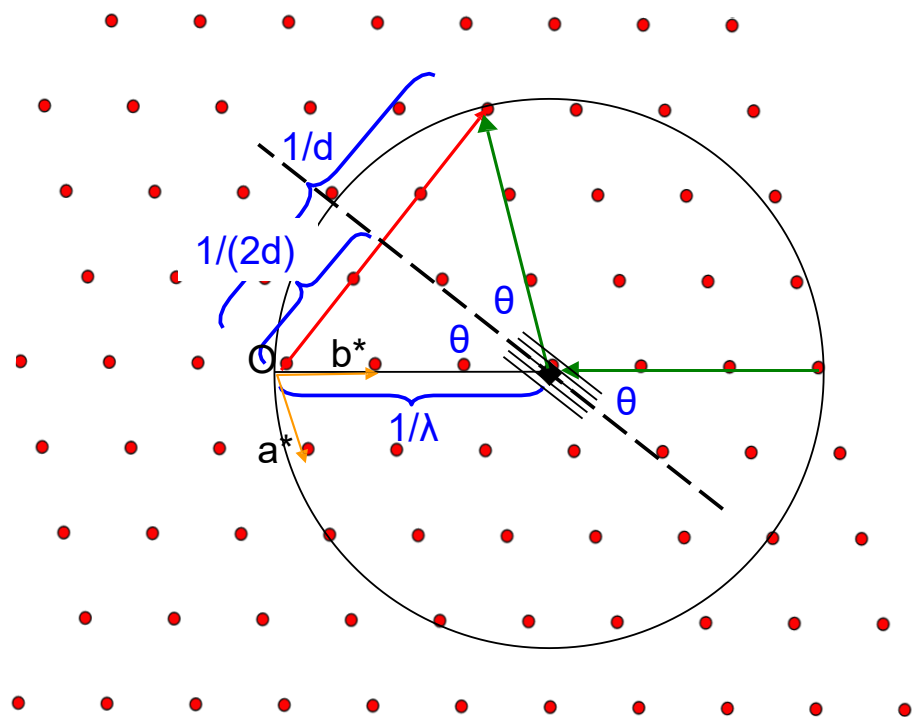


Intercepts	$\frac{a}{h}, \frac{b}{k}, \frac{c}{l}$
Fractional intercepts	$\frac{1}{h}, \frac{1}{k}, \frac{1}{l}$
Reciprocals of the fractional intercepts	h, k, l
Miller Indices (prime integers)	h, k, l

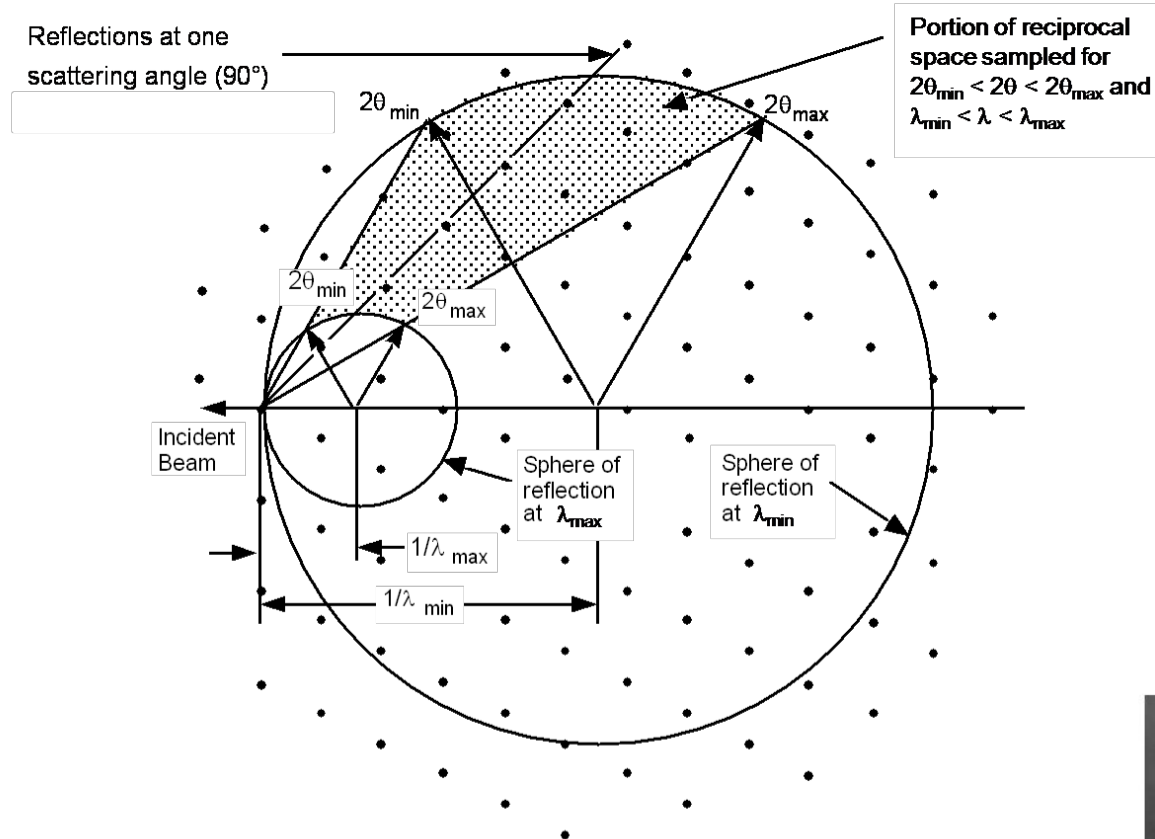
d -spacing = spacing between origin and first plane or between neighboring planes in the family of planes.

The Ewald Sphere

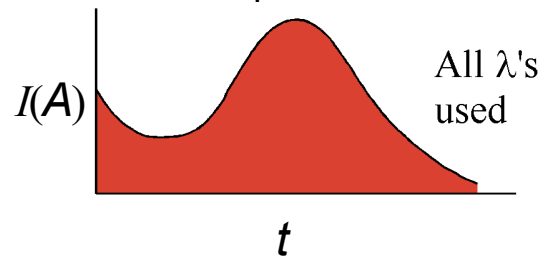
Constant wavelength = monochromatic



Wavelength range = polychromatic



Neutron spectrum:



Polychromatic "white" spectrum

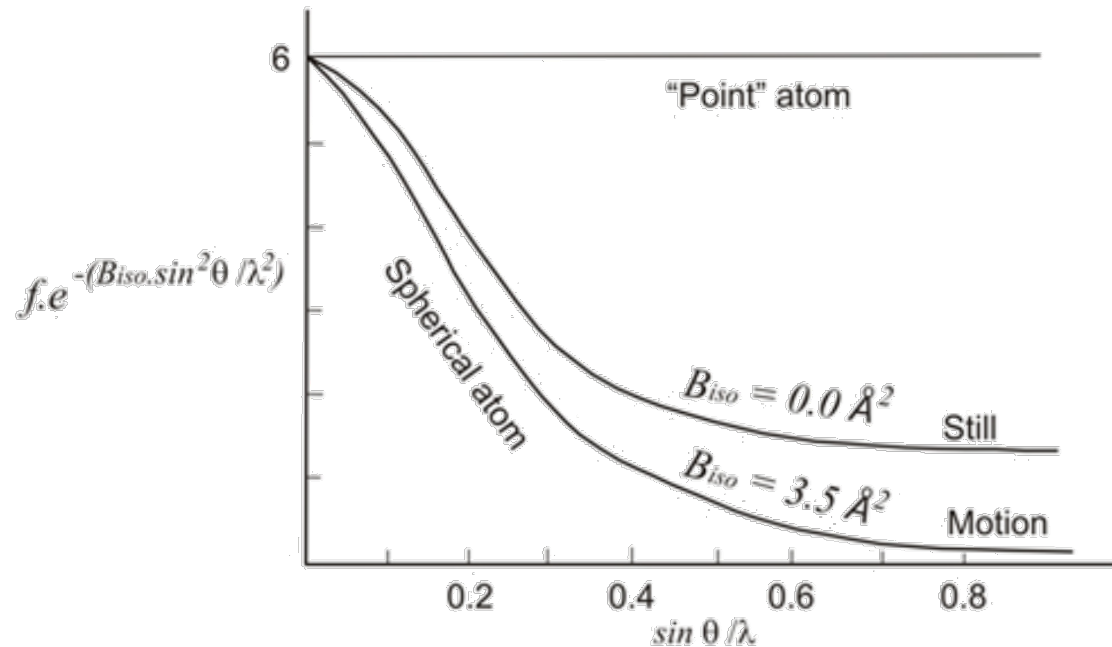
From A.J. Schultz



Paul Peter Ewald

Atomic form-factor

X-ray
magnetic



Scattering angle dependence and thermal motion

$$s = \frac{\sin \theta}{\lambda}$$

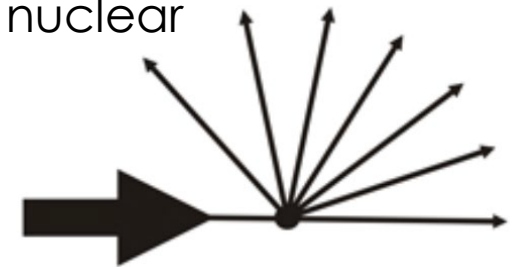
$$Q = \frac{4\pi \sin \theta}{\lambda} = 4\pi s.$$

$$f_j(Q) = \int \rho_j(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d\mathbf{r}.$$

$$f_j(0) = Z_j,$$

$$f_j(Q) < Z_j$$

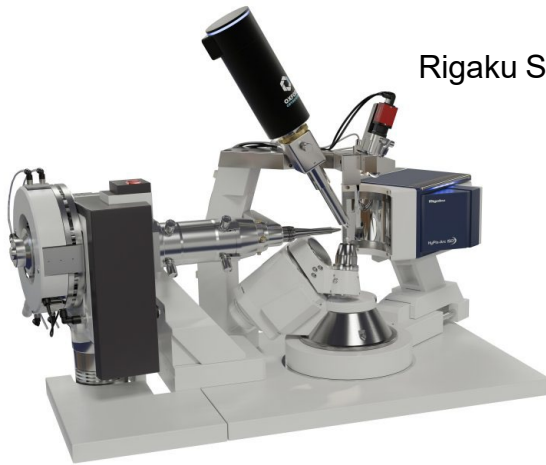
nuclear



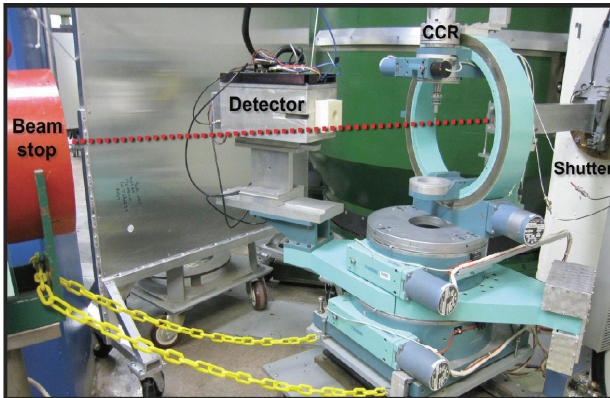
Single Crystal Diffraction

Single crystal structure analysis and investigation

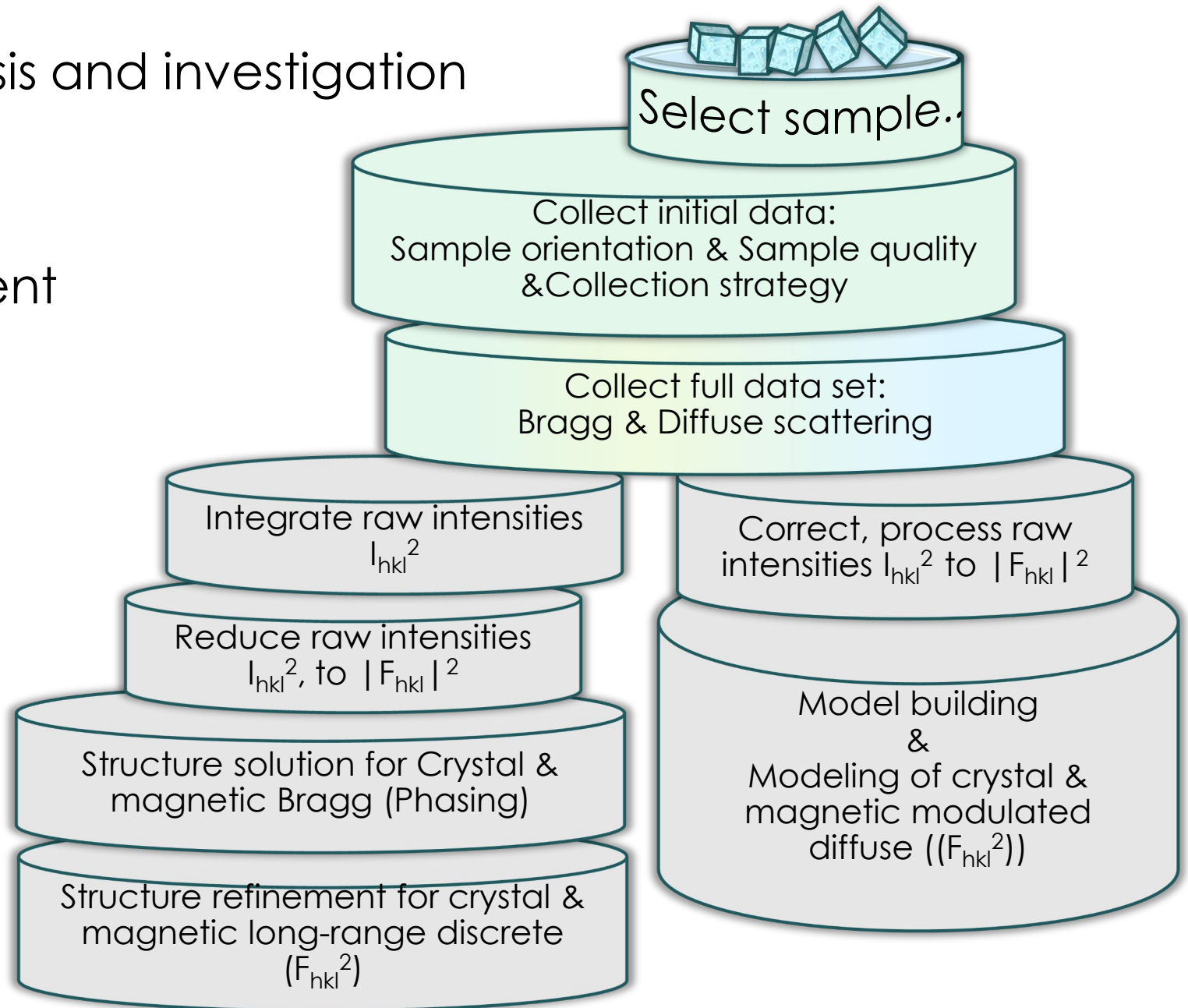
- A single crystal
- Diffraction experiment
- Data collection at instrument



Rigaku Synergy DW

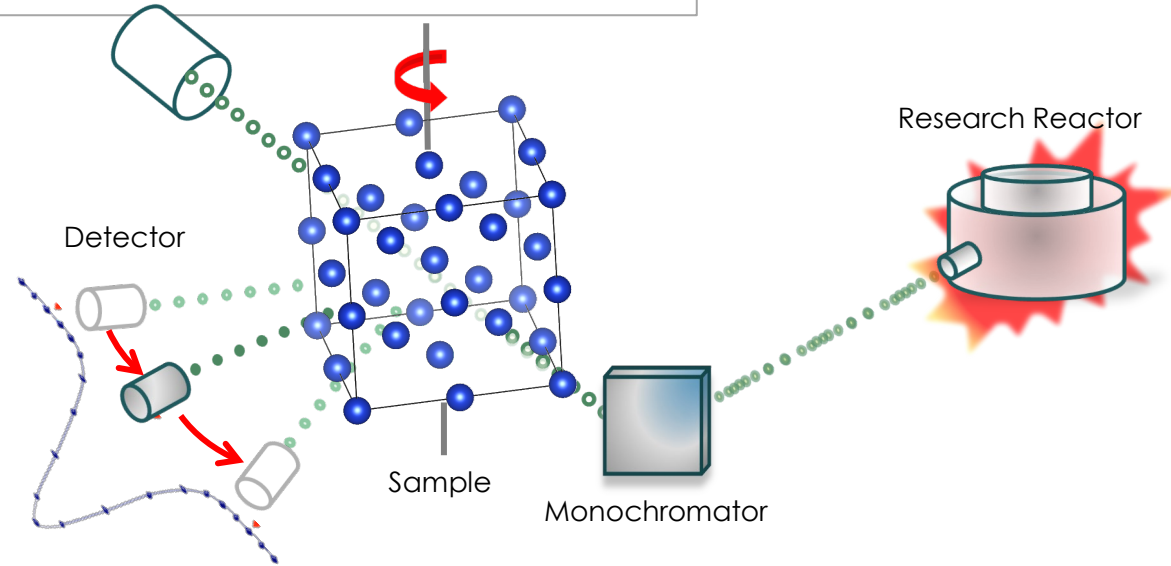


HFIR Demand



Single Crystal Diffraction

Constant Wavelength = Monochromatic
from a continuous neutron source



B. Wollan & C. Shull

The Nobel Prize in Physics 1994. NobelPrize.org.

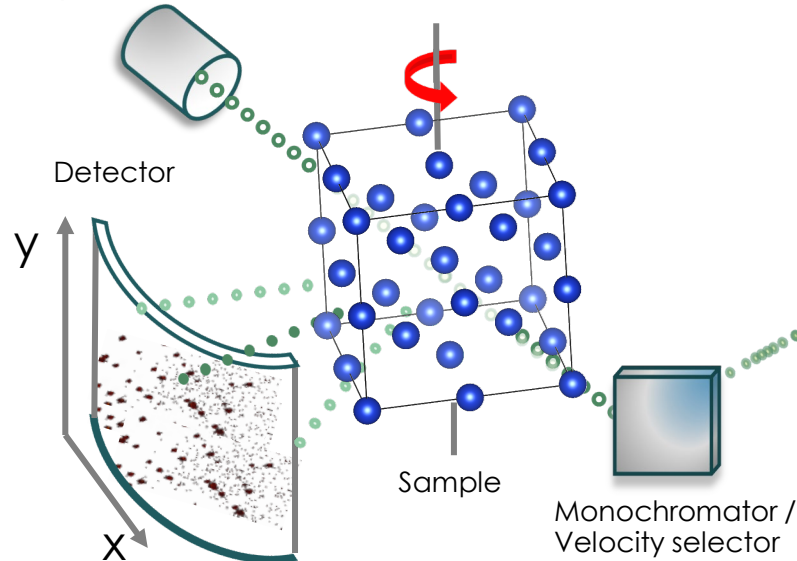
<https://www.nobelprize.org/prizes/physics/1994/summary/>

Single Crystal Diffraction

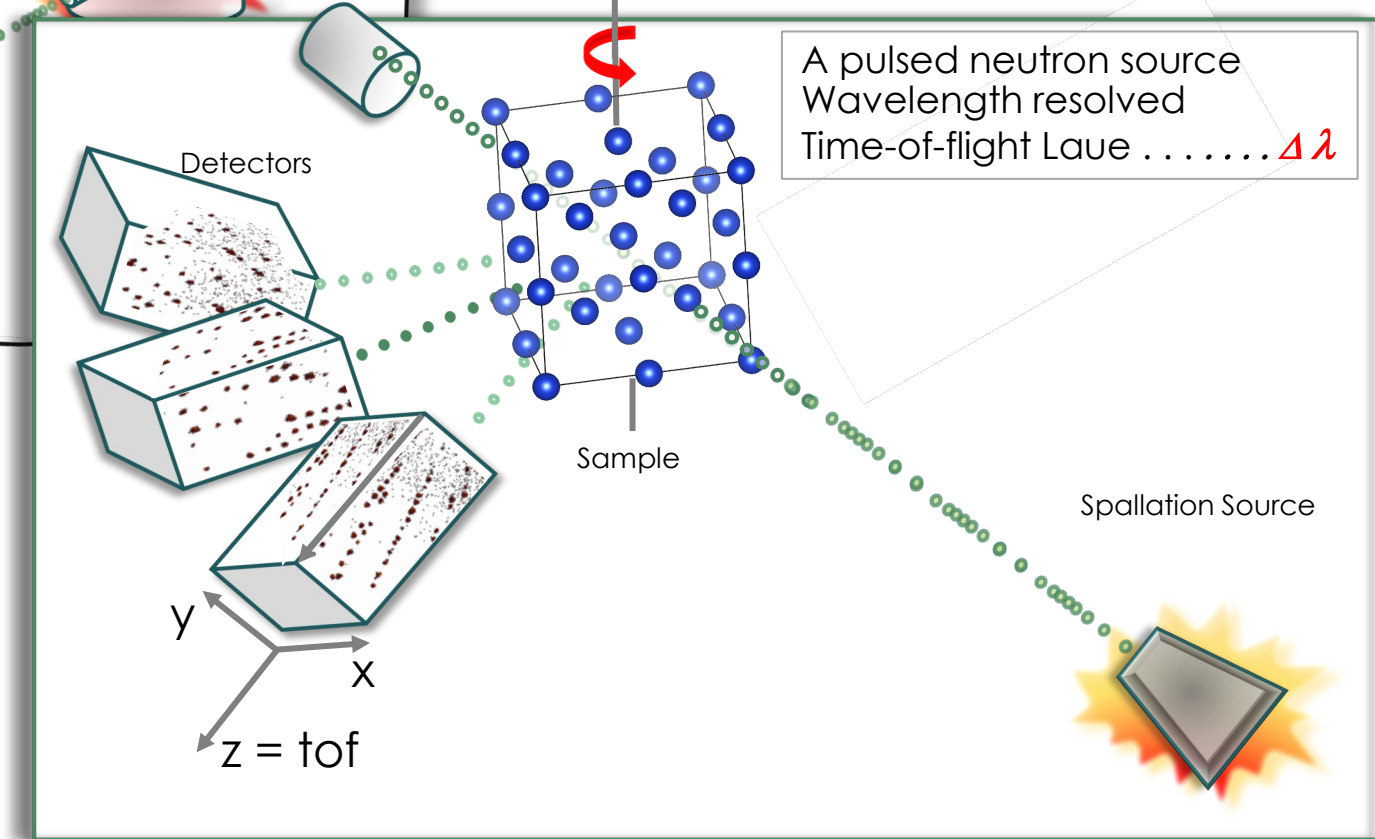
A continuous neutron source

Constant Wavelength = Monochromatic $\Delta \sin \theta$

Laue = Polychromatic $\text{sum}(\Delta \lambda)$



Research Reactor



Braggs law / momentum transfer

$$2d \sin \theta = \lambda = (4\pi/|\vec{Q}|) \sin \theta$$

$$\lambda = \frac{h}{mv} = \frac{ht}{m(L_1 + l_2)} = 2d \sin \theta$$

$$t = \frac{m}{h}(L_1 + l_2) \times 2d \sin \theta$$

Measure intensities:

$$I_{hkl} = I_{coh} + I_{bkg} + I_{inc}$$

The Nobel Prize in Physics 1994. NobelPrize.org.

<https://www.nobelprize.org/prizes/physics/1994/summary/>

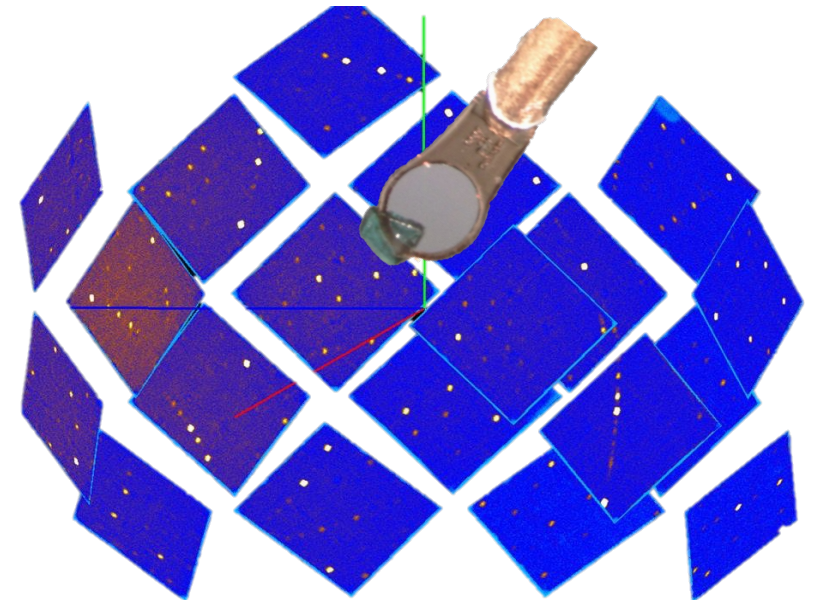
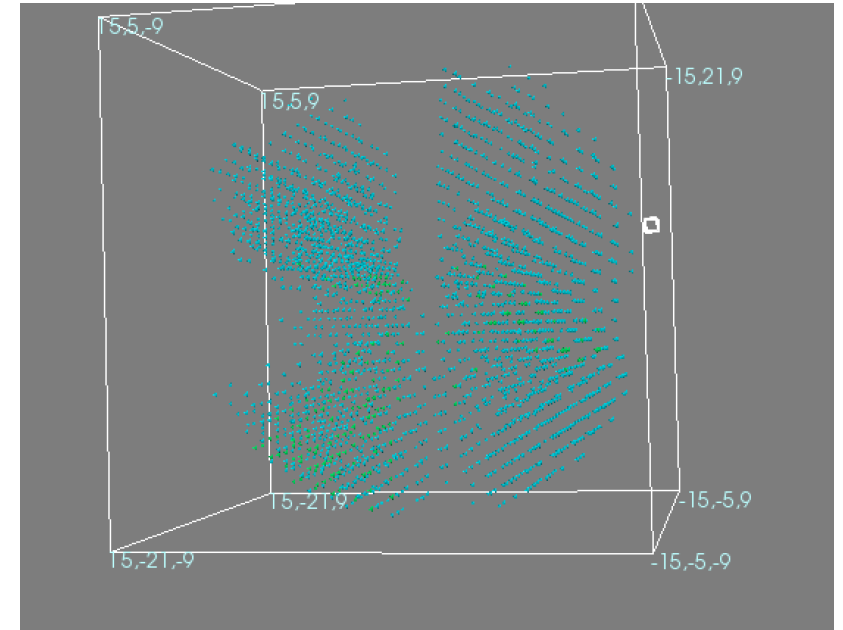
↗ National Laboratory

Collect a Representative Set of Data

Employ data collection strategy to cover required **volume of reciprocal space**

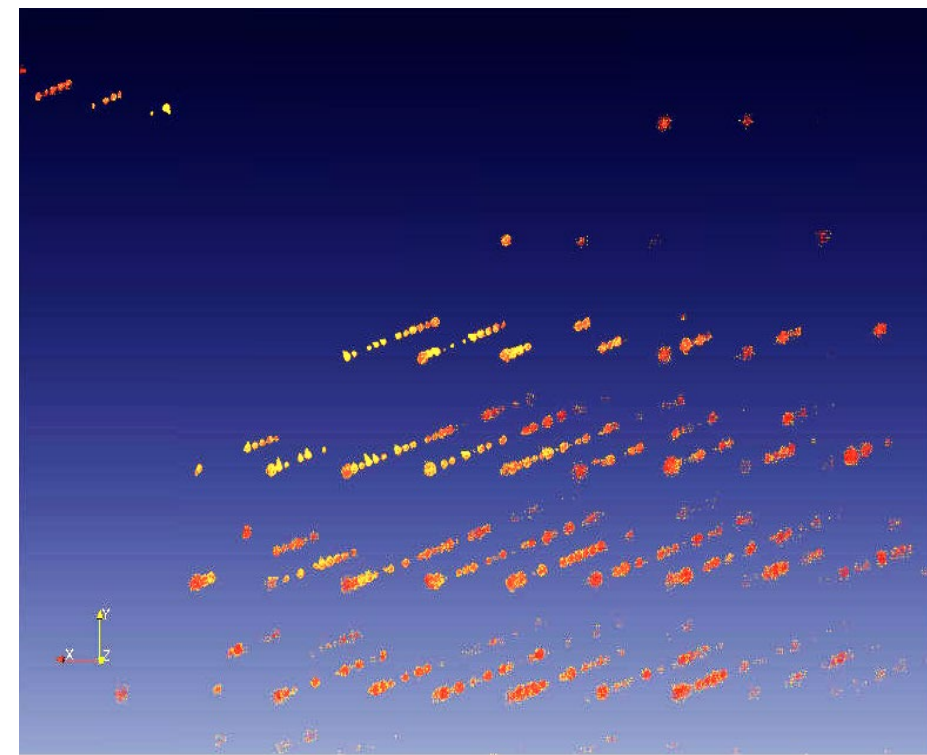
Resolution considerations due to

- crystal quality
- Sample stability
- Aim of study
 - Full structure analysis
 - Partial analysis to find hydrogen
 - Magnetic structure
 - Order parameter with ΔT , ΔE , ΔH
 - Phase transition
 - Stroboscopic measurement



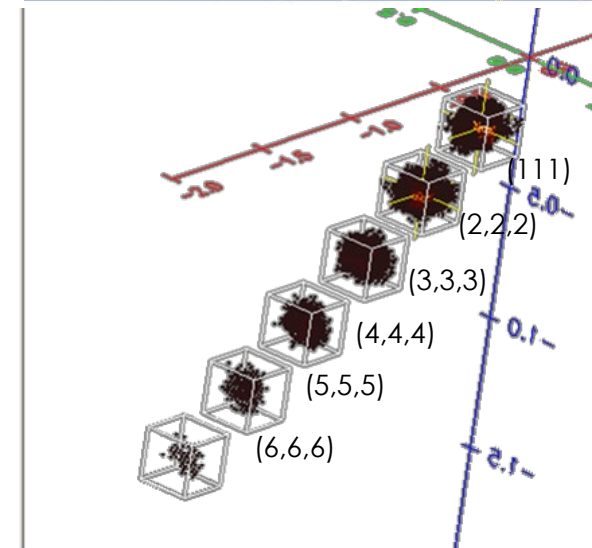
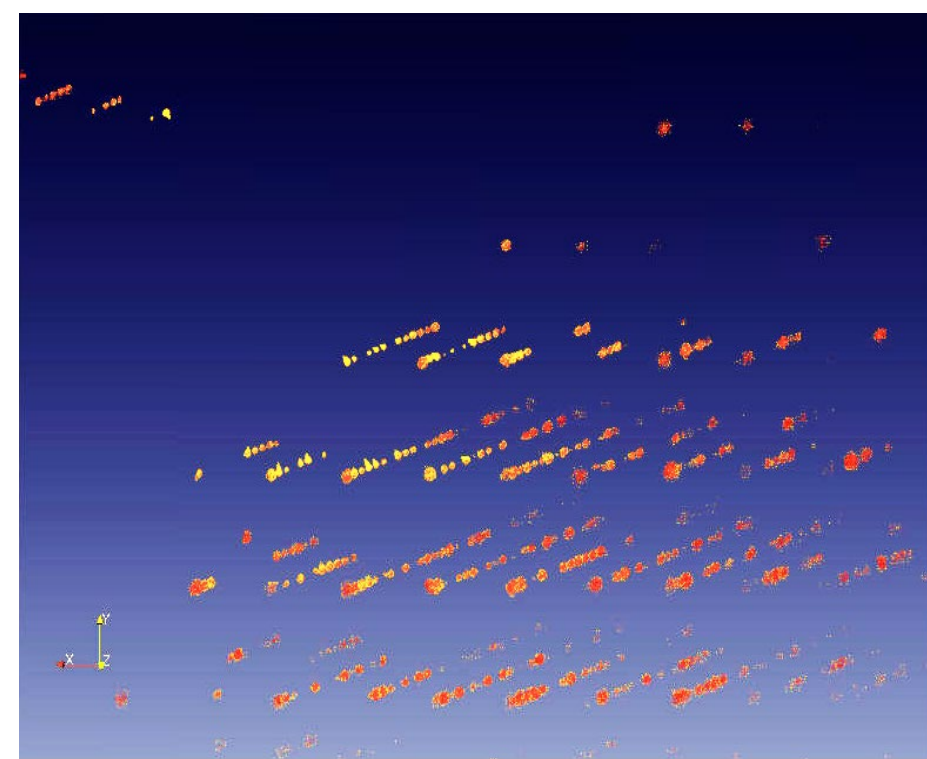
Integration and Corrections

- Integration of raw/measured integrated intensities – background
 - **Load raw/measured intensity**
 - Find peaks → locate peak centers of strong peaks
 - Find UB = unit cell and its orientation with respect to the incident neutron beam
 - Using FFT
 - Index peaks
 - Choose Cell = determine system symmetry
 - Predict all possible peak positions
 - 2-D or 3-D peak fitting – background at peak position



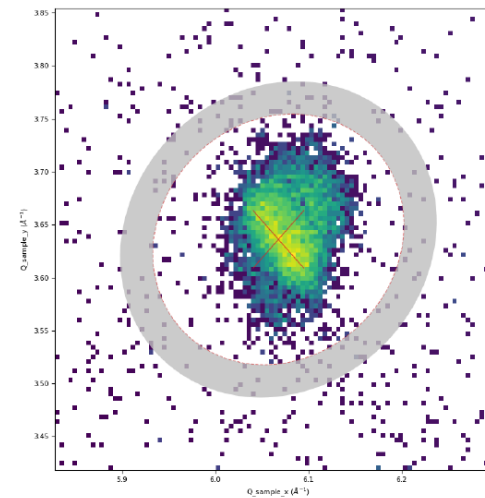
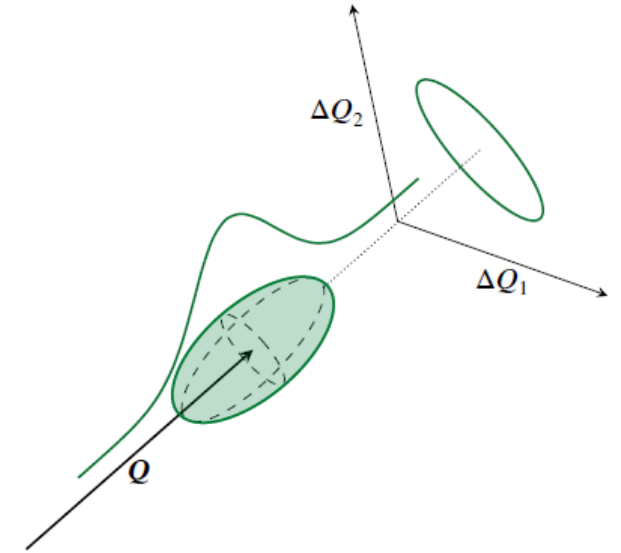
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 - **Choose Cell = determine system symmetry**
 - **Predict all possible peak positions**
 - 3-D profile peak fitting – background at peak position

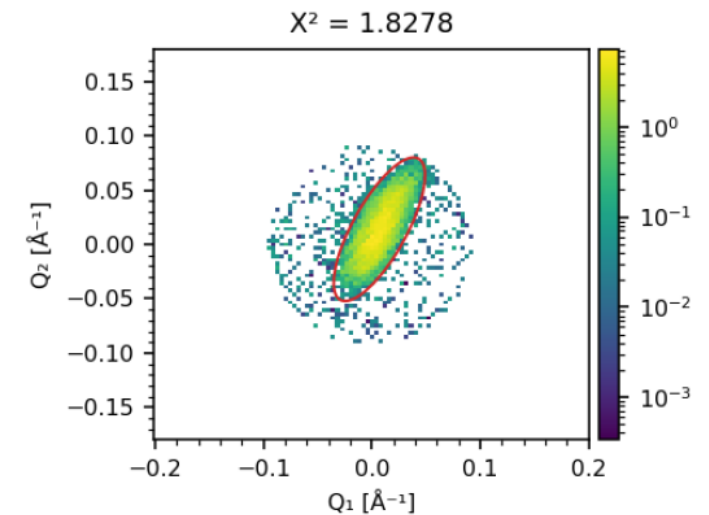


Integration and Corrections

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 - **3-D profile peak fitting – background at peak position**



A. J. Schultz *et al.*, J Appl Crystallogr **47**, 915 (2014).



Z. Morgan *et al.*, (2026).

Integration and Corrections

- Integration of raw/measured integrated intensities – background

- Load raw/measured intensity
- Find peaks → locate peak centers of strong
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 - Using FFT
- Index peaks
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- Predict all possible peak positions
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➔ Integrated raw intensities I_{hkl}

File		Edit																	
Version: 2.0 Facility: SNS Instrument: SNAP																			
6	L1	TO_SHIFT																	
7	1505.5382	4.168																	
4	DETNUM	NROWS	NCOLS	WIDTH	HEIGHT	DEPTH	DETD	CenterX	CenterY	CenterZ	BaseX	BaseY	BaseZ	UpX	UpY	UpZ			
5	10	256	256	16.1725	16.2027	0.2000	55.26	-50.0977	16.6157	-16.3538	-0.00594	-0.00142	-0.99998	-0.00179	1.00000	-0.00137			
5	11	256	256	16.1142	16.0675	0.2000	52.69	-49.9941	16.6391	0.4007	-0.00623	-0.00138	-0.99998	-0.00194	1.00000	-0.00137			
5	12	256	256	16.0775	16.1339	0.2000	55.33	-49.8906	16.6626	17.1552	-0.00637	-0.00140	-0.99998	-0.00189	1.00000	-0.00139			
5	13	256	256	16.1362	16.1297	0.2000	52.66	-50.0661	-0.1391	-16.3305	-0.00604	-0.00142	-0.99998	-0.00194	1.00000	-0.00141			
5	14	256	256	16.0790	16.1810	0.2000	49.96	-49.9625	-0.1156	0.4239	-0.00623	-0.00140	-0.99998	-0.00189	1.00000	-0.00139			
5	15	256	256	16.1808	16.0856	0.2000	52.74	-49.8589	-0.0922	17.1784	-0.00613	-0.00138	-0.99998	-0.00203	1.00000	-0.00137			
5	16	256	256	16.1341	16.2021	0.2000	55.27	-50.0344	-16.8938	-16.3073	-0.00618	-0.00133	-0.99998	-0.00199	1.00000	-0.00132			
5	17	256	256	16.1124	16.1506	0.2000	52.71	-49.9308	-16.8704	0.4472	-0.00618	-0.00142	-0.99998	-0.00194	1.00000	-0.00141			
5	18	256	256	16.0624	16.1940	0.2000	55.34	-49.8272	-16.8469	17.2016	-0.00604	-0.00142	-0.99998	-0.00184	1.00000	-0.00141			
0	NRUN	DETNUM	CHI	PHI	OMEGA	MONCNT													
1	235	10	0.00	0.00	0.00	10000													
2	SEQN	H	K	L	COL	ROW	CHAN	L2	2_THETA	AZ	WL	D	IPK	INTI	SIGI	RFLG			
3	1	-1	2	-3	17.47	18.13	724.64	51.811	1.75187	2.95129	1.839285	1.1972	63	0.00	0.00	1			
3	2	-1	5	-8	241.83	202.56	335.71	59.342	1.97832	2.74006	0.847206	0.5070	30	0.00	0.00	1			
3	3	-2	5	-7	11.33	64.30	307.81	52.369	1.74247	2.89565	0.780158	0.5098	28	0.00	0.00	1			
3	4	-2	4	-6	17.01	18.32	362.73	51.807	1.75131	2.95106	0.919942	0.5989	18	0.00	0.00	1			
3	5	-1	3	-5	203.01	102.98	521.14	56.397	1.95347	2.85092	1.318462	0.7955	15	0.00	0.00	1			
3	6	-1	4	-6	154.85	162.51	414.28	56.463	1.89565	2.78328	1.047764	0.6451	12	0.00	0.00	1			
3	7	-1	6	-9	204.84	227.24	288.00	59.035	1.93784	2.71383	0.726736	0.4408	10	0.00	0.00	1			
0	NRUN	DETNUM	CHI	PHI	OMEGA	MONCNT													
1	235	11	0.00	0.00	0.00	10000													
2	SEQN	H	K	L	COL	ROW	CHAN	L2	2_THETA	AZ	WL	D	IPK	INTI	SIGI	RFLG			
3	8	-1	5	-6	240.19	193.41	345.21	54.564	1.69270	2.74934	0.873882	0.5835	16	0.00	0.00	1			
0	NRUN	DETNUM	CHI	PHI	OMEGA	MONCNT													
1	235	12	0.00	0.00	0.00	10000													
2	SEQN	H	K	L	COL	ROW	CHAN	L2	2_THETA	AZ	WL	D	IPK	INTI	SIGI	RFLG			
3	9	-1	2	-2	232.69	19.17	686.49	51.962	1.36494	2.94845	1.742187	1.3811	67	0.00	0.00	1			
3	10	-1	4	-3	110.80	151.79	379.47	56.134	1.23938	2.79297	0.959806	0.8263	62	0.00	0.00	1			
3	11	-1	5	-4	180.80	189.91	322.00	55.727	1.31935	2.75144	0.814426	0.6644	17	0.00	0.00	1			
3	12	-2	4	-3	23.96	18.81	311.47	56.053	1.13366	2.94822	0.787569	0.7334	17	0.00	0.00	1			
3	13	-2	6	-5	164.37	96.93	246.58	54.106	1.29171	2.85567	0.623979	0.5184	13	0.00	0.00	1			
3	14	-1	7	-5	108.22	224.90	231.54	57.843	1.24670	2.71396	0.584425	0.5006	11	0.00	0.00	1			
3	15	-2	4	-4	232.83	19.09	344.00	51.959	1.36510	2.94855	0.872276	0.6914	10	0.00	0.00	1			
0	NRUN	DETNUM	CHI	PHI	OMEGA	MONCNT													
1	235	13	0.00	0.00	0.00	10000													
2	SEQN	H	K	L	COL	ROW	CHAN	L2	2_THETA	AZ	WL	D	IPK	INTI	SIGI	RFLG			
3	16	-1	1	-2	23.73	98.37	1101.55	50.999	1.76264	-3.10107	2.798183	1.8133	132	0.00	0.00	1			
3	17	-2	2	-5	215.00	92.70	535.53	54.677	1.98049	-3.09367	1.356384	0.8111	49	0.00	0.00	1			
3	18	-2	2	-4	24.05	98.19	551.23	51.004	1.76303	-3.10084	1.399508	0.9068	48	0.00	0.00	1			
3	19	-2	3	-5	22.98	211.03	439.47	51.217	1.76108	3.04061	1.115306	0.7232	31	0.00	0.00	1			
3	20	-4	3	-8	126.63	23.61	309.90	53.041	1.88125	-3.00759	0.785118	0.4859	13	0.00	0.00	1			
0	NRUN	DETNUM	CHI	PHI	OMEGA	MONCNT													
1	235	14	0.00	0.00	0.00	10000													
2	SEQN	H	K	L	COL	ROW	CHAN	L2	2_THETA	AZ	WL	D	IPK	INTI	SIGI	RFLG			
3	21	-2	2	-4	107.71	212.60	422.72	50.264	1.52652	2.02785	1.101258	0.7025	46	0.00	0.00	1			

Integration and Corrections

- **Convert to structure factor amplitudes from intensities:**

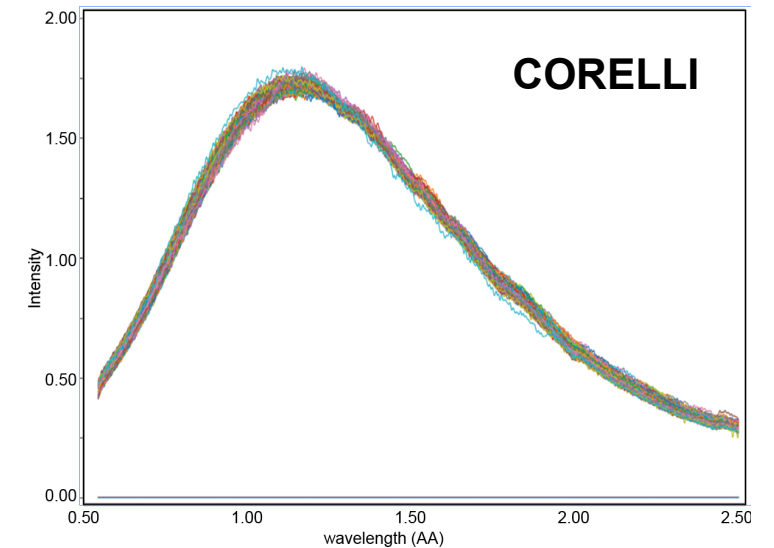
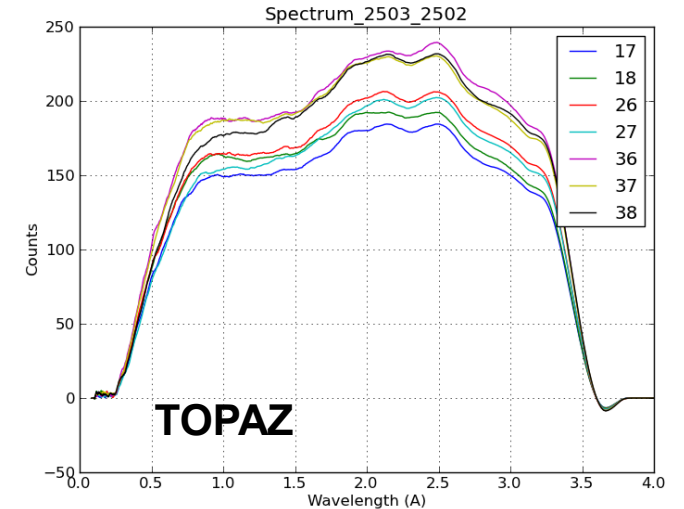
- Instrument specific corrections:

- Incident spectrum correction
- Detector efficiency correction
- Normalization (vanadium)
- Scaling

- Sample dependent corrections:

- Absorption correction
 - Density, chemical composition, volume
 - Linear attenuation coefficient
- Pathlength correction
 - Sample size, shape
- Lorentz correction
 - Geometric or Lambda contribution

$$I(t) = I_0 e^{-\mu t}, \quad \mu = \left[\mu_s + \frac{\mu_a}{1.798} \times \lambda \right] \text{ cm}^{-1}$$



Single crystal data **reduction**

Convert raw integrated intensities, I_{hkl} , into relative structure factor amplitudes, $|F_{hkl}|^2$.

TOF Laue:

$$I_{hkl} = k \phi(\lambda) \varepsilon(\lambda) A(\lambda) y(\lambda) (V_s/V_c^2) |F_{hkl}|^2 \lambda^4 / \sin^2 \theta$$

Lorentz factor

Constant Wavelength:

$$I_{hkl} = k \phi(\lambda) \varepsilon(\lambda) A(\lambda) y(\lambda) (V_s/V_c^2) |F_{hkl}|^2 \lambda^3 / \sin 2\theta$$

k = scale factor

$\phi(\lambda)$ = incident flux spectrum

$\varepsilon(\lambda)$ = detector efficiency as a function of wavelength λ

$A(\lambda)$ = sample absorption

$y(\lambda)$ = secondary extinction correction

V_s = sample volume

V_c = unit cell volume

F_{hkl} = structure factor

λ = wavelength

h, k, l, $ F_{hkl} ^2$, $\sigma_{(F_{hkl} ^2)}$, batch, λ , ...											
-2	0	-4	4298.42	193.58	1	2.50807	0.09279	-0.73894	-0.42849	0.58255	-0
-3	1	-5	589.48	60.36	1	1.96898	0.09435	-0.73894	-0.56656	0.58255	-0
-3	-1	-5	606.79	61.36	1	1.79364	0.09198	-0.73894	-0.45063	0.58255	-0
-4	0	-8	788.90	70.91	1	1.25404	0.09281	-0.73894	-0.42849	0.58255	-0
-4	0	-6	73.17	21.31	1	1.50857	0.09348	-0.73894	-0.55873	0.58255	-0
-4	0	-5	35.24	16.30	1	1.65971	0.09375	-0.73894	-0.63059	0.58255	-0
-5	1	-11	2530.43	144.21	1	0.95726	0.09317	-0.73894	-0.40875	0.58255	-0
-5	1	-10	522.83	63.81	1	1.02775	0.09350	-0.73894	-0.45720	0.58255	-0
-5	1	-9	2122.75	125.25	1	1.10622	0.09384	-0.73894	-0.50912	0.58255	-0
-5	-1	-9	2180.89	127.34	1	1.04810	0.09232	-0.73894	-0.44370	0.58255	-0
-5	1	-8	679.26	65.36	1	1.19332	0.09418	-0.73894	-0.56573	0.58255	-0
-5	-1	-8	555.22	58.64	1	1.12724	0.09256	-0.73894	-0.49355	0.58255	-0
-5	1	-7	2152.15	126.31	1	1.28935	0.09446	-0.73894	-0.62574	0.58255	-0
-5	-1	-7	2153.33	126.42	1	1.21387	0.09276	-0.73894	-0.54506	0.58255	-0
-6	0	-12	245.58	68.94	1	0.83602	0.09280	-0.73894	-0.42849	0.58255	-0
-6	2	-11	3080.88	173.37	1	0.92416	0.09430	-0.73894	-0.51903	0.58255	-0
-6	-2	-11	3360.52	193.75	1	0.84529	0.09168	-0.73894	-0.41194	0.58255	-0
-6	2	-10	2341.73	138.04	1	0.98449	0.09458	-0.73894	-0.56656	0.58255	-0
-6	0	-10	3770.93	187.90	1	0.94440	0.09329	-0.73894	-0.51311	0.58255	-0
-6	-2	-10	2515.08	152.95	1	0.89682	0.09186	-0.73894	-0.45063	0.58255	-0
-6	2	-9	283.57	52.43	1	1.05015	0.09486	-0.73894	-0.61690	0.58255	-0
-6	-2	-9	306.43	53.69	1	0.95238	0.09204	-0.73894	-0.49076	0.58255	-0
-6	0	-8	673.79	65.07	1	1.07177	0.09374	-0.73894	-0.60703	0.58255	-0
-7	1	-12	521.36	93.17	1	0.81034	0.09380	-0.73894	-0.52385	0.58255	-0
-7	-1	-12	352.75	85.24	1	0.77900	0.09265	-0.73894	-0.47567	0.58255	-0
-7	3	-11	531.37	85.59	1	0.88442	0.09511	-0.73894	-0.60876	0.58255	-0
-7	1	-11	715.23	99.60	1	0.85555	0.09404	-0.73894	-0.56432	0.58255	-0
-7	-1	-11	710.42	98.91	1	0.82117	0.09282	-0.73894	-0.51235	0.58255	-0
-7	-3	-11	511.19	94.04	1	0.78192	0.09148	-0.73894	-0.45254	0.58255	-0
-7	1	-10	272.83	65.57	1	0.90397	0.09427	-0.73894	-0.60596	0.58255	-0

Fourier Transform:

Real Space $\leftrightarrow$ Reciprocal Space

Structure Factor amplitudes $\rightarrow$ Density $\leftrightarrow$ Structure Factors

Relative phase shifts related to atomic/molecular structure

h, k, l, $|F_{hkl}|^2$, $\sigma_{(|F_{hkl}|^2)}$, batch, λ , ...

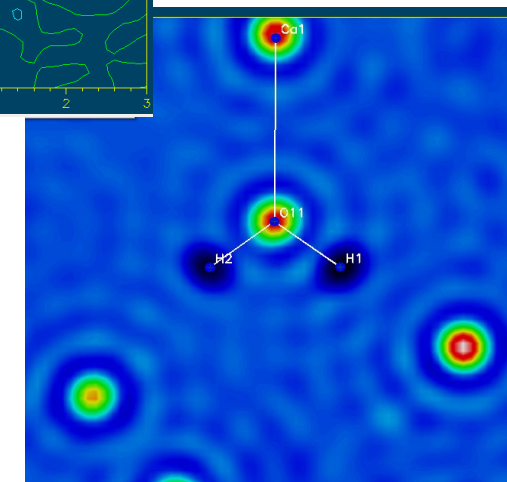
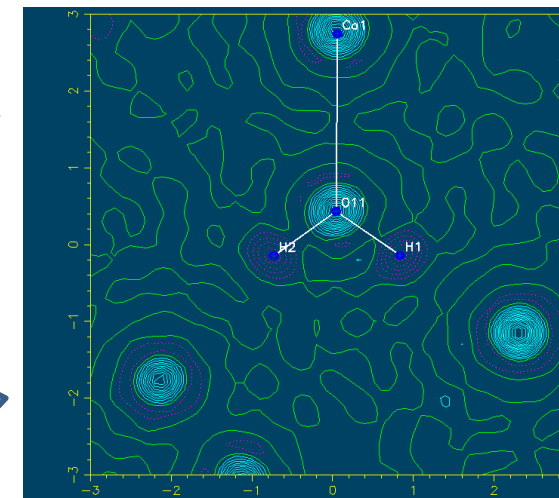
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-5	1	-11	2530.43	144.21	1	0.95726	0.09317	-0.73894	-0.40875	0.58255	-0
-5	1	-10	522.83	63.81	1	1.02775	0.09350	-0.73894	-0.45720	0.58255	-0
-5	1	-9	2122.75	125.25	1	1.10622	0.09384	-0.73894	-0.50912	0.58255	-0
-5	-1	-9	2180.89	127.34	1	1.04810	0.09232	-0.73894	-0.44370	0.58255	-0
-5	1	-8	679.26	65.36	1	1.19332	0.09418	-0.73894	-0.56573	0.58255	-0
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-6	2	-11	3080.88	173.37	1	0.92416	0.09430	-0.73894	-0.51983	0.58255	-0
-6	-2	-11	3360.52	193.75	1	0.84529	0.09168	-0.73894	-0.41194	0.58255	-0
-6	2	-10	2341.73	138.04	1	0.98449	0.09458	-0.73894	-0.56656	0.58255	-0
-6	0	-10	3770.93	187.90	1	0.94440	0.09329	-0.73894	-0.51311	0.58255	-0
-6	-2	-10	2515.08	152.95	1	0.89682	0.09186	-0.73894	-0.45863	0.58255	-0
-6	2	-9	283.57	52.43	1	1.05015	0.09486	-0.73894	-0.61698	0.58255	-0
-6	-2	-9	306.43	53.69	1	0.95238	0.09204	-0.73894	-0.49876	0.58255	-0
-6	0	-8	673.79	65.07	1	1.07177	0.09374	-0.73894	-0.60783	0.58255	-0
-7	1	-12	521.36	93.17	1	0.81034	0.09380	-0.73894	-0.52385	0.58255	-0
-7	-1	-12	352.75	85.24	1	0.77900	0.09265	-0.73894	-0.47567	0.58255	-0
-7	3	-11	531.37	85.59	1	0.88442	0.09511	-0.73894	-0.60876	0.58255	-0
-7	1	-11	715.23	99.60	1	0.85555	0.09404	-0.73894	-0.56432	0.58255	-0
-7	-1	-11	710.42	98.91	1	0.82117	0.09282	-0.73894	-0.51235	0.58255	-0
-7	-3	-11	511.19	94.04	1	0.78192	0.09148	-0.73894	-0.45254	0.58255	-0
-7	1	-10	272.83	65.57	1	0.90397	0.09427	-0.73894	-0.60506	0.58255	-0

$$\rho(xyz) = \frac{1}{V} \sum_{hkl} |F_{hkl}| e^{-2\pi i (hx+ky+lz)}$$

$$I_{hkl} \propto |F_{hkl}|^2$$

$$F_{hkl} = |F_{hkl}| e^{i\phi}$$

$$F_{hkl} = \rho_{xyz} e^{2\pi i (s \cdot r)} dv = \sum_j b_j e^{2\pi i (hx_j + ky_j + lz_j)}$$



Amplitude

Phase angle

$$F_{hkl} = |F_{hkl}| e^{i\phi} = |F_{hkl}| \cos \phi + i |F_{hkl}| \sin \phi = A + iB$$

$$\phi = \tan^{-1} \frac{B}{A}$$

Sum over j atoms in the unit cell.

Neutron scattering length of the j^{th} atom,

Structure Solution (phase problem)

- Direct methods (**SHELXT**, **SIR**, **Olex2**)
 - the structure consists of discrete atoms;
 - electron density is positive;
 - the density is concentrated near atomic positions.
 - The probability that the phase of a third peak is equal to the sum of the phases of two other related peaks.
 - J. Karle and H. Hauptman received the 1985 Nobel Prize in Chemistry
- Patterson synthesis (**WINGX**, **Olex2**, **SIR**, **JANA2020**)
 - using the $|F_{\text{obs}}|^2$ values as Fourier coefficients
 - Map **of interatomic vectors**
 - Also called the heavy atom method
- Charge flipping / Band flipping (**JANA2020/SUPERFLIP**, **SHELXT**,)
 - Start with measured $|F|$ with random phases;
 - Fourier-transform to obtain a trial density map;
 - Modify the map, flip weak density or impose positivity;
 - Transform back to reciprocal space;
 - Replace the calculated amplitudes with the measured $|F|$, while retaining the newly calculated phases;
 - Repeat until a solution is obtained.

$$\phi_{\mathbf{h}} + \phi_{\mathbf{k}} + \phi_{-\mathbf{h}-\mathbf{k}} \approx 0.$$

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{h}} |E(\mathbf{h})| e^{i\phi(\mathbf{h})} e^{-2\pi i \mathbf{h} \cdot \mathbf{r}}.$$

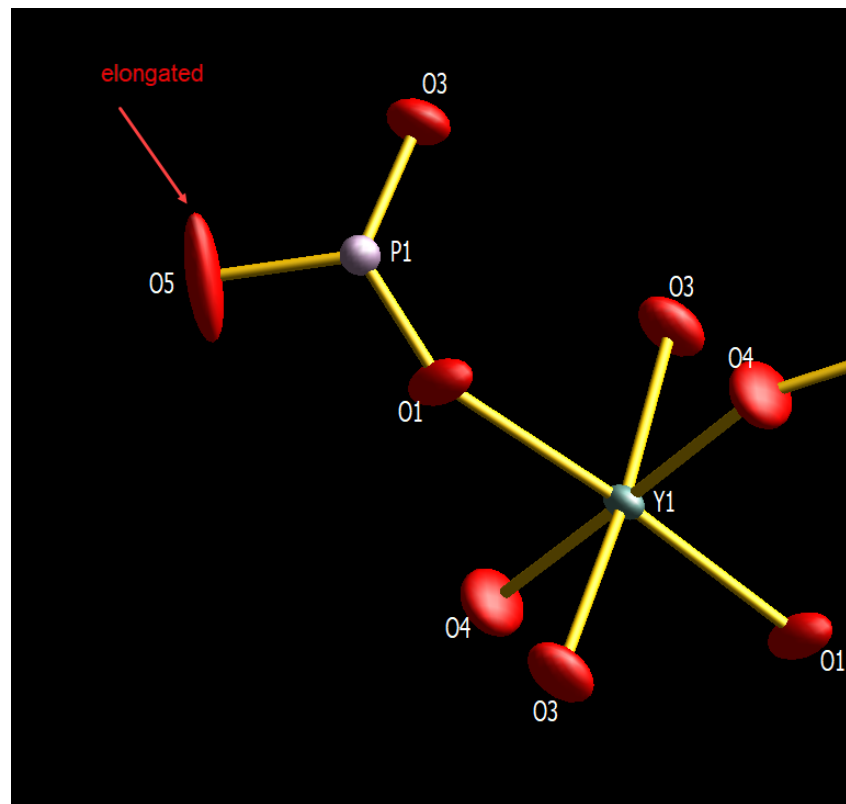
$$P(\mathbf{u}) = \frac{1}{V} \sum_{\mathbf{h}} |F(\mathbf{h})|^2 e^{-2\pi i \mathbf{h} \cdot \mathbf{u}}.$$

$$F_{hkl} = \sum_i b_i \exp(2\pi i \mathbf{s} \cdot \mathbf{r})$$

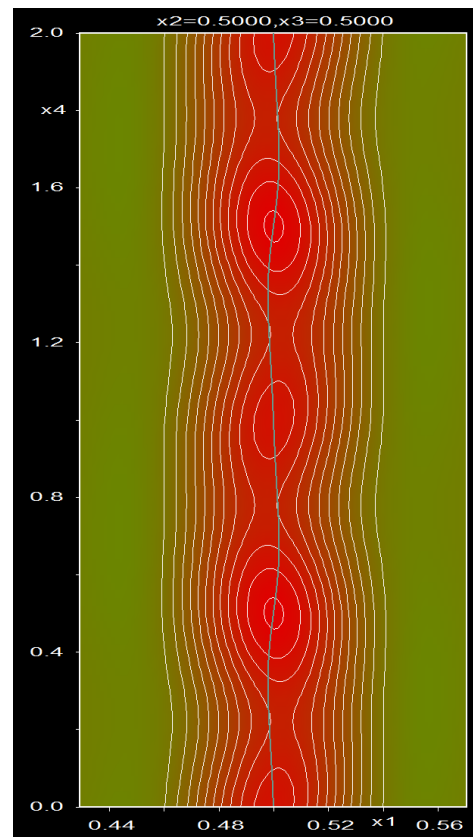
$$F_{hkl} = \sum_i b_i \exp[2\pi i (hx + ky + lz)]$$

$$F_{hkl}^2 \sim I_{hkl}$$

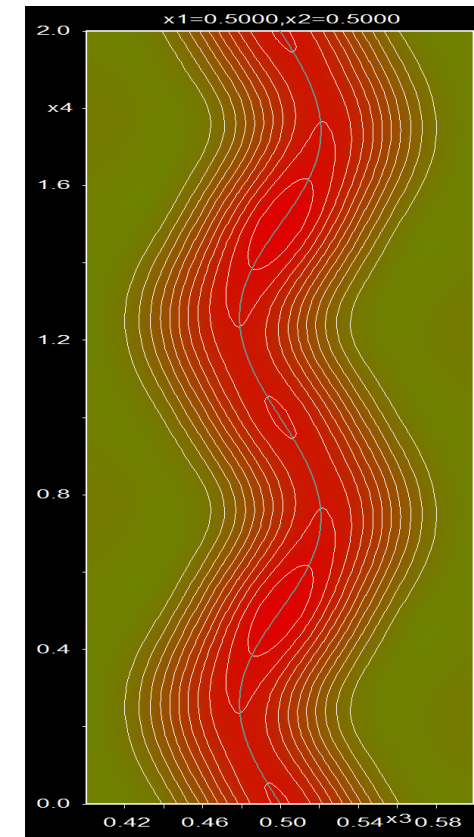
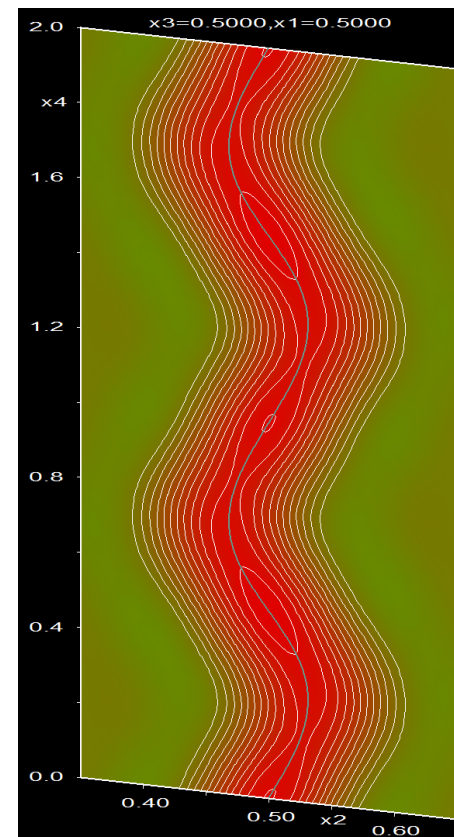
Example of structure solution (YP_3O_9) using JANA2020



Fourier map shows the location of the atoms



Detailed de Wolff sections for specific atom (Y1) shows the features of modulation



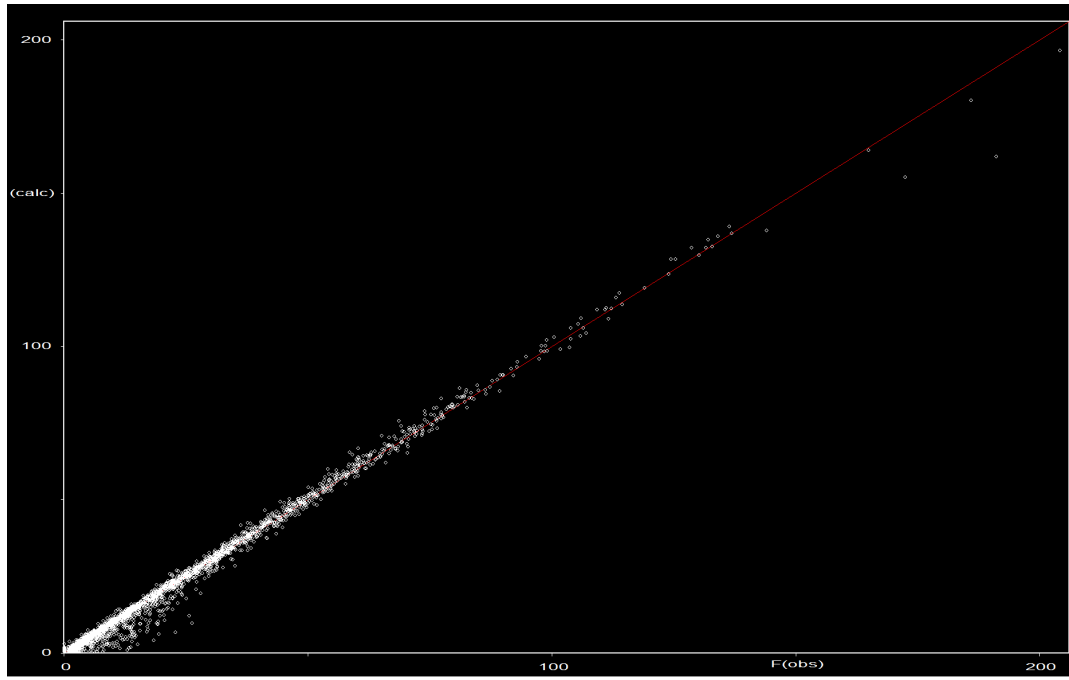
Structure refinement

- JANA2020, GSAS/GSAS-II, Fullprof, SHELX, CRYSTALS, OLEX2, Phenix...
- Nonlinear least squares refinement:
 - Adjust atomic fractional coordinates x, y, z & temperature factors U (isotropic) or u_{ij} (anisotropic)
- best fit between observed and calculated structure factors.

$$\chi^2 = \sum_{hkl} w(|F_o| - |F_c|)^2$$
$$F_{hkl} = \sum_i b_i \exp[2\pi i(hx_i + ky_i + lz_i)] \exp[-8\pi^2 U_i \sin^2 \theta / \lambda^2]$$

$$wR_2 = \sqrt{\frac{\sum_{hkl} w(F_{obs}^2 - F_{calc}^2)^2}{\sum_{hkl} w(F_{obs}^2)^2}}$$

$$R_1 = \frac{\sum_{hkl} ||F_{obs}| - |F_{calc}||}{\sum_{hkl} |F_{obs}|}$$



Refinement statistics: $R_{int}(obs)/R_{int}(all) = 6.62/6.05$, $R_{sigma}(obs)/R_{sigma}(all) = 2.18/2.02$, Redundancy = 14.153, $\langle I \rangle / \langle \sigma(I) \rangle = 19.34/19.37$, GOF = 1.506



References and Online Resources

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- J. P. Glusker and K. N. Trueblood, *Crystal Structure Analysis: A Primer*, 2nd ed., Oxford University Press, 1985.
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- Chick C. Wilson, *Single Crystal Neutron Diffraction From Molecular Crystals*, World Scientific, 2000.
- D.S. Sivia, *Elementary Scattering Theory (for X-ray and Neutron Users)*, Oxford University Press, 2011, ISBN: 9780199228683.
- G. L. Squires, *Introduction to the Theory of Thermal Neutron Scattering*, reprinted as a Dover Publication, 1978.
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- W. Massa, *Crystal Structure Determination*, ISBN-13: 978-3540206446
- Stout and Jensen, *X-ray Structure Determination*, ISBN-13: 978-0471607113
- **Bilbao Crystallography Server** <https://www.crist.ehu.es/#msgtop>
- **The Collaborative Computational Project (CCP14)** <http://www.cristal.org/DU-SDPD/nexus/ccp14/web/about.htm>
- **An Introductory Course by Rudolf Winter:** <http://users.aber.ac.uk/ruw/>
- **An Introductory Course by Bernhard Rupp:** <http://www.ruppweb.org/Xray/101index.html>
- **Spanish National Research Council (CSIC) - Crystallography** <https://www.xtal.iqfr.csic.es/Cristalografia/index-en.html>

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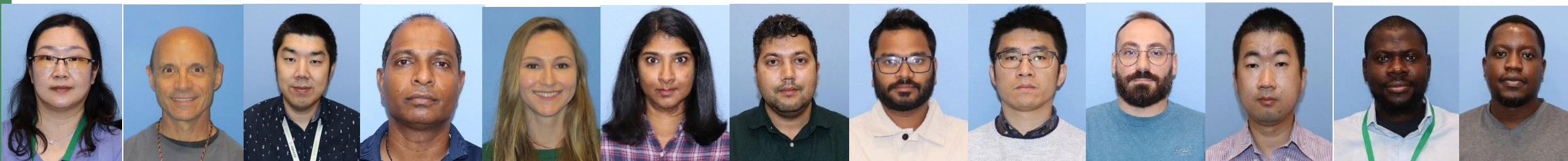
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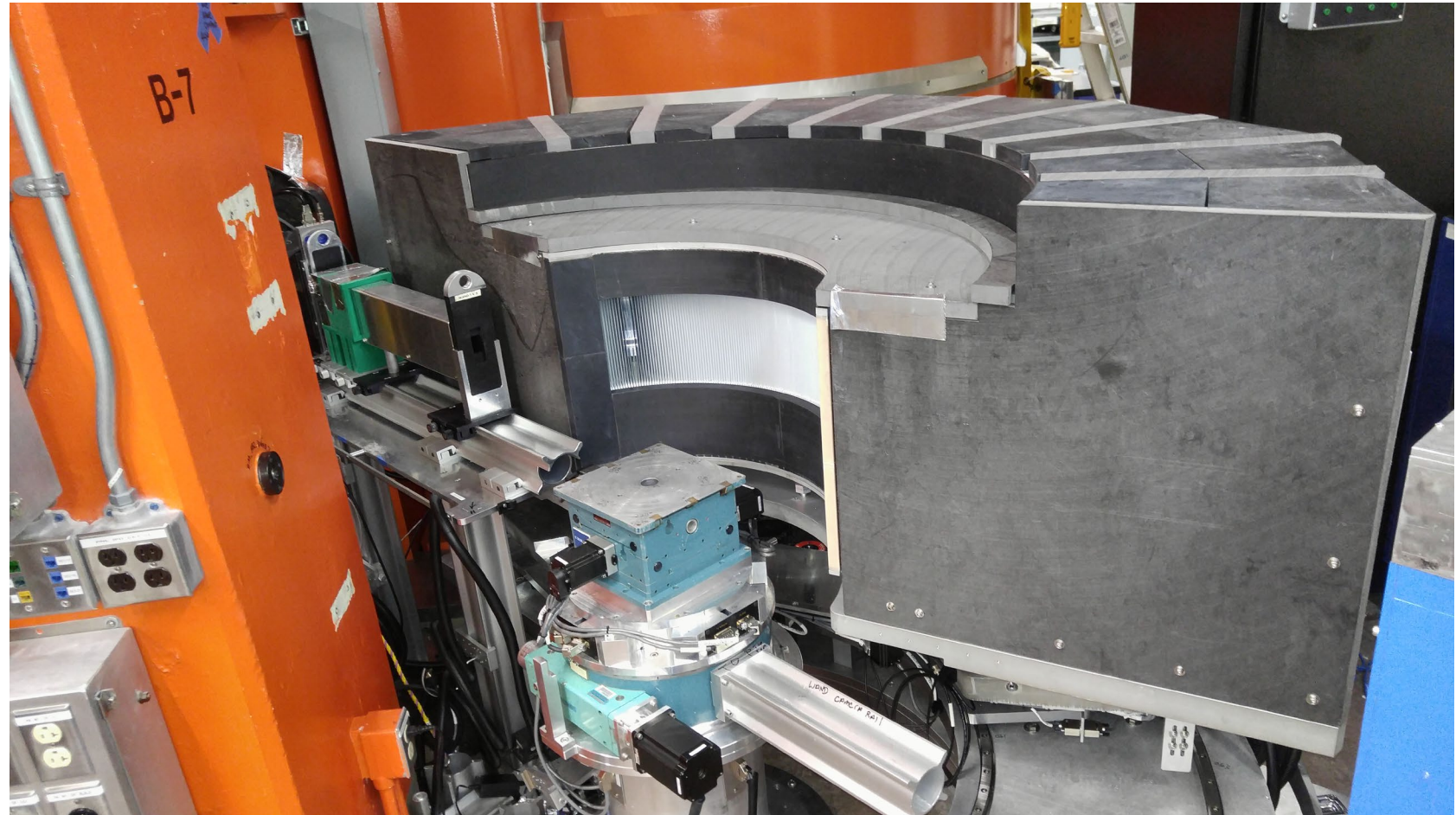
Students: Brianna Billingsley (Arizona), Aneesa Sawh (Fisk), Sam Miller (NC State), Tatenda Kanyowa (UTK)



WAND²: Fast medium resolution powder/single crystal diffractometer

Key features:

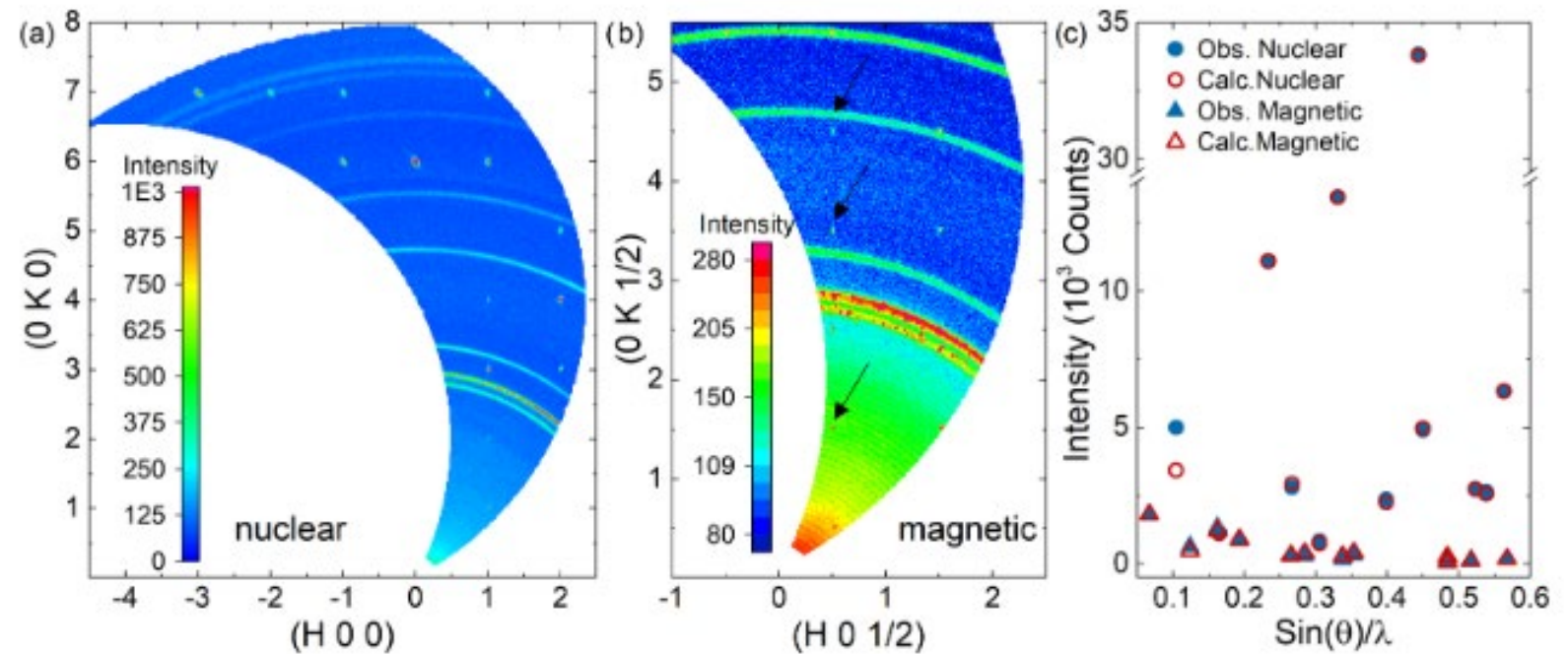
- Wide angle (120° in-plane, 15° out of plane) seamless coverage
- High-efficient ³He detector with 0.03125° sub-wire resolution
- 10⁷ n/cm² s @ 1.486Å
- Event mode data collection
- Sample Environment+



WAND²

Science - Single Crystal

- Magnetic structure determination
- Small samples (1.22mg BaNd₂PtO₅ single crystal)
- Out of plane coverage of 1st BZ

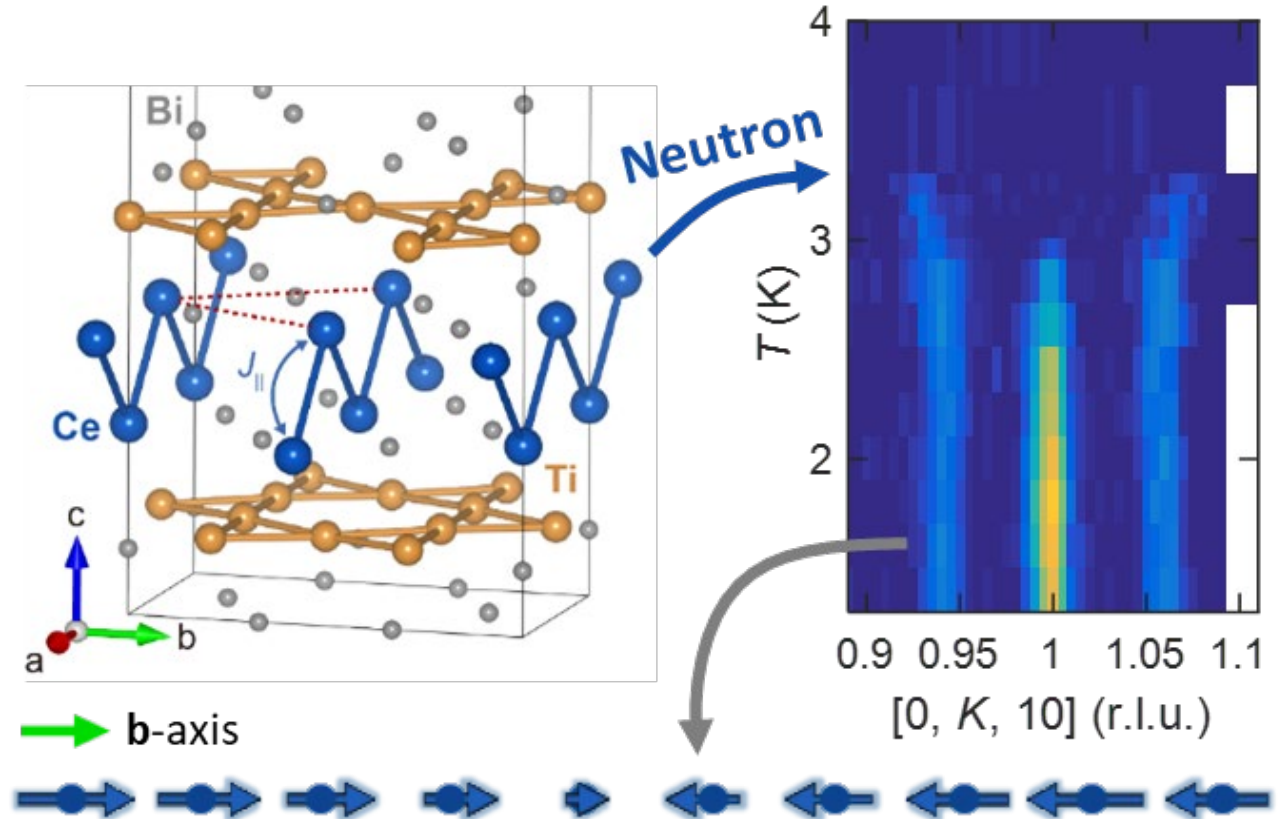
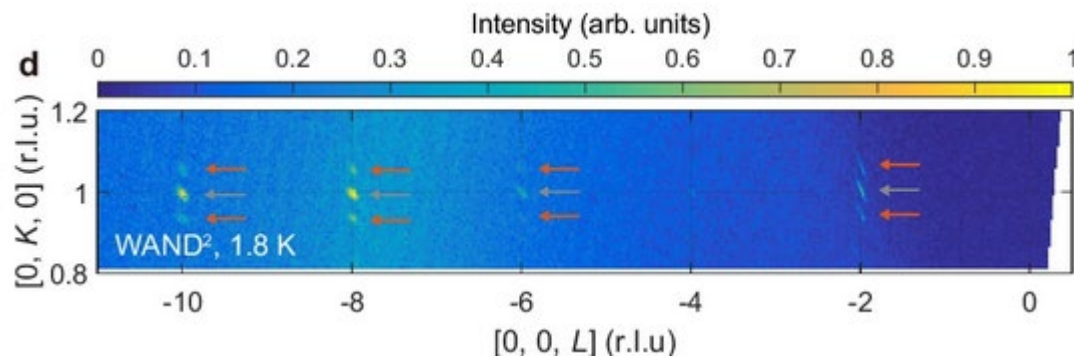


Pasco C., Rai B., Frontzek M., Sala G., Stone M.B., Chakoumakos B.C., Garlea V.O., Christianson A.D., May A.F., ["Anisotropic magnetism of the Shastry-Sutherland lattice material BaNd₂PtO₅"](#), *Physical Review Materials*, **7**, 074407 (2023)

WAND²

Science - Single Crystal

- Magnetic structure determination
- Reciprocal space mapping allows tracking of unknown propagation vector
- Out of plane coverage of 1st BZ



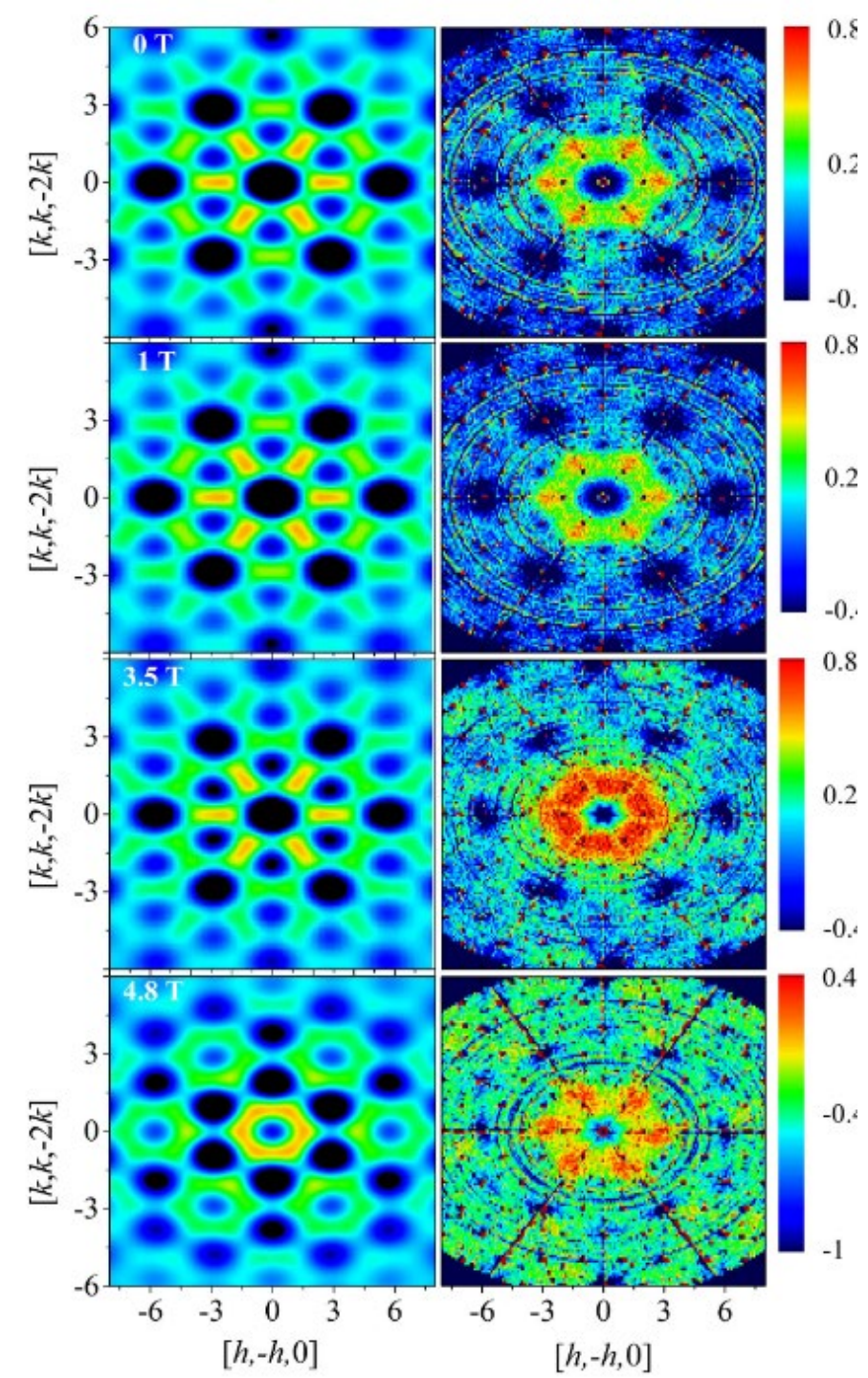
P. Park, B. R. Ortiz, M. Sprague, A. P. Sakhya, S. A. Chen, M. D. Frontzek, W. Tian, R. Sibille, D. G. Mazzone, C. Tabata, K. Kaneko, L. M. DeBeer-Schmitt, M. B. Stone, D. S. Parker, G. D. Samolyuk, H. Miao, M. Neupane, & A. D. Christianson, "Spin density wave and van Hove singularity in the kagome metal CeTi₃Bi₄", *Nat. Commun.* **16**, 4384 (2025).

WAND²

Science - Single Crystal

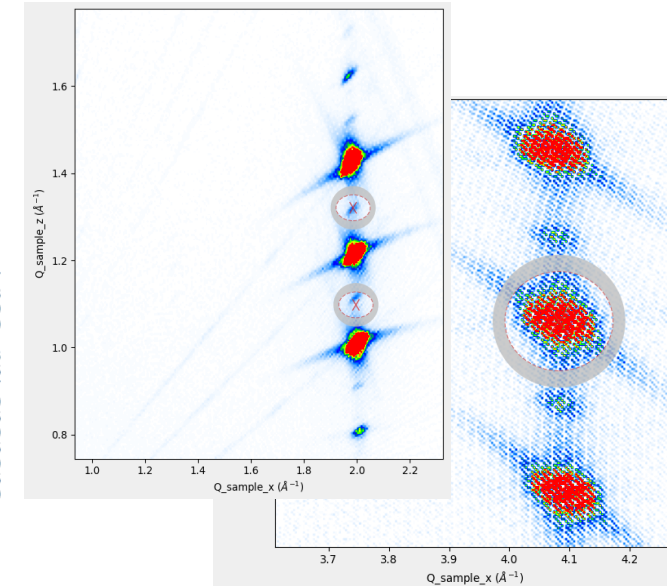
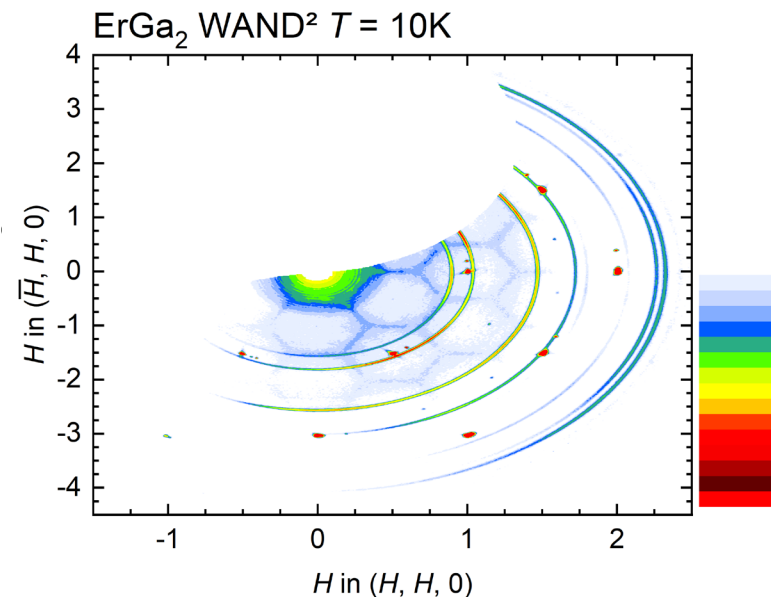
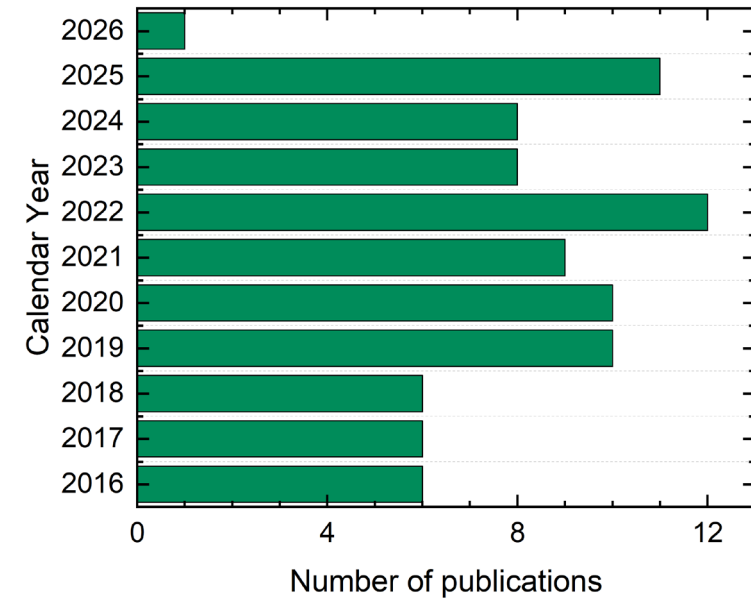
- Diffuse Scattering
- Reciprocal space mapping allows optimization of magnetic exchange coupling parameter
- 70mK data in 6T cryomagnet (minus 50K, 0T background)
- Out of plane coverage of 1st BZ

Dissanayake S., Shi Z., Rau J.G., Bag R., Steinhardt W., Butch N.P., Frontzek M., Podlesnyak A., Graf D., Marjerrison C.A., Liu J., Gingras M., Haravifard S., ["Towards understanding the magnetic properties of the breathing pyrochlore compound Ba₃Yb₂Zn₅O₁₁ through single-crystal studies"](#), *npj Quantum Materials*, **7**, 77 (2022).



WAND²: Effectiveness of beam time use

- Experiment to publication rate is about 30%
- SE reliability, instrument issues and sample quality are NOT main issues
- Data reduction is script based and cumbersome, albeit well documented
- CIs have developed software for many problems, less documented
- Auto-reduction + Peak integration
- Inexperienced users, insufficient support
- Slowly seeing returning users



DEMAND Instrument Overview

1) four-circle mode



2) two-axis mode



Extreme sample environment



Ultra-low temperature
 $T \sim 0.05$ to 700 K

High magnetic field
 $H \sim -6$ to 6 T (vertical)

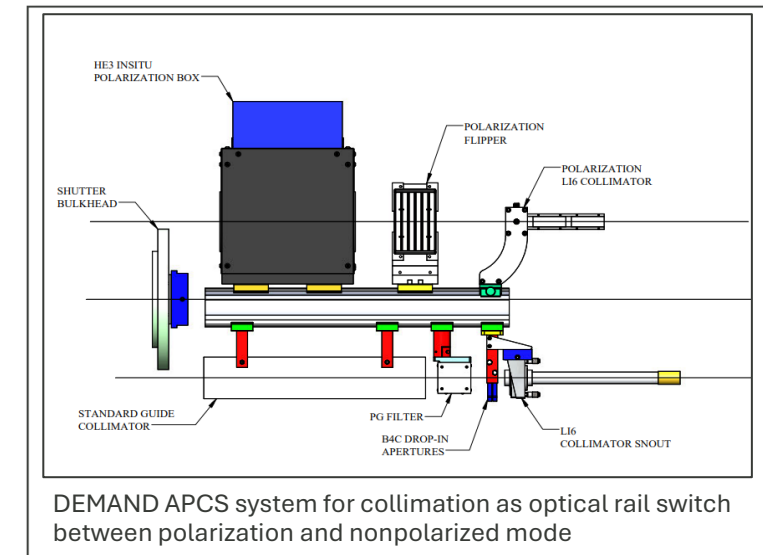
High pressure
 $P \sim 0$ to 10 GPa

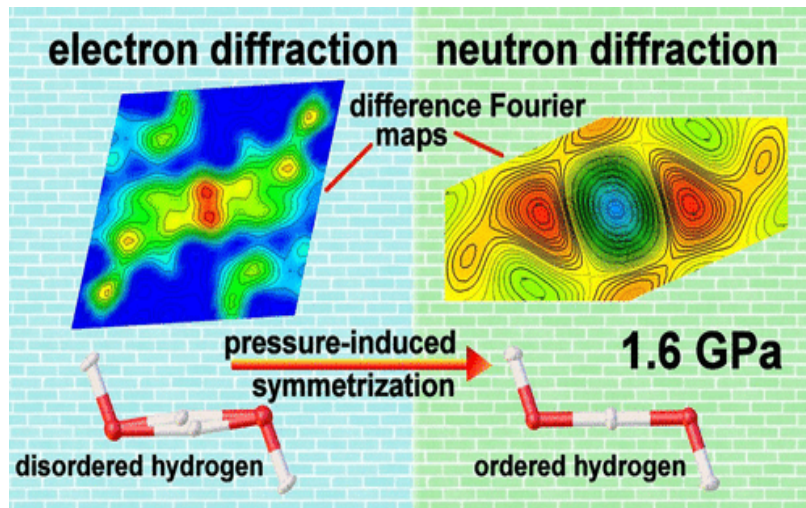
Electric field
 $E \sim 0$ - 10^4 voltage/cm

Large area detector: position-sensitive but magnetic field insensitive.

Beam:

- a) High Flux: 2.2×10^7 n/cm²s at 1.54 Å.
- b) High Resolution: $\delta d/d = \delta Q/Q \sim 0.2\%$
- c) Unpolarized neutrons
- d) Polarized neutrons by S-bender and He-3 polarizer





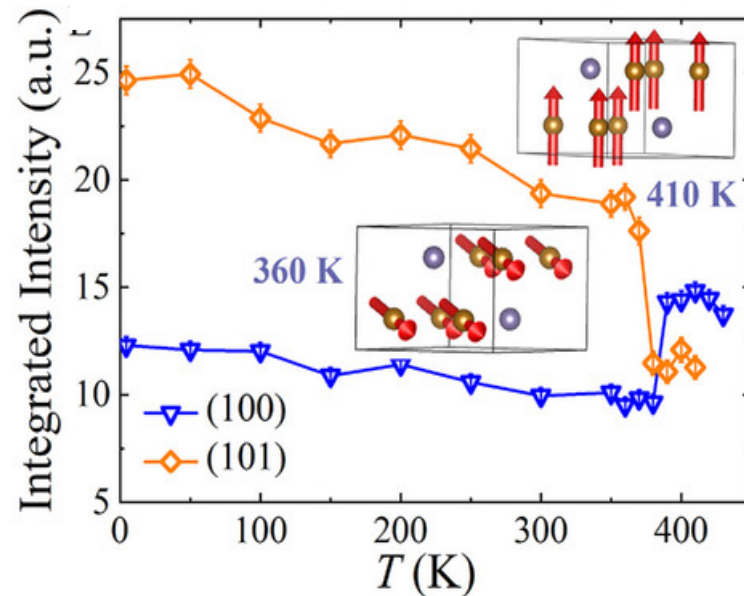
Charge density analysis with single-crystal electron diffraction and neutron diffraction studies reveal that the bihydroxide anion in natrochalcite undergoes HB summarization at low pressure below 1.6 GPa in $[\text{NaCu}_2(\text{SO}_4)_2 \cdot \text{H}_3\text{O}_2]$ natrochalcite.

- A second-order phase transition was found in bihydroxide anions of $[\text{NaCu}_2(\text{SO}_4)_2 \cdot \text{H}_3\text{O}_2]$ that hydrogen bond (HB) symmetrized at the lowest pressure reported so far among inorganic compounds.
- This research brought important insights to understand the process of water transport to the deeper part of Earth's mantle and superconductivity in hydrogenous superconductor systems.

P. Rejnhardt, R. Gajda, M. Woińska, J. Parafiniuk, G. Giester, R. Miletich, Y. Wu, T. Poręba, M. Mezouar, S. Sutuła, T. Góral, P. Dera, K. Woźniak, *J. Am. Chem. Soc.*, **147**, 30, 26830–26843, (2025), doi:[10.1021/jacs.5c08310](https://doi.org/10.1021/jacs.5c08310).

Science Highlights

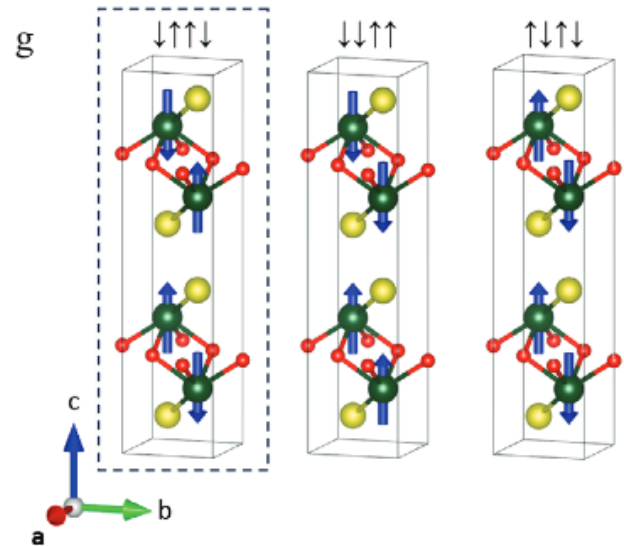
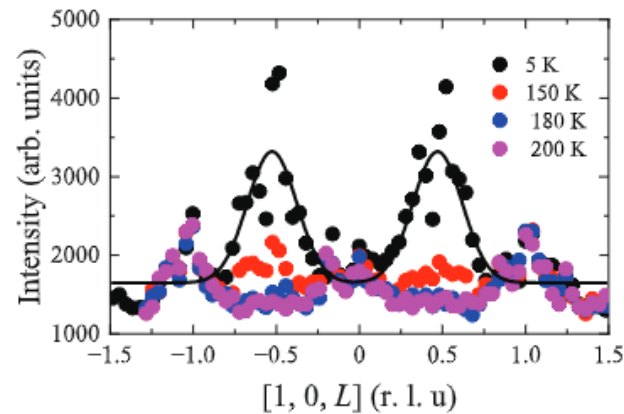
2025 DOE Conference Call :
DEMAND science highlights



Neutron diffraction data collected at DEMAND instrument displays the peak intensity change along with magnetic transition; the insets show the schematic diagram of spin configurations of the magnetic phases.

- The Kagome lattice Fe₃Ge exhibits topological Hall resistivity and Nernst effect. These phenomena are attributed to the Berry phase associated with the field-induced nonzero scalar spin chirality.
- The results highlight the synergic effects of the Berry phases in both momentum and real space. With high magnetic ordering temperature, Fe₃Ge could be a promising candidate for thermoelectric applications based on the Nernst effect.

C. Xu, S. Gupta, H. Tan, H. Bae, O. O. Emmanuel, M. Xu, Y. Wu, X. Xu, P. Zhang, W. Xie, B. Yan, X. Ke, *Advanced Functional Materials*, **1**, 11059 (2025),
doi:[10.1002/adfm.202511059](https://doi.org/10.1002/adfm.202511059)



Single-crystal neutron diffraction data of UTeO (upper-panel) and the symmetry-allowed magnetic structures (lower-panel). The $\uparrow\downarrow\uparrow\downarrow$ structure agrees with the neutron data

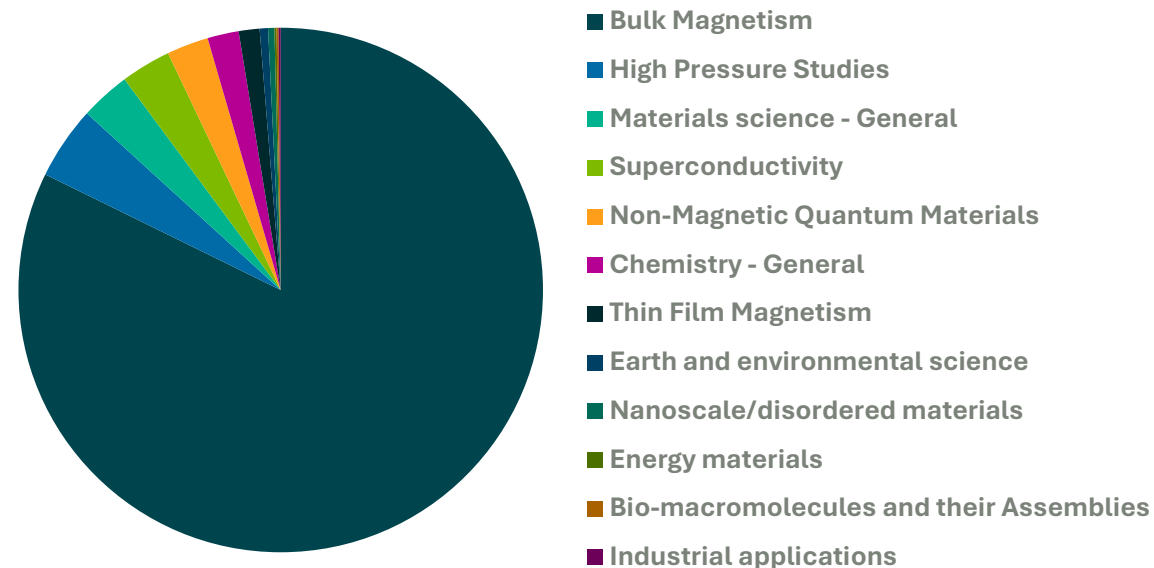
- Magnetic structure of the topological antiferromagnet UOTe is revealed using single crystal neutron diffraction. A fully compensated AFM Chern insulator is discovered based on experiment evidences and theoretical predictions.
- These results show breaking of combined parity and time-reversal (PT) symmetry, allowing for non-zero Chern number responsible of quantum anomalous Hall effects.

Christopher Broyles, Sougata Mardanya, Mengke Liu, Junyeong Ahn, Thao Dinh, Gadeer Alqasseri, Jalen Garner, Zackary Rehfuss, Ken Guo, Jiahui Zhu, David Martinez, Du Li, Yiqing Hao, Huibo Cao, Matt Boswell, Weiwei Xie, Jeremy G. Philbric, Tai Kong, Li Yang, Philip Kim, Su-Yang Xu, Ashvin Vishwanath, Jennifer E. Hoffman, Jonathan D. Denlinger, Sugata Chowdhury, and Sheng Ran, *Advanced Materials*, 2414966 (2024).

Beamline productivity

- **DEMAND** keeps developing new capabilities to satisfy emergent science needs and sustain productivity in the long-term.
- Over 1000 unique authors on Push publications has reached at DEMAND in 2025.

HB-3A Research Areas 2020-2025



Instrument H-index 46

★Specially Recognized

Citation Count 20-49 (48)

Citation Count > 50 (44)

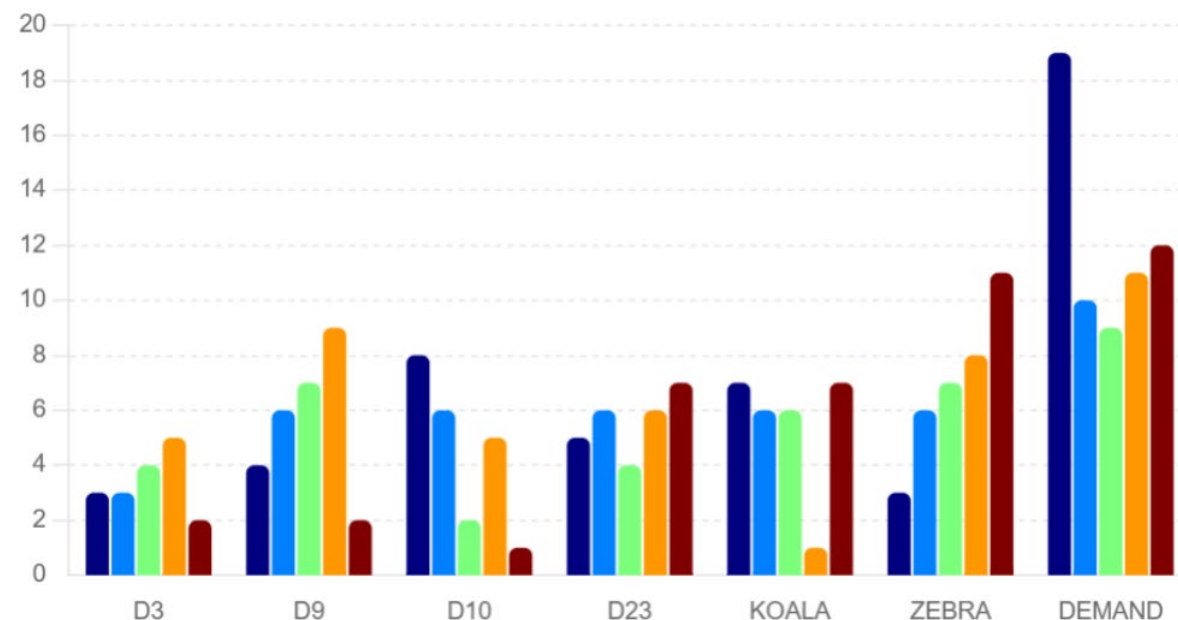
DOE Highlight (19)

Editor's Choice (1)

Journal Impact Factor >7 (53)

Rapid Communication (5)

Publications by year for 2021, 2022, 2023, 2024, and 2025



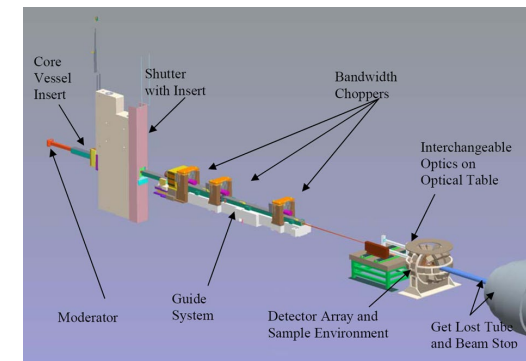
TOPAZ Instrument Overview

Neutron Source

Moderator	Hydrogen Decoupled poisoned
Source to sample distance	18 m
Bandwidth (1 st Frame)	0.30 – 3.5 Å
Resolution	> 0.2% $\Delta d/d$
d spacing range	0.25 Å - 14 Å
Q range	0.45 – 25 Å ⁻¹
Neutron beam sizes	2.0 – 4.0 mm diameter
Neutron beam divergence	15 – 25 mrad

Detector

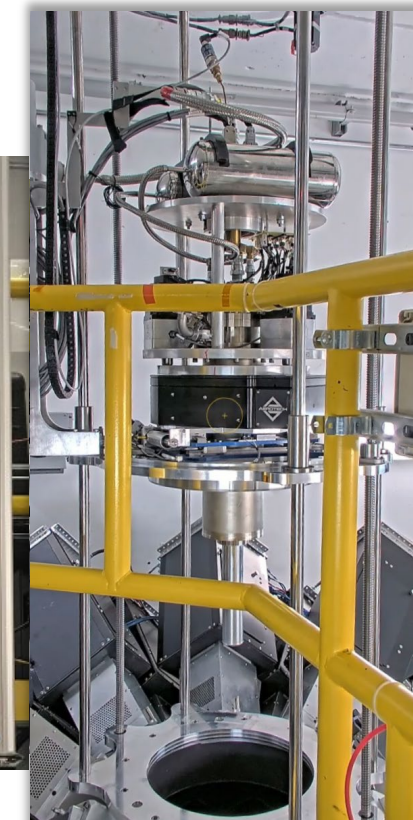
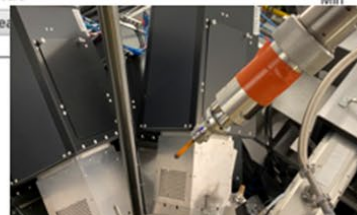
Sample to detector distance	39.5 – 45.5 cm
Detector coverage	3.2 sr for 25 detectors
Detector size	15 x 15 cm ² with 256 by 256 pixels
Detector angular range	15° – 160° 2θ
	0 +/- 32° out-of-plane



Instrument Status
 Beam Power (kW): 1378.06 kW
 Primary Shutter: ●
 Acquisition Software Status: ●
 Data/Reduction Status: ●

Proposal Information
 Proposal #: IPTS-12132
 Proposal Title: NX School: High-resolution single crystal structure
 Team Members: Xiaoping Wang, Justin Paloni, Ashley Cardenal, (XCAMS/UCAMS)

Run Information
 Scan Status: Scanning
 Run Status: Run Abort
 Run Number: 40731
 Run Time: 7.3 s
 Total Neutron Counts: 835132
 Count Rate (counts/s): 121473
 Total Proton Charge: 0.0102 C
 Beam Monitor 1 Counts: 18959
 Beam Monitor 2 Counts: 17957



Quantum Crystallography

J|A|C|S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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Open Access



Article

Intermolecular Interactions in Direct Air Capture Materials: Insights from Charge Density Analysis

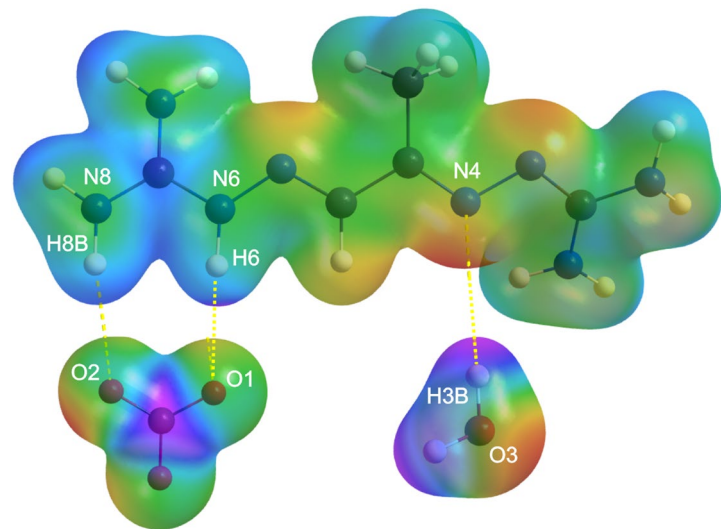
Sylvia Pawledzio,* Jeffrey Einkauf, Radu Custelcean, and Xiaoping Wang*



Cite This: *J. Am. Chem. Soc.* 2025, 147, 27299–27313

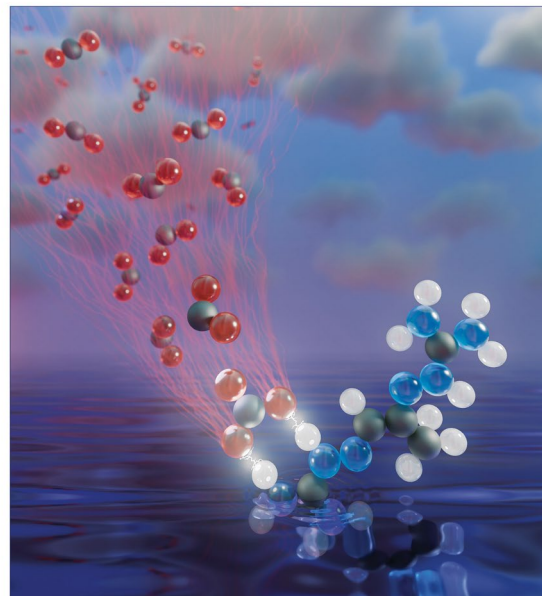


Read Online



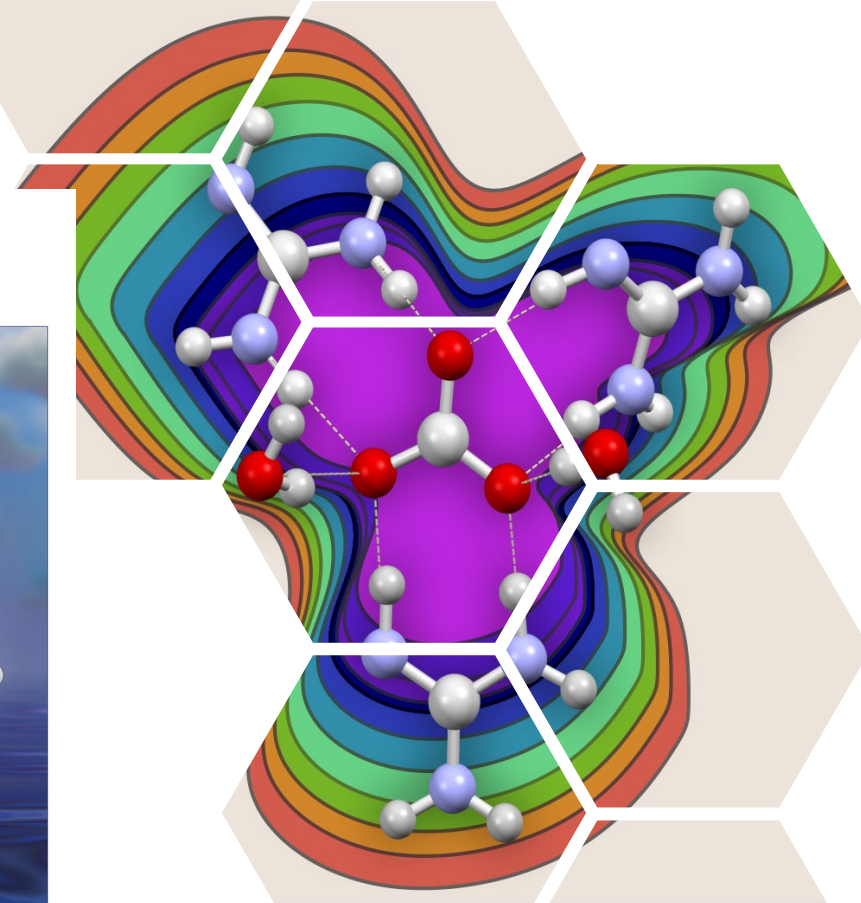
August 6, 2025
Volume 147
Number 31
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NSD Postdoc Project Quantum crystallography integrating neutron and X-ray diffraction reveals the electron-density distribution and hydrogen-bonding interactions between CO₂ and a guanidine-based sorbent, providing mechanistic insights to guide the rational design of next-generation Direct Air Capture materials.

Magnetic Swirls

J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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Article

Skyrmion-like Spin Textures Emerging in the Material Derived from Structural Frustration

YiXu Wang,[▽] Ian Campbell,[▽] Zachary P. Tener, Judith K. Clark, Jacnel Graterol, Andrei Rogalev, Fabrice Wilhelm, Hu Zhang, Yi Long, Richard Dronskowski, Xiaoping Wang,* and Michael Shatruk*

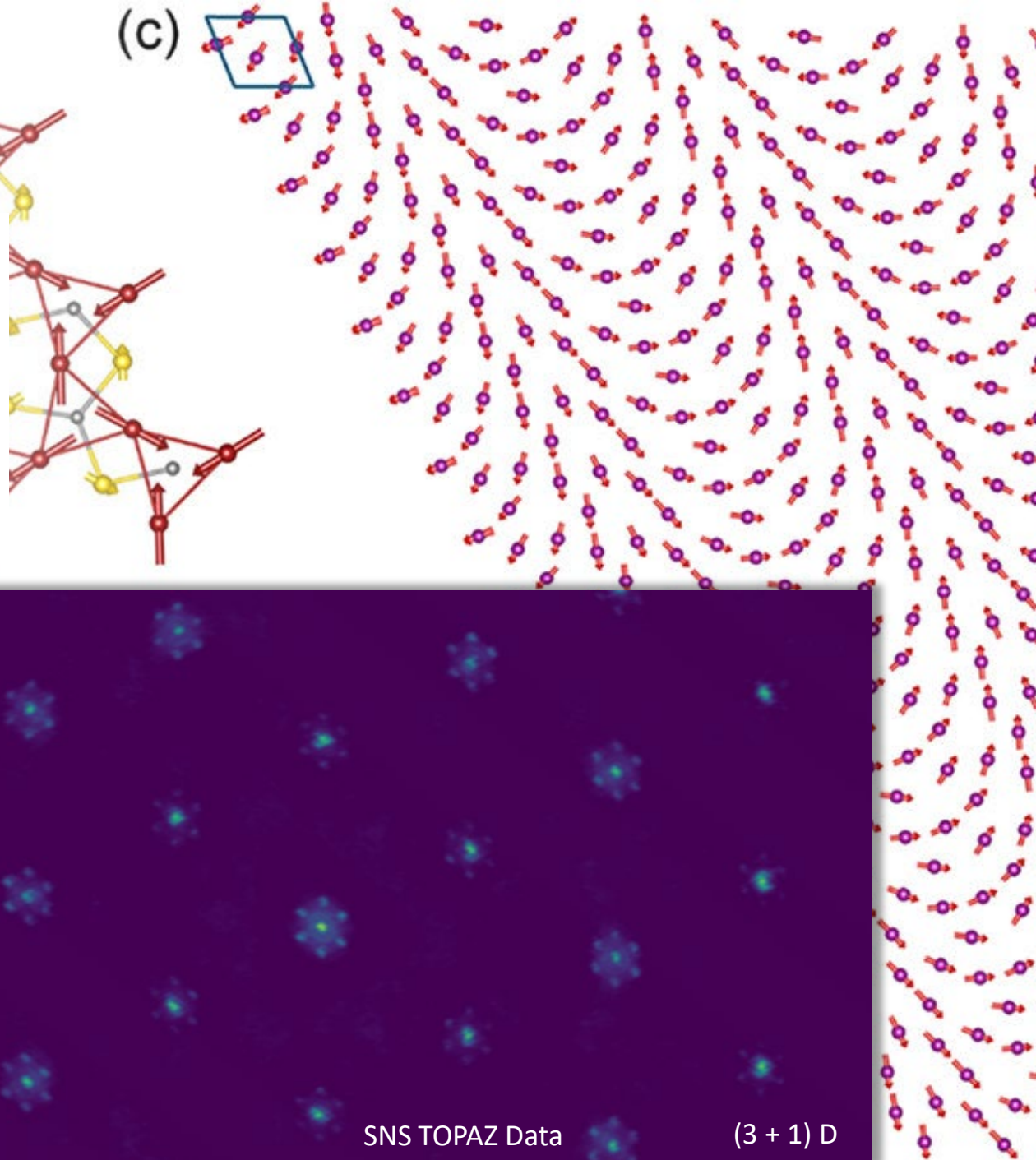
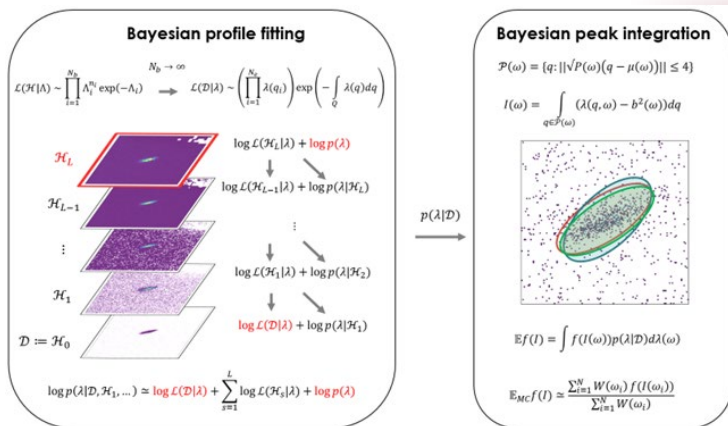


Cite This: *J. Am. Chem. Soc.* 2025, 147, 43550–43559



Read Online

- **AI-Assisted Peak Integration (LDRD)**
- Multiresolution Bayesian optimization
- Use global prior from ML/AI for integrating weak magnetic peaks near strong Bragg reflections



Single Crystal Diffraction Beyond Three Dimensions

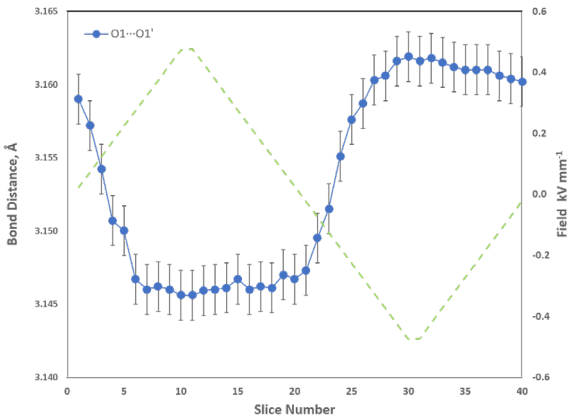
RESEARCH ARTICLE | FEBRUARY 08 2021

Operando single crystal neutron diffraction reveals insight into the field response mechanisms in the hydrogen-bonded KH_2PO_4 ferroelectric

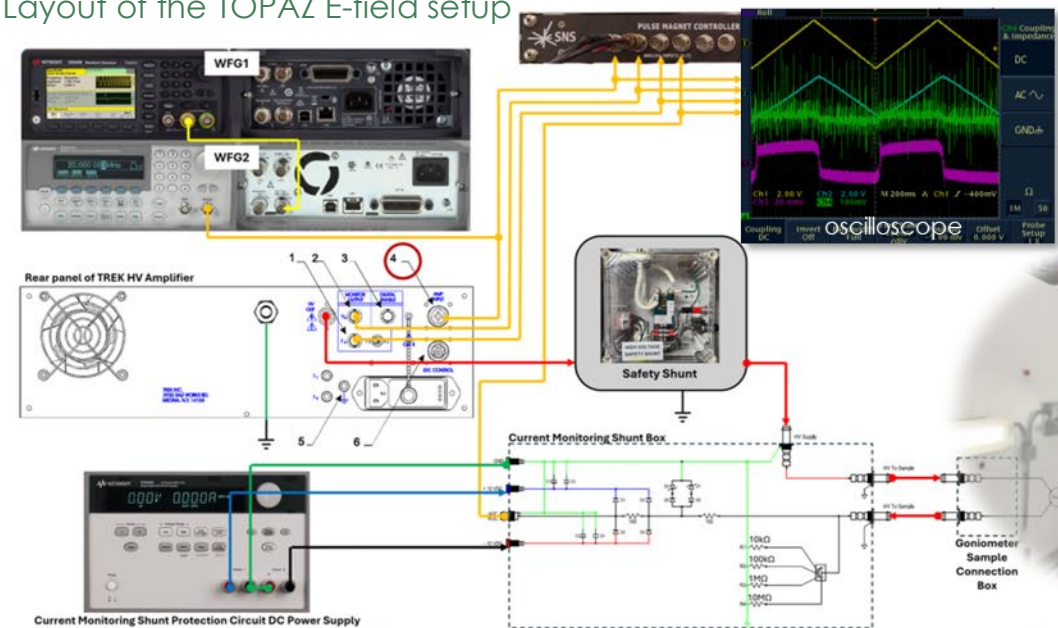
Special Collection: 100 Years of Ferroelectricity — a Celebration

C. M. Fancher ; C. M. Hoffmann ; X. P. Wang ; L. L. Daemen; A. J. Schultz

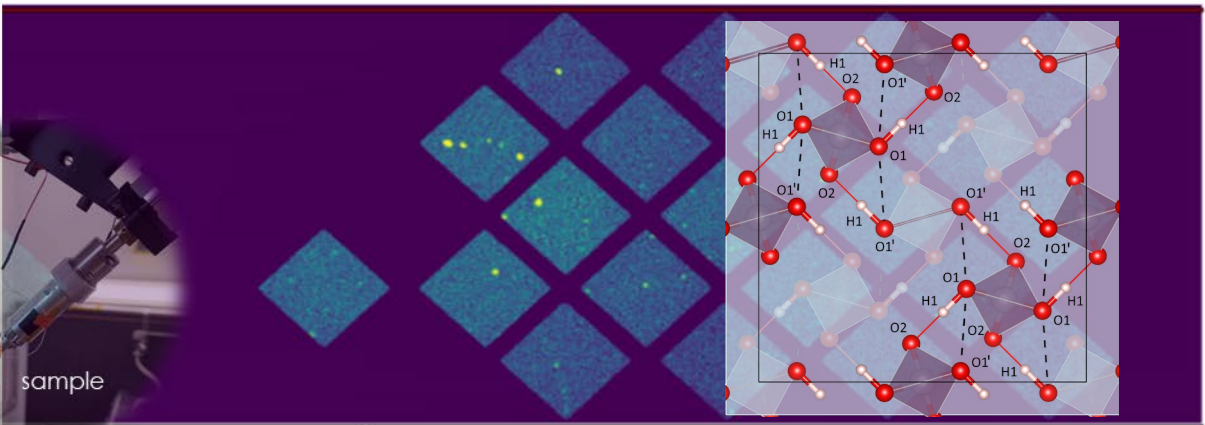
(3+d)
Diffraction Space
+
Parameter Space
(T, E, Stress, P, B)



Layout of the TOPAZ E-field setup



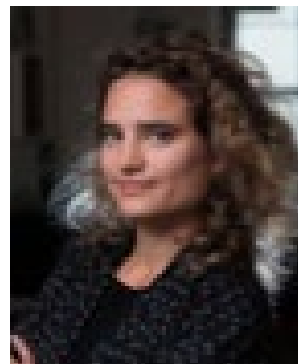
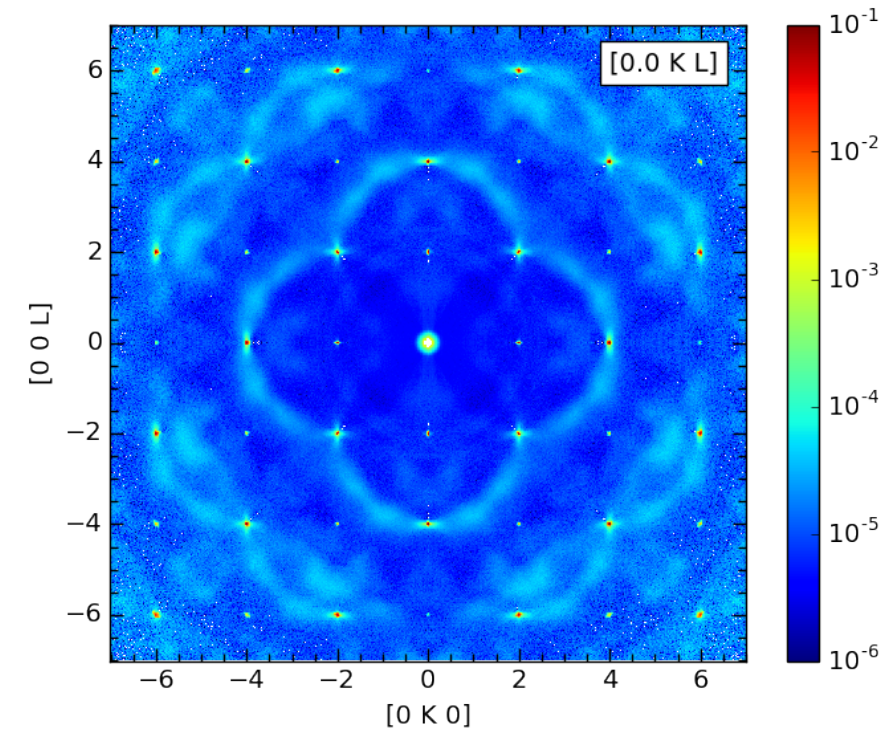
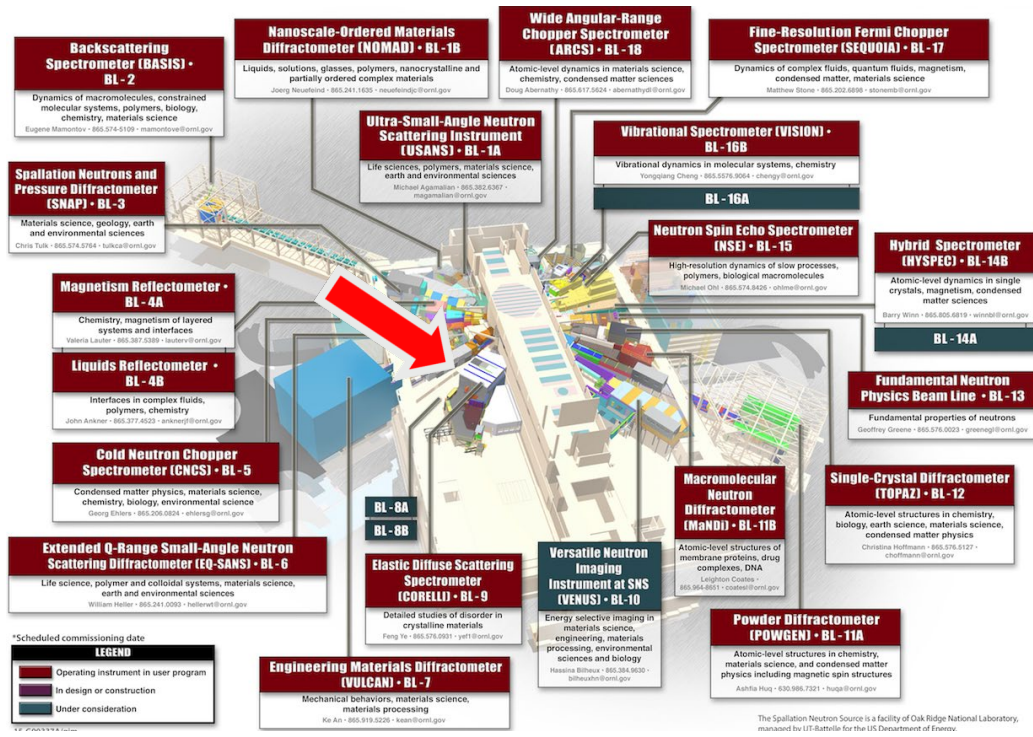
Run Number:	52542
Run Time:	10.2 s
Total Neutron Counts:	892700
Count Rate (counts/s):	87899
Total Proton Charge:	0.0133 C



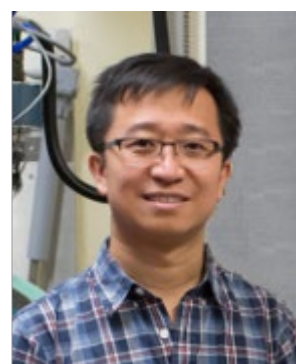
Min	Max	Mean	Total	Rate
0	390	3.570	800387	79872 e/s

Sub-atomic resolution structure at 0.019 sec. time-resolution

CORELLI Instrument Overview



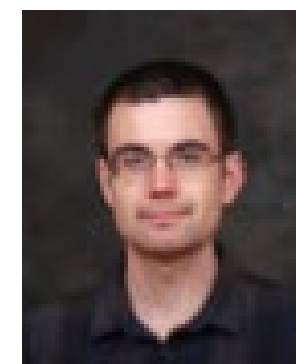
Arianna Minelli



Huibo Cao



Feng Ye

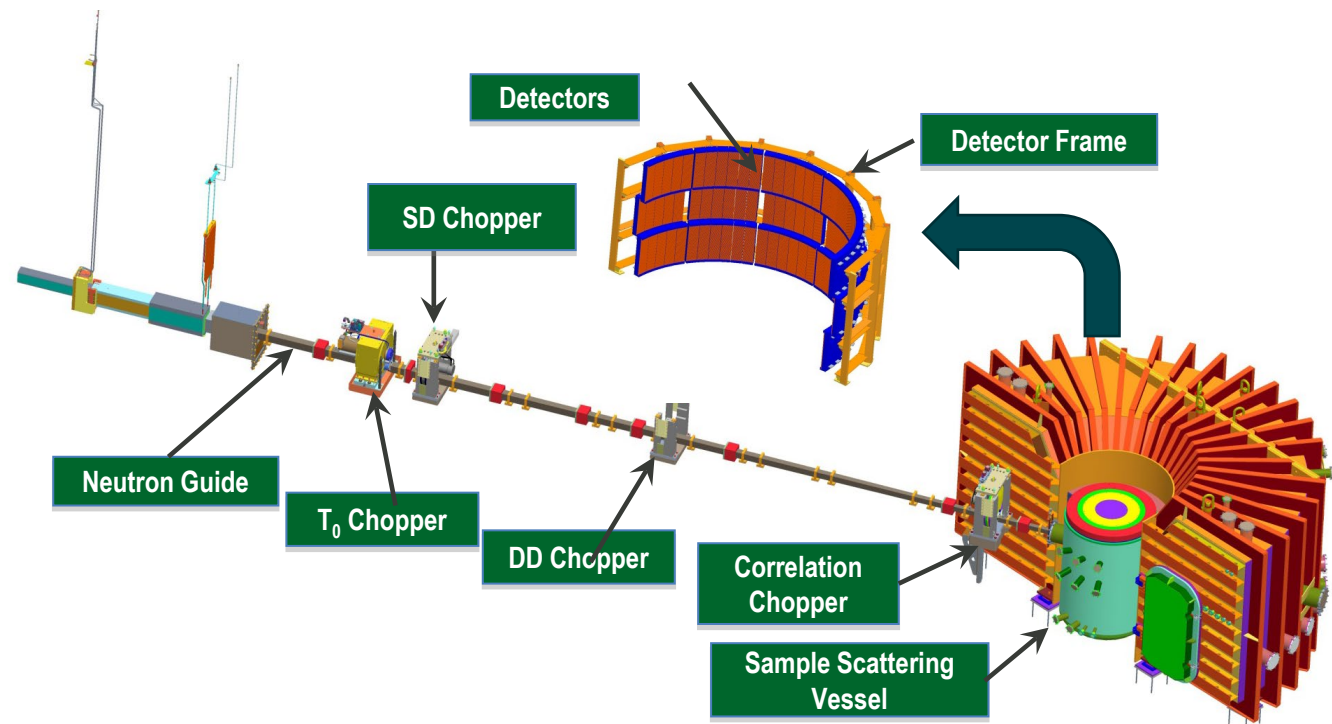


Zachary Morgan



Duminda Liurukara

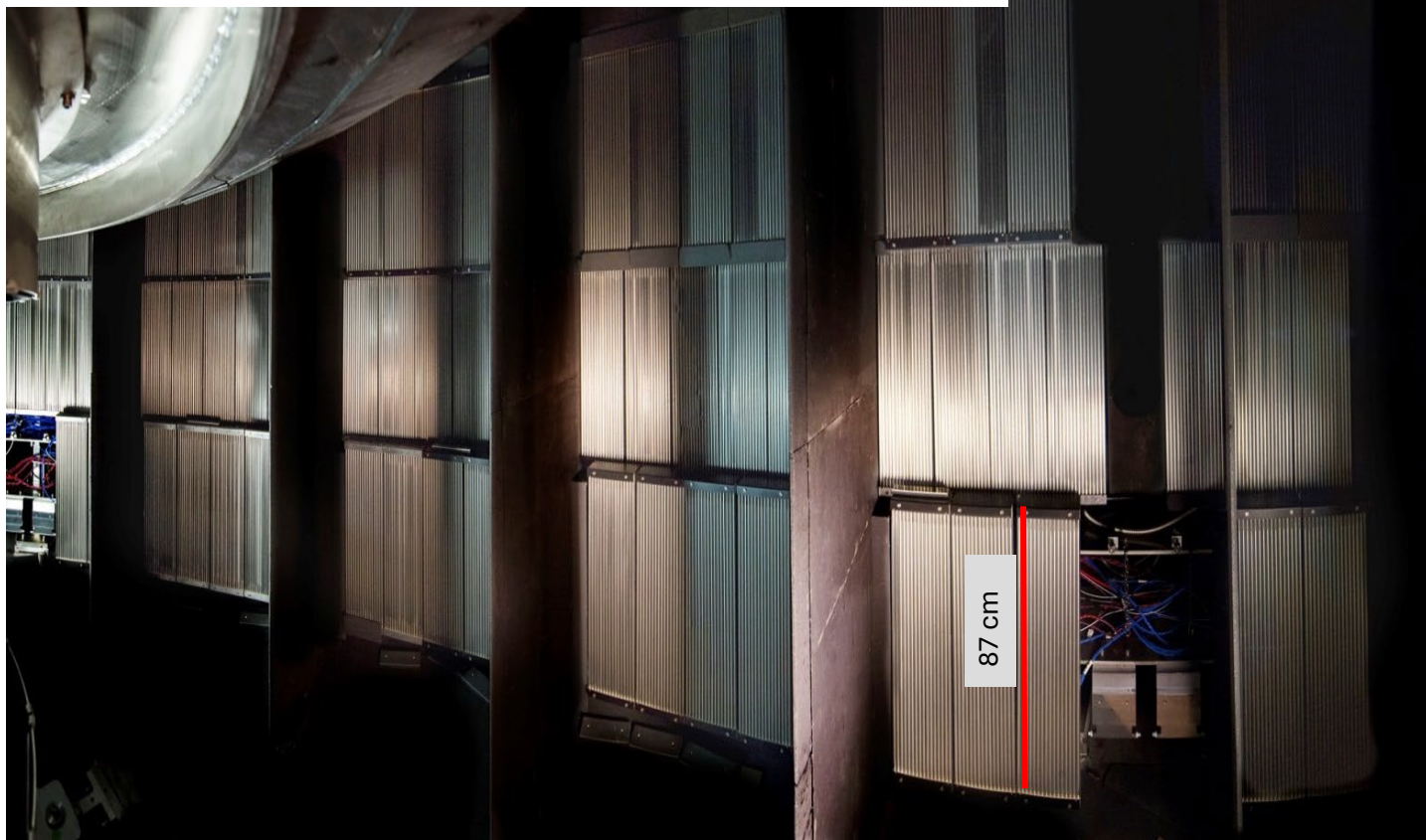
Neutronic optics and Specifications



Moderator	decoupled poisoned H ₂ O
Source to sample	20 m
Sample to detector	2.5 m
Detector angular coverage	-21.9° < 2θ < 148.2° (Horizontal) ± 28.5° (Vertical)
Detector solid angle coverage	2.0 ster. (76 modules installed)
Incident energy range	10 – 200 meV
Momentum transfer	0.5 – 16 Å ⁻¹
Beam size	8 mm (H) X 12 mm (V)
Energy resolution	0.9 meV at E _{inc} = 25 meV
Momentum resolution	ΔQ/Q ≤ 7x10 ⁻³ at 90° for Q=10 Å ⁻¹

^3He detectors inside the scattering vessel

370,000 pixels, time resolved, < 0.001 ms

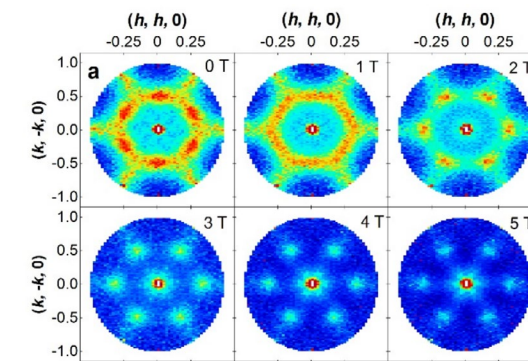
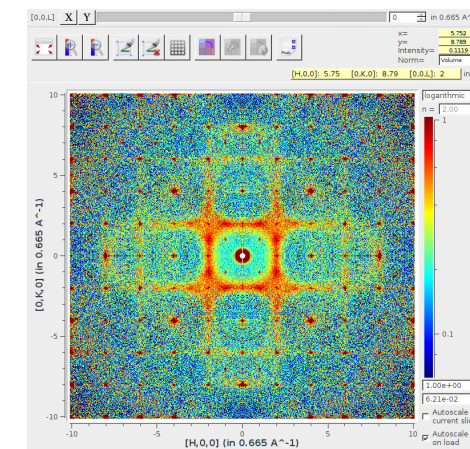
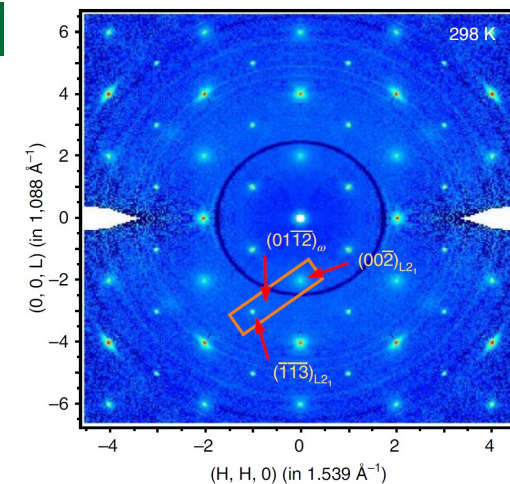


Elastic assumption:
 $\lambda[\text{\AA}] = 3.596 * \text{t.o.f. [ms]} / L_{\text{m-d [m]}}$

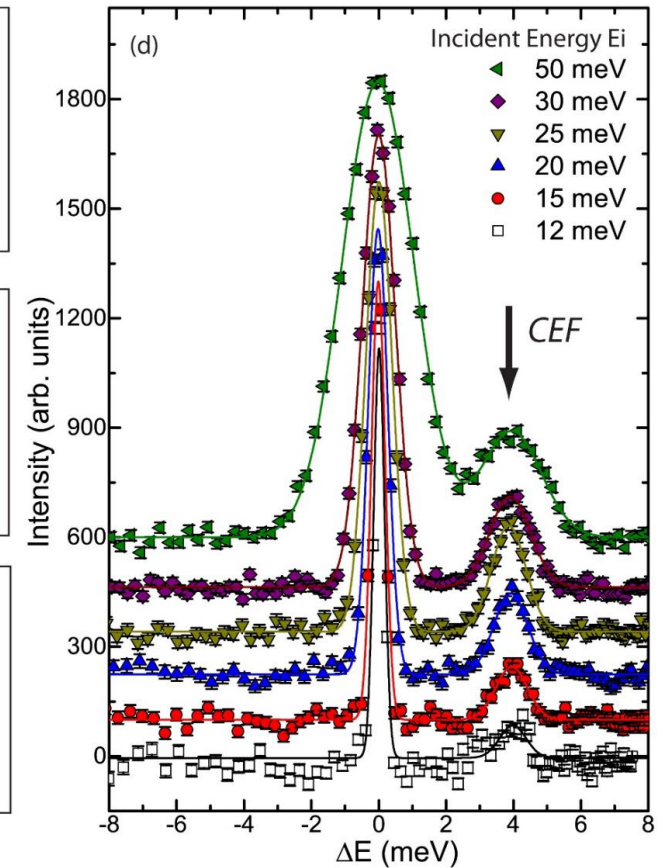
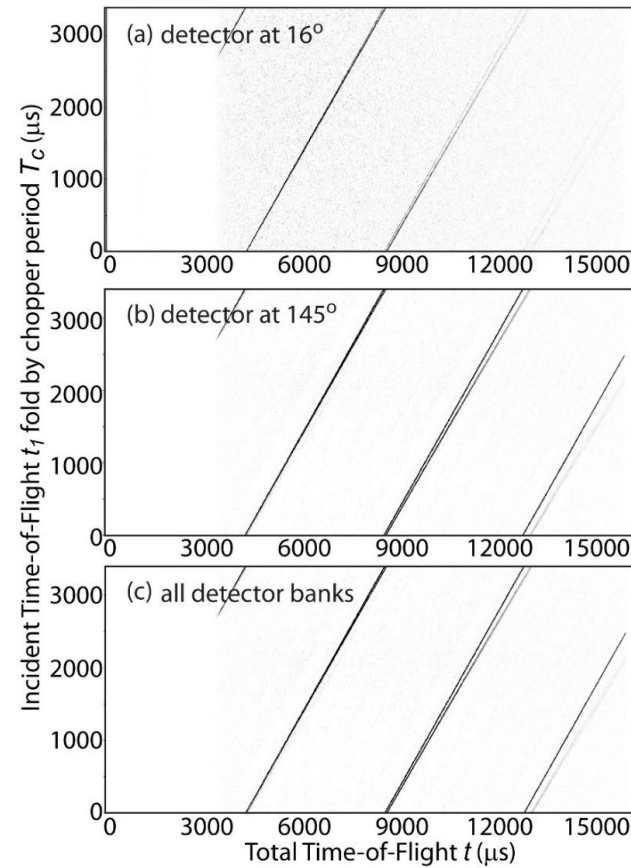
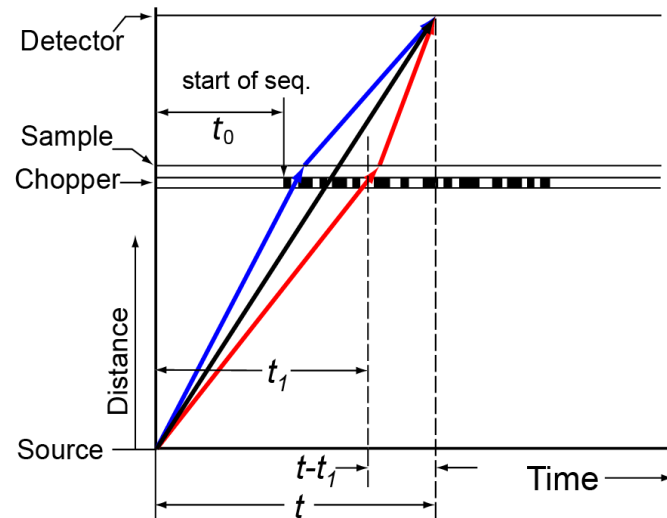
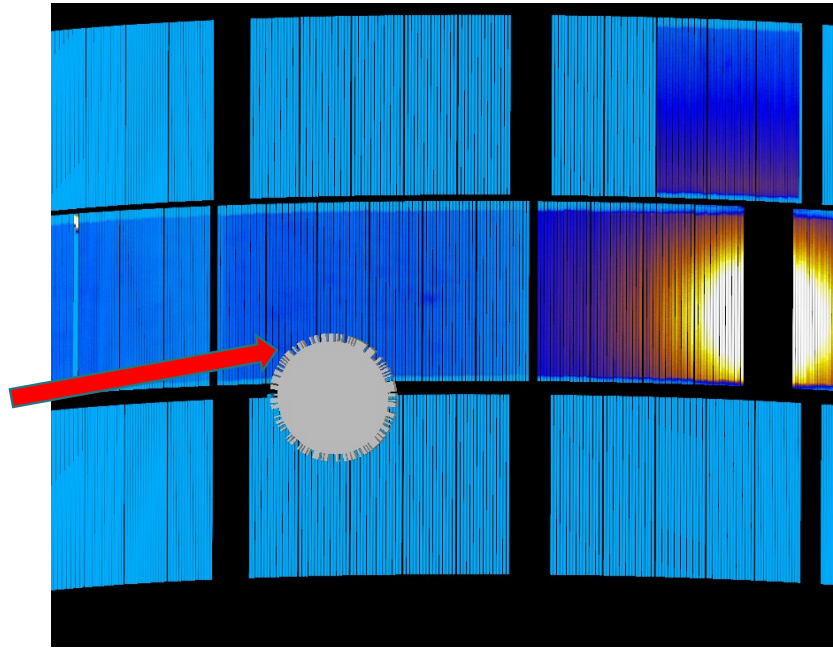
$L_{\text{m-d}} = 22.5$ m for CORELLI

$1 \text{ \AA} \sim 82 \text{ meV} \sim 3956 \text{ m/s} = 3.956 \text{ m/ms}$

$\text{t.o.f [1 \AA]} = 5.687 \text{ ms}$

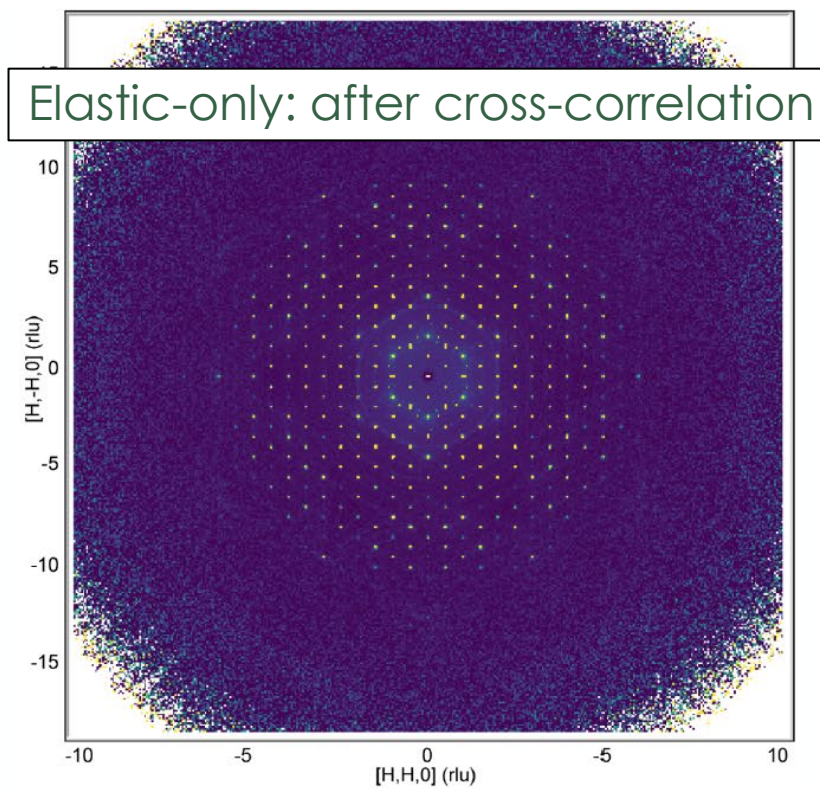
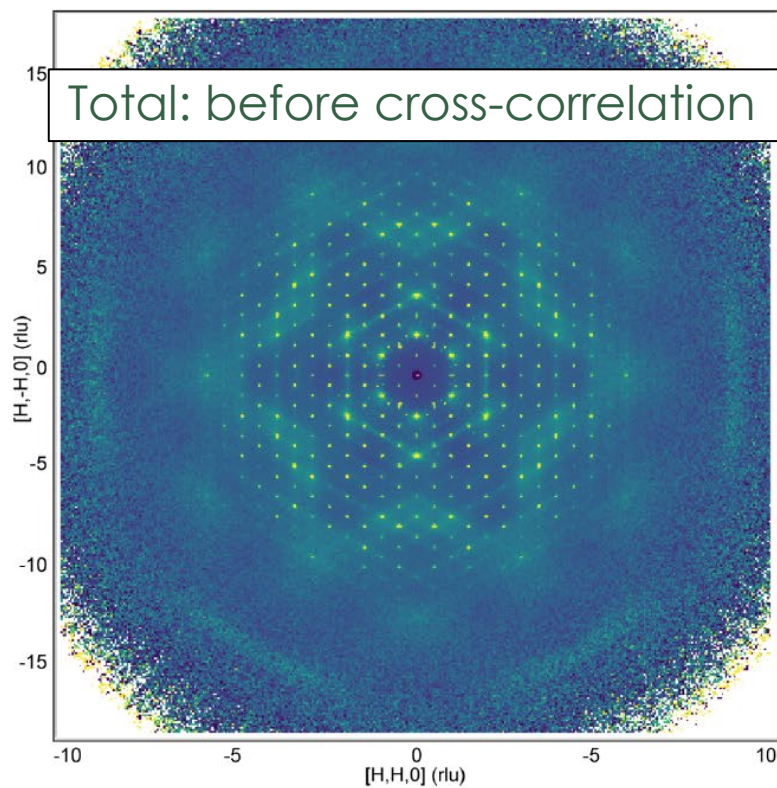


Cross-correlation enables energy discrimination

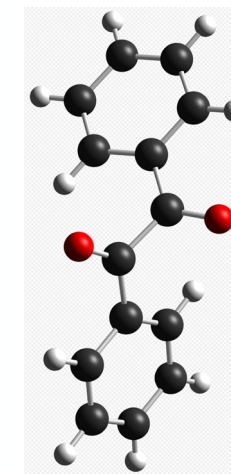
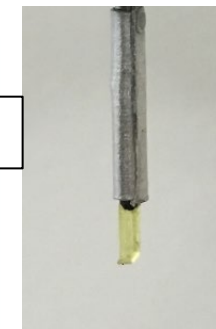


PrAl₃ powder sample, CEF ~ 4 meV
 F. Ye, Y. Liu, R. Whitfield *et al.*,
 J. Appl. Crystallogr. 51, 315 (2018)

Nature of diffuse scattering from molecular Benzil crystal

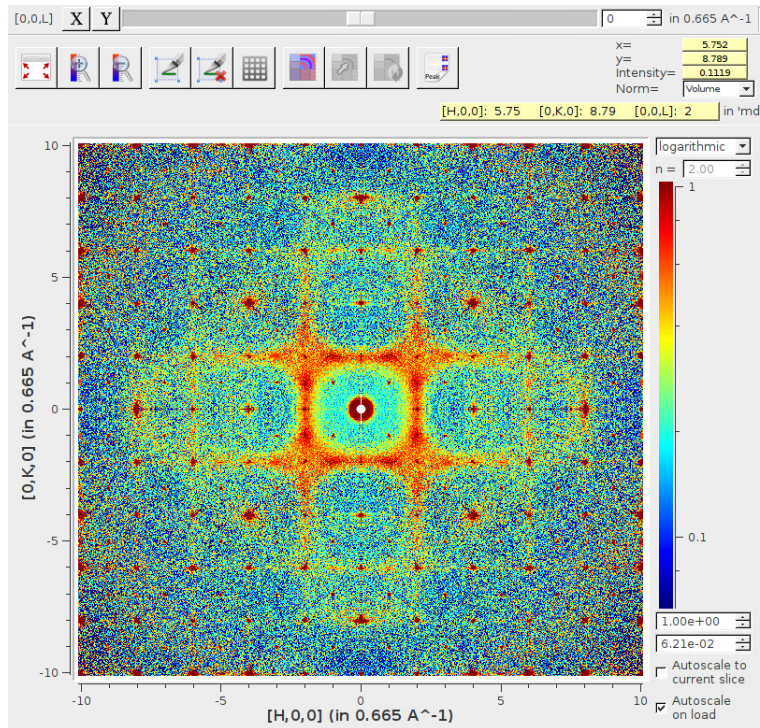


Benzil ($C_{14}D_{10}O_2$) taken at 300 K

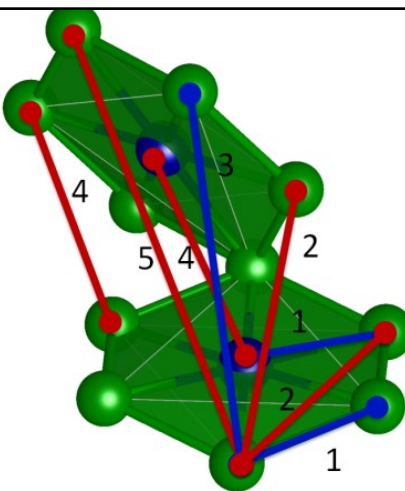
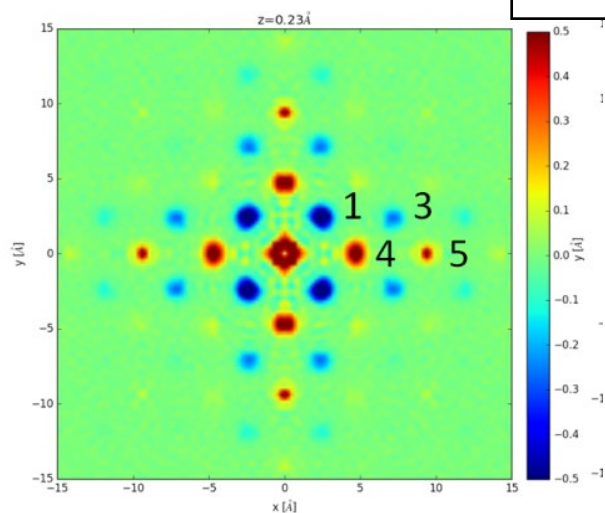
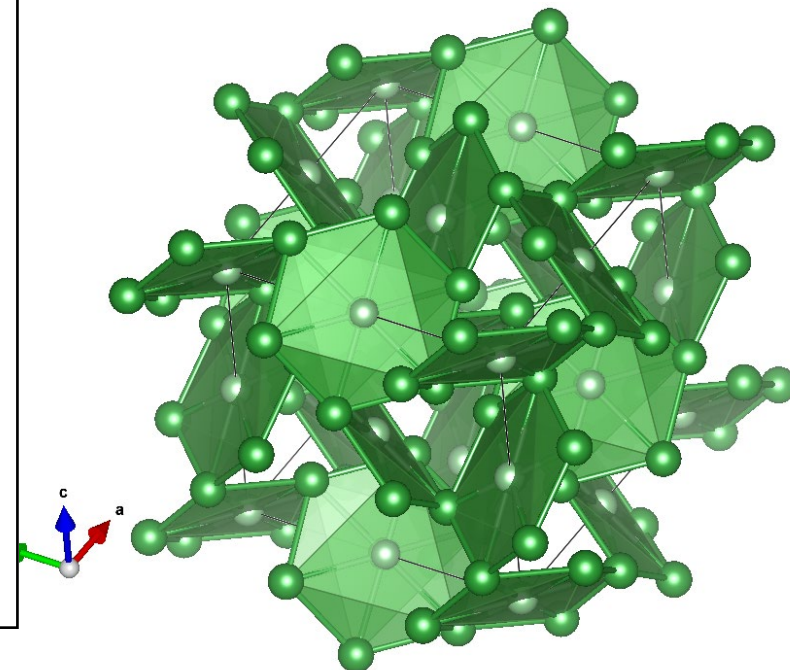


The diffuse scattering features observed in the total scattering channel do not exist in the elastic-only channel.

Model free analysis for magnetic diffuse scattering

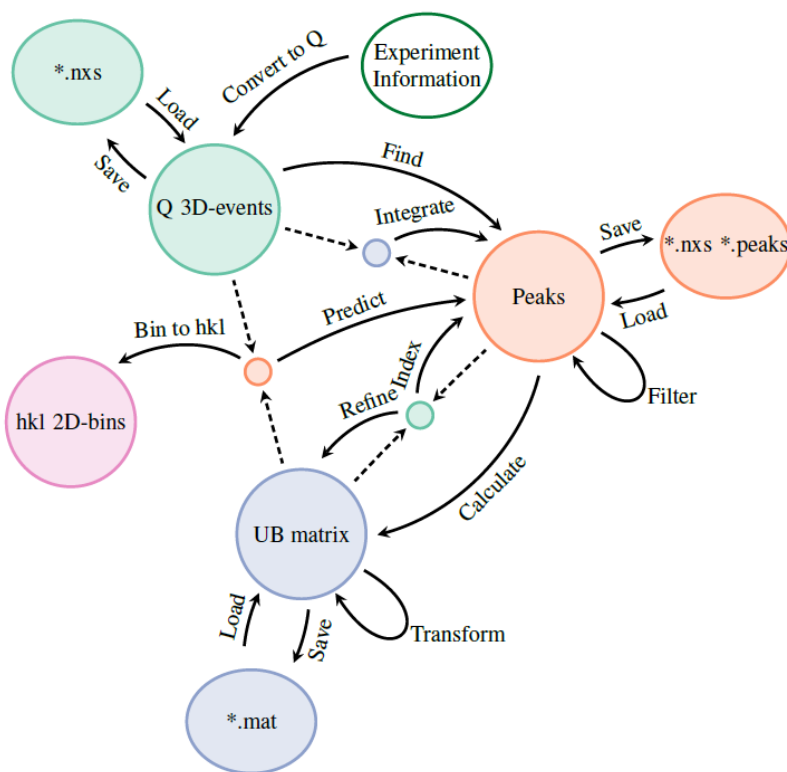
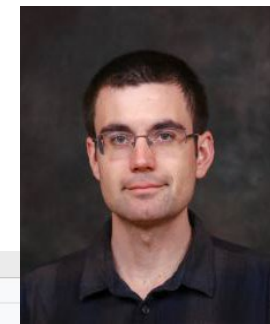


Frustrated Bixbyite ($\text{Mn}^{3+}, \text{Fe}^{3+}$)₂O₃

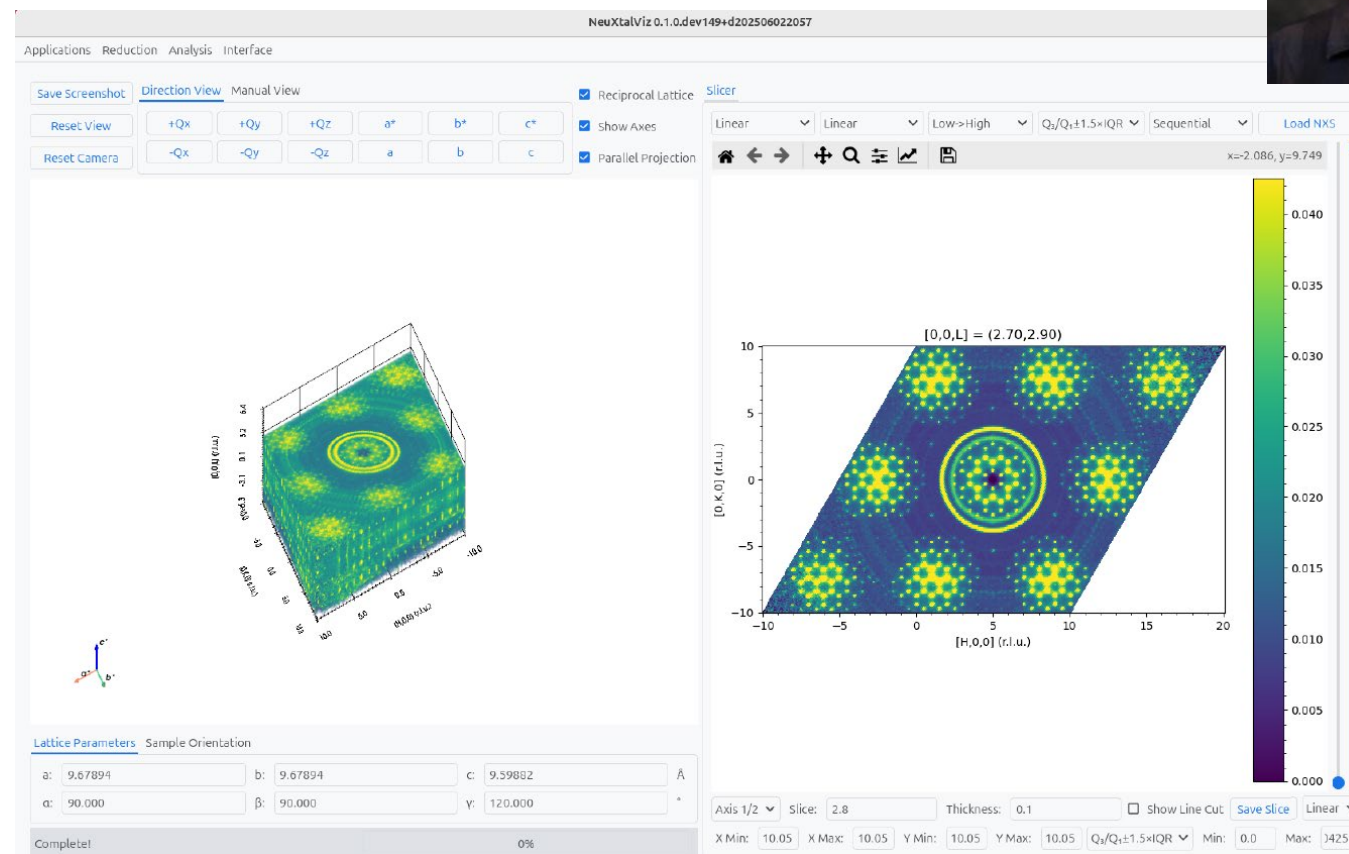


Three-dimensional magnetic differential pair distribution function 3D-mΔPDF

Enhancing neutron single crystal visualization with NeuXtalViz



Complete interactive pathways between reciprocal space data, peaks, and UB-matrix

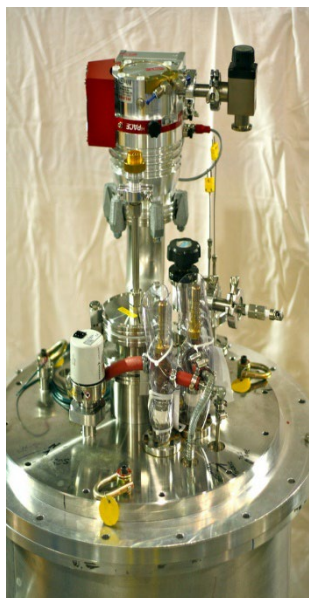


Normalized reciprocal space data showing diffuse/modulated scattering features

A large variety of selection of sample environments



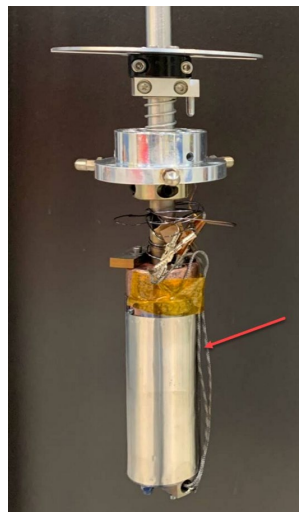
low background
CCR 6 K – 750 K



MICAS Furnace
RT - 1400 °C



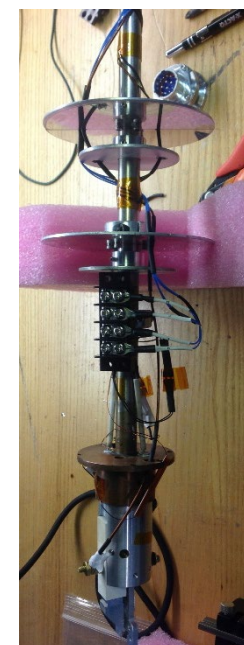
³He insert
0.3 – 300K
or
Dilfridge insert
0.05 K – 300K



Dual heater
stick 750 K



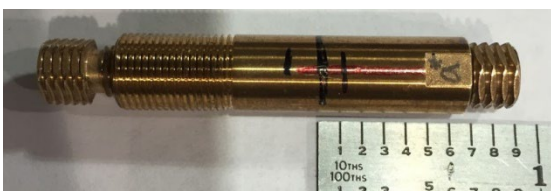
Static Vertical Magnetic
Field, $B_{max} = 5$ T



High Voltage
 $V_{max} = 10$ kV



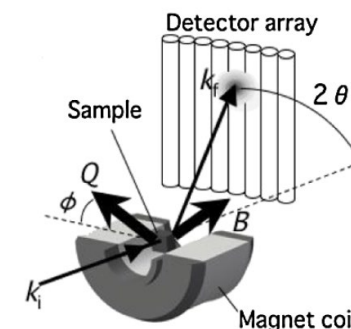
McWhan, $P_{max} \sim 5$ GPa



Pressure Cell, $P_{max} = 1.8$ GPa



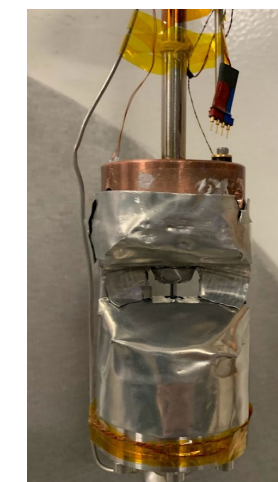
Orange Cryostat



Pulsed Magnetic Field
 $B_{peak} = 30$ T



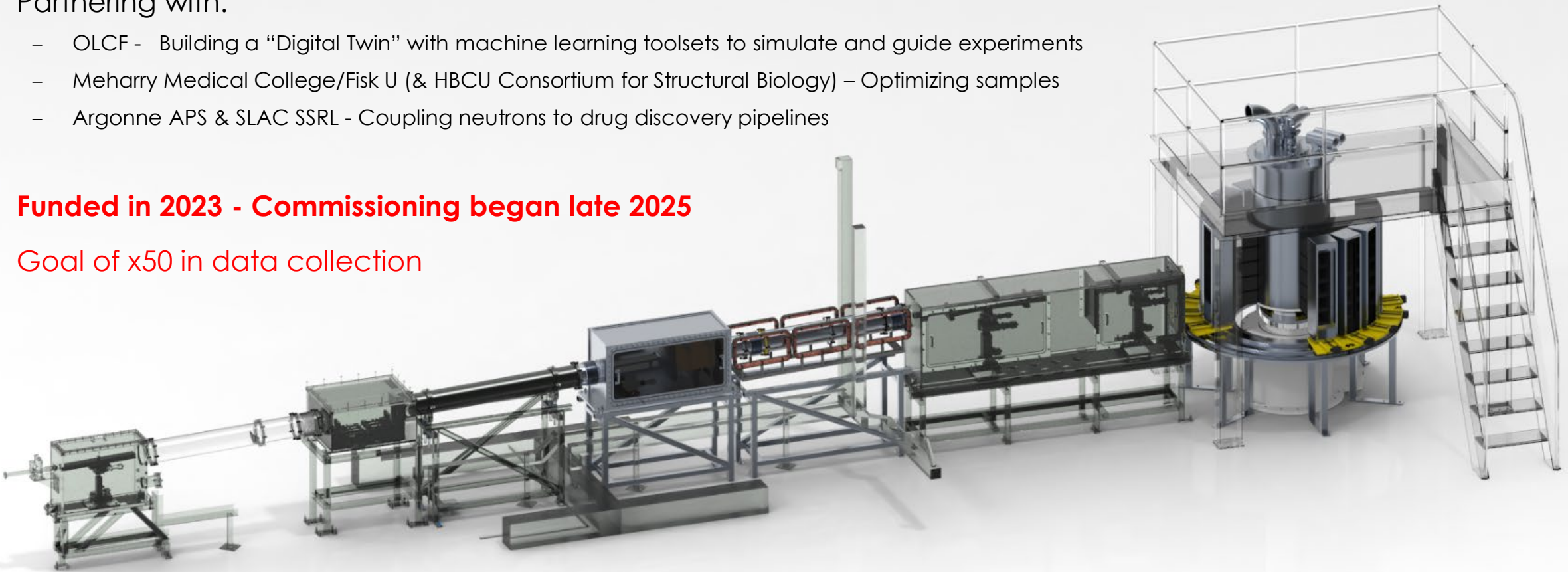
14 T magnet



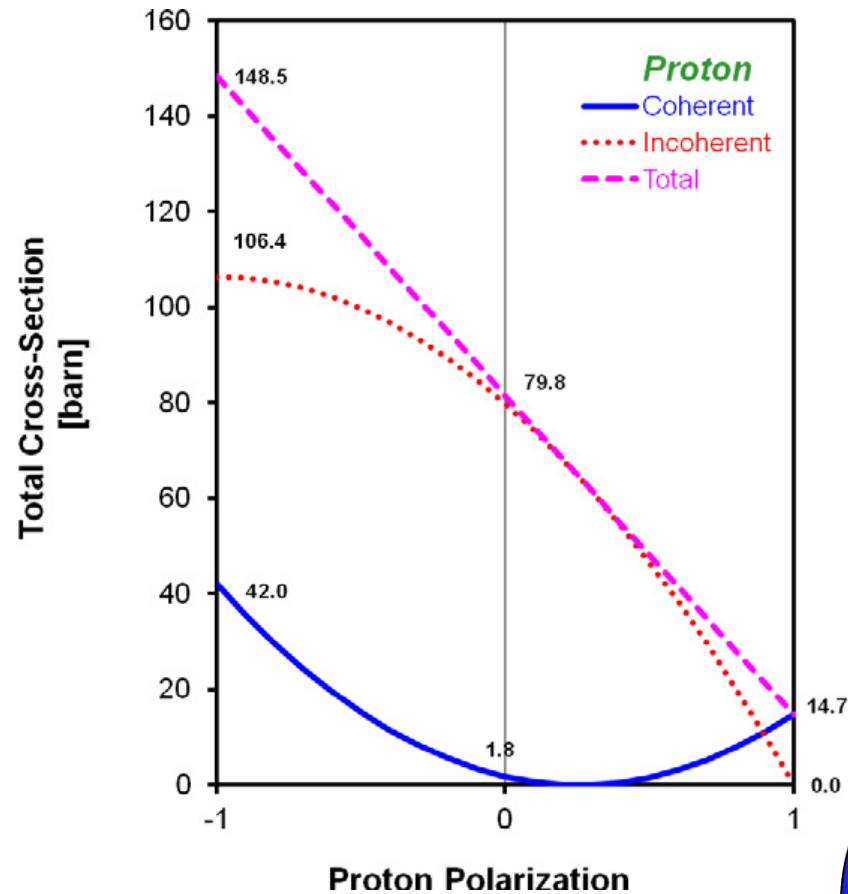
Strain-cell
OAK RIDGE
National Laboratory

BRaVE: DNP-IMAGINE-X - Accelerating drug discovery

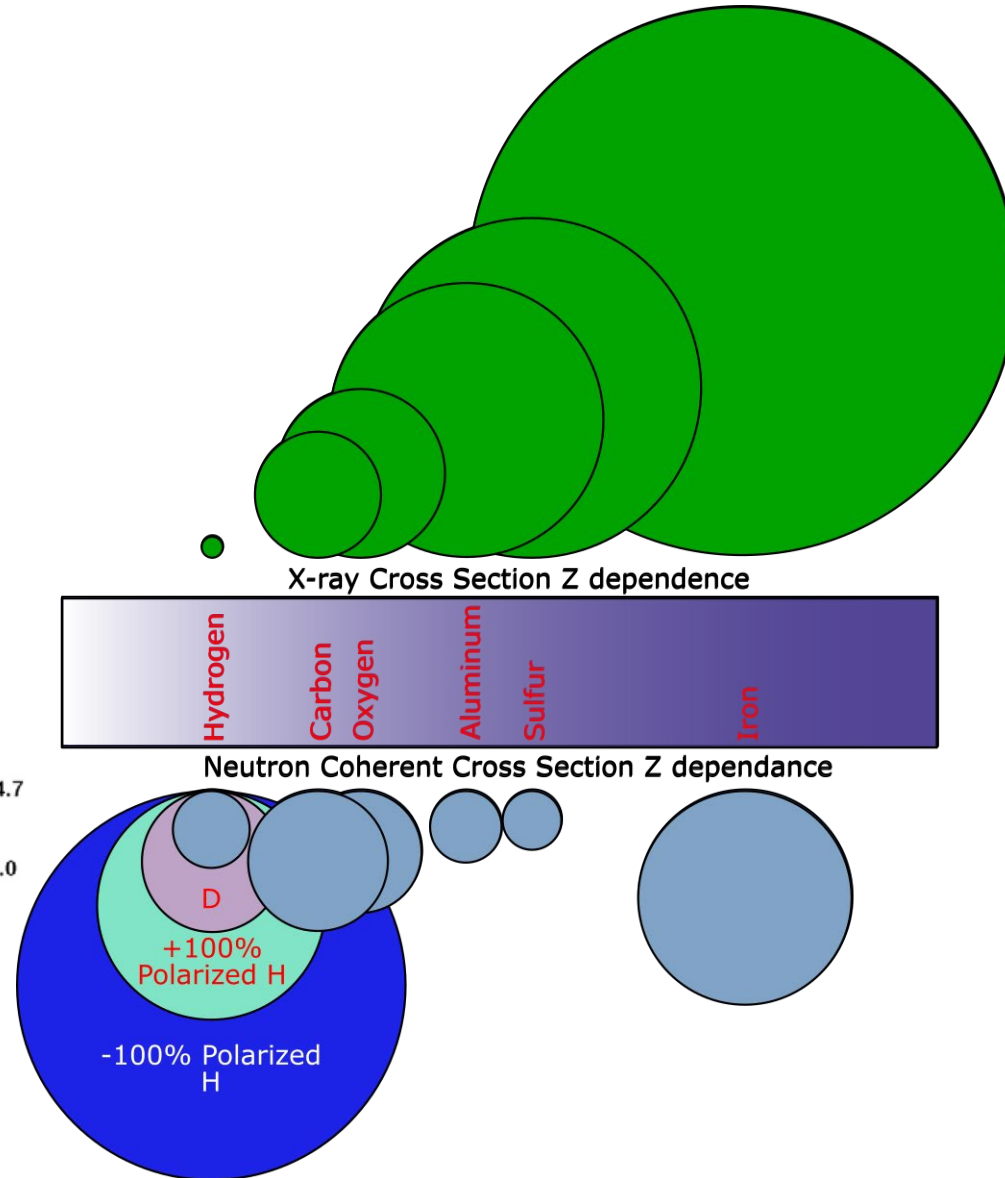
- New DNP system, detectors and polarizing optics on the imagine beamline at HFIR
 - Along with new computational tools and sample preparation protocols as part of a DOE BRAVE project
 - Amplifying the diffracted intensity and minimizing incoherent scattering background
 - Measure radically smaller crystals ($< 0.01 \text{ mm}^3$) of ANY hydrogenated proteins
- Partnering with:
 - OLCF - Building a "Digital Twin" with machine learning toolsets to simulate and guide experiments
 - Meharry Medical College/Fisk U (& HBCU Consortium for Structural Biology) – Optimizing samples
 - Argonne APS & SLAC SSRL - Coupling neutrons to drug discovery pipelines
- **Funded in 2023 - Commissioning began late 2025**
- **Goal of x50 in data collection**



Spin Dependence of Neutron Scattering



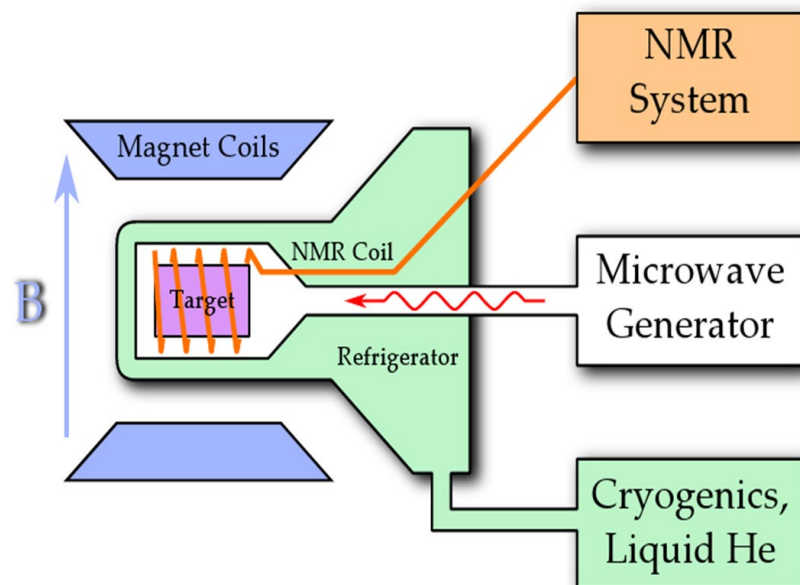
Coherent, incoherent and total scattering cross section of hydrogen as a function of the proton polarization for fully polarized neutrons. (JK Zhao et al., 2013)



Dynamic Nuclear Polarization - DNP

- Produces very high nuclear polarization in samples by using a combination of:

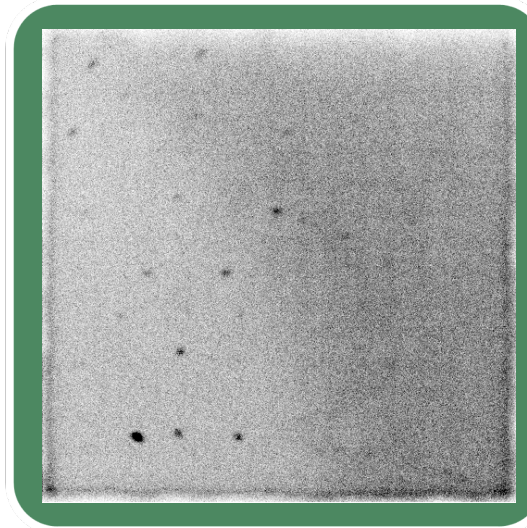
- High Magnetic field
 - Superconducting magnets – 5T or 2.5T being the most common
- Low Temperature
 - 100mk using a dilution refrigerator
- Microwaves
 - Near the electron Larmor frequency
- Prepared sample material
- NMR system for polarization measurement



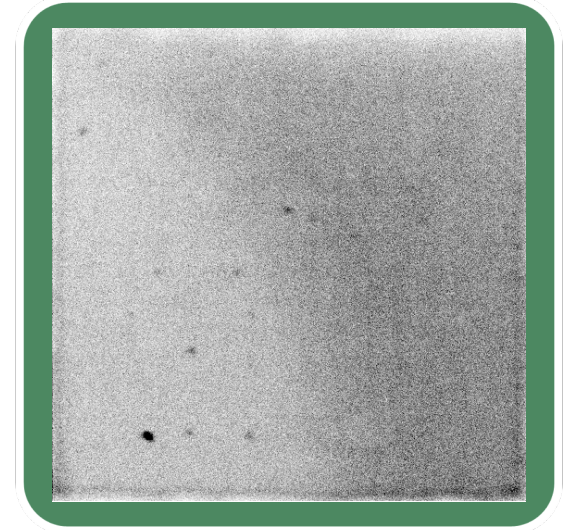
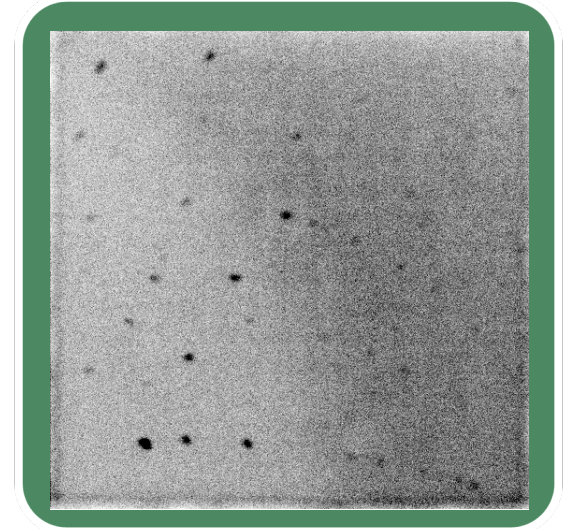
DNP Modulated Diffraction

- T4 Lysozyme Results
- Doped with TEMPO (10-100mM)
- Large crystals
 - ~0.9 mm on edge
- Single prototype anger camera
- Short hold times in “frozen spin” mode
 - ~120-240 min T_1
 - Low temperatures
 - ~200 mK
- DNP modulated diffraction
- **Enhancements of 200-300% in integrated diffraction pattern for anti-aligned spins**
 - The enhancement of individual reflections varies depending on the relative contribution of hydrogen
- Consistent with maximum polarizations of around 50%

Unpolarized



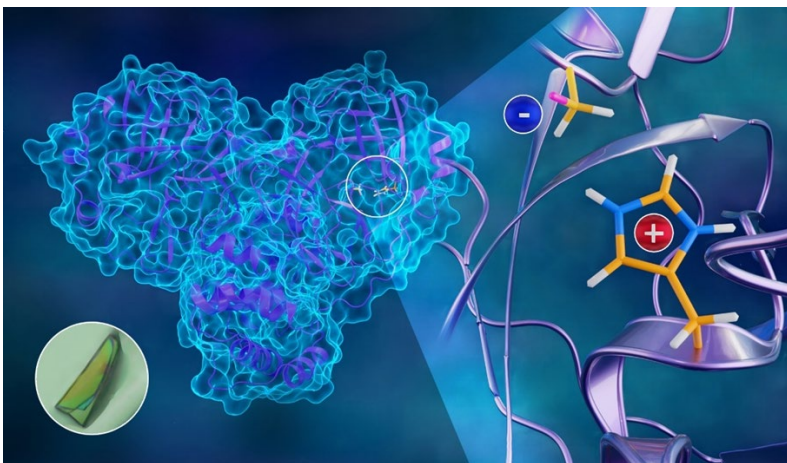
Anti-aligned



Aligned

Why - Chemistry & electrostatics: drug binding & design

Mapping hydrogen atoms in SARS-CoV-2 main protease (3CL Mpro)

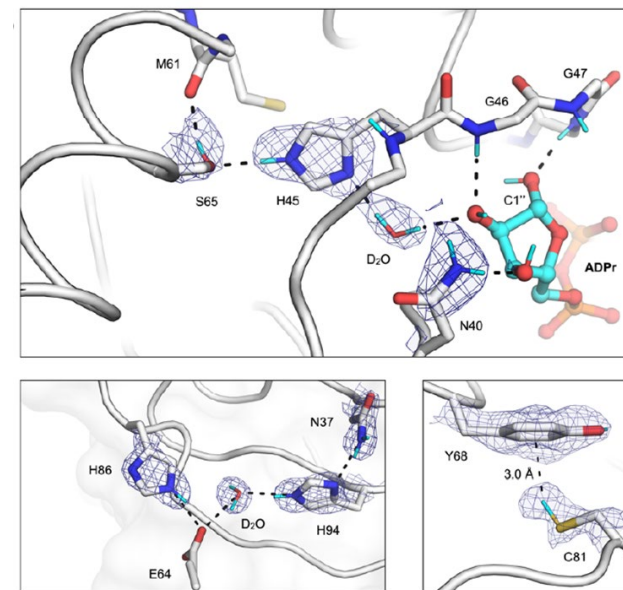


Research Details

- Neutron crystallography directly visualized the hydrogen bonding and protonation states of all ionizable amino acid residues in the from SARS-CoV-2
- Structure shows that the catalytic dyad adopts a zwitterionic charge-separated reactive state, details important for computational drug design.

D.W. Kneller, (2020) J. Biol. Chem.

Neutron structures of SARS-CoV-2 macrodomain guide design of novel antivirals



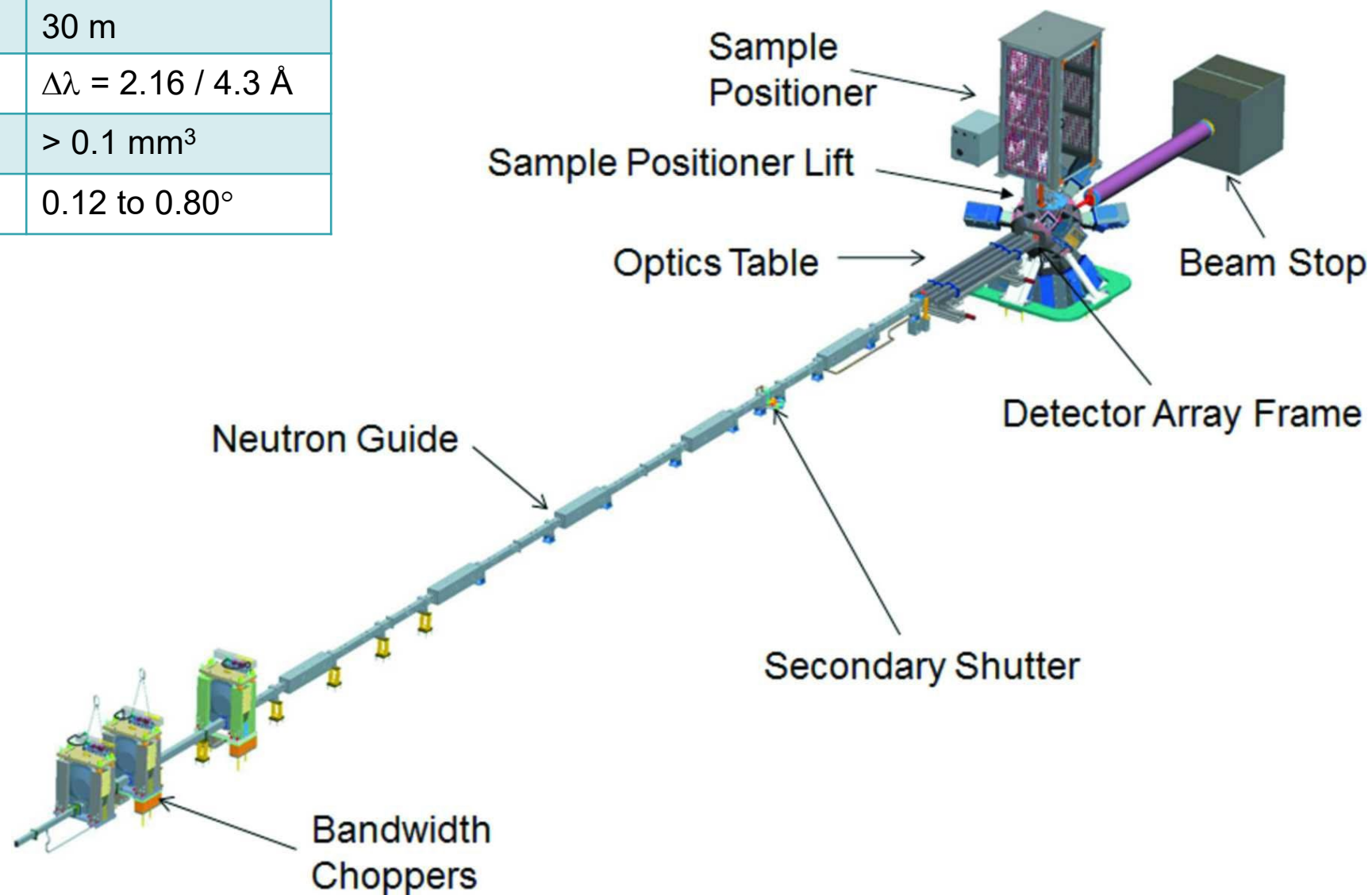
Research Details

- Determined the protonation states of Mac1 residues that control catalytic activity.
- Clarified H-bond networks that govern protein flexibility
- Re-evaluated the catalytic mechanism of Mac1
- Informed the design of new Mac1 inhibitors

G.J. Correy et al. (2022) *Science Advances*.

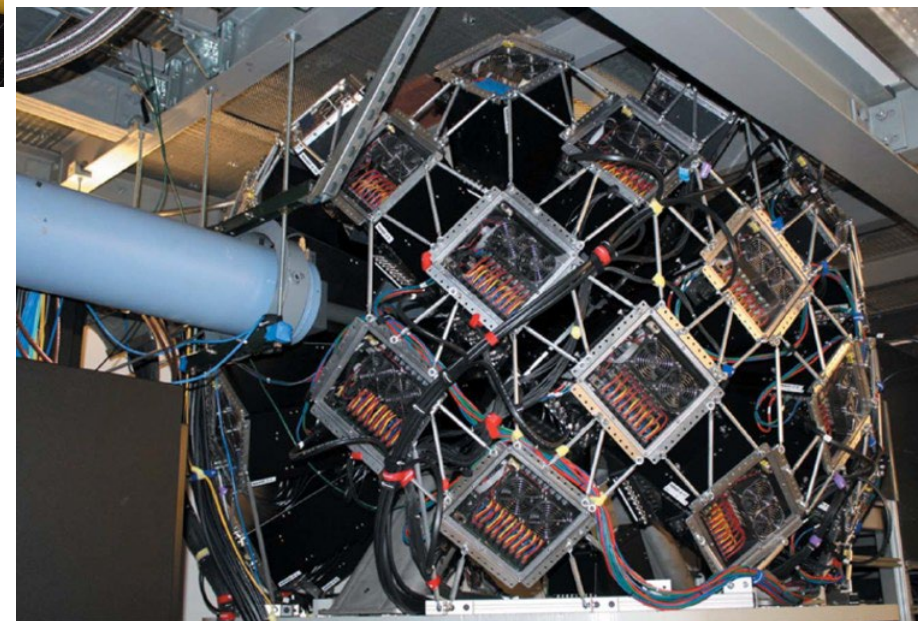
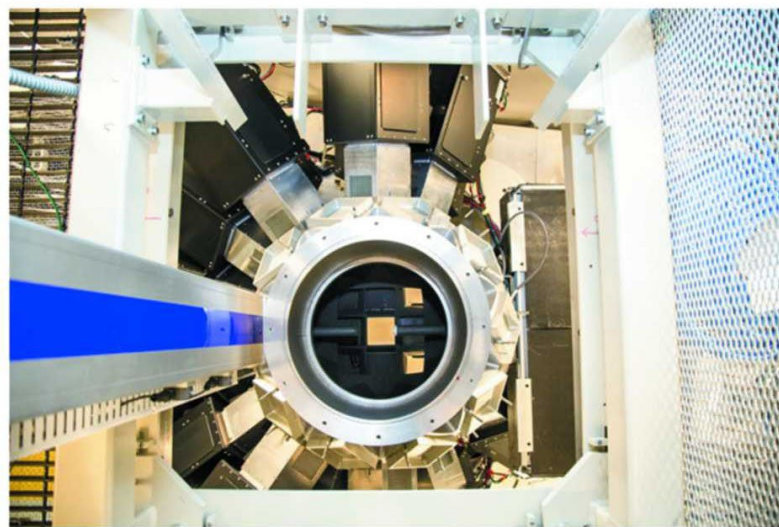
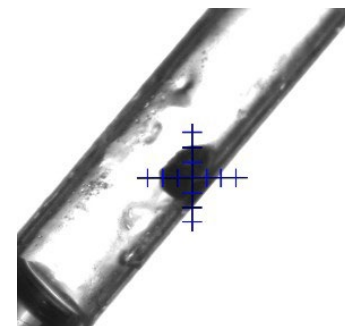
Beamline BL11B: **Macromolecular Neutron Diffractometer**

Source-to-sample distance	30 m
Wavelength bandwidth	$\Delta\lambda = 2.16 / 4.3 \text{ \AA}$
Sample size	$> 0.1 \text{ mm}^3$
Divergence	0.12 to 0.80°

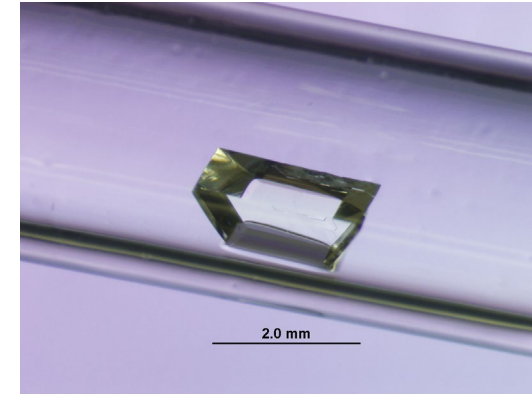
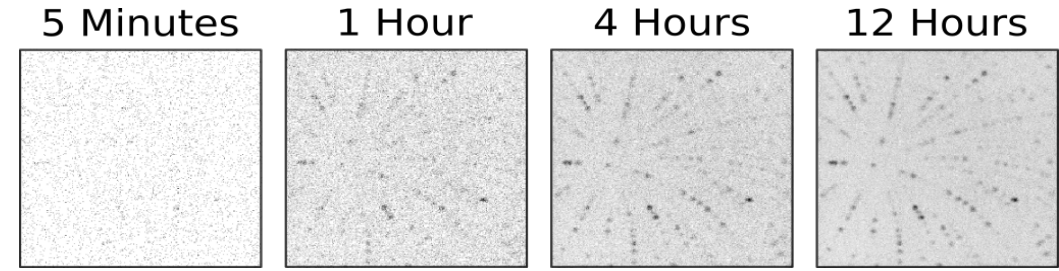
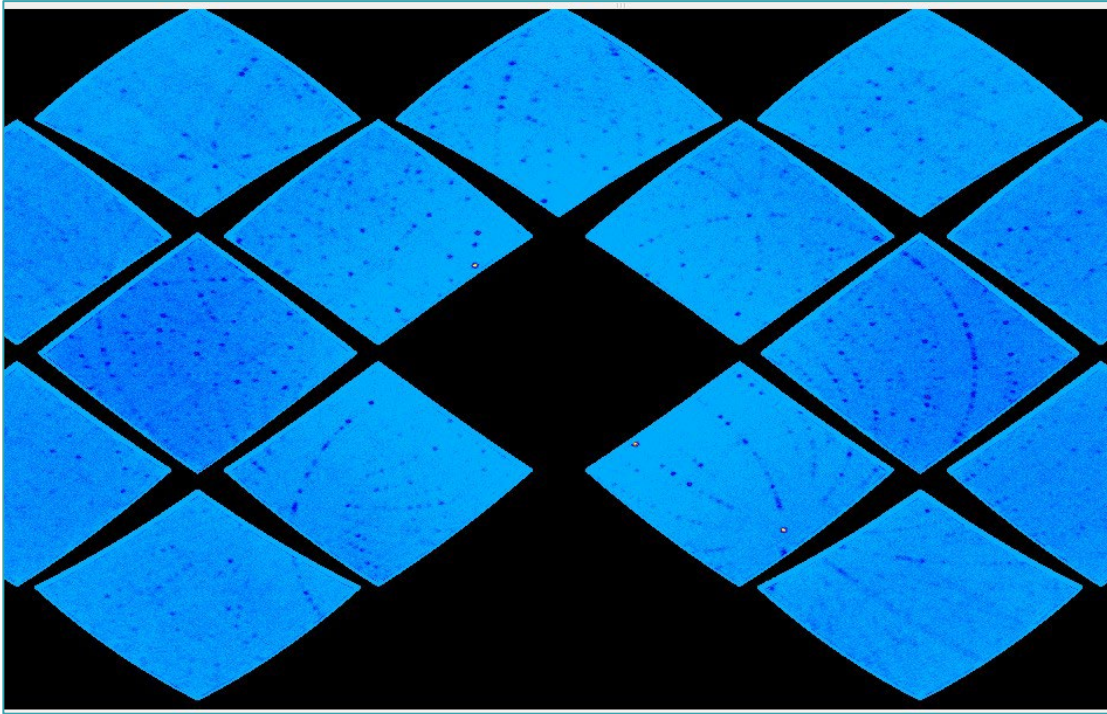


Beamline BL11B: Macromolecular Neutron Diffractometer

Sample-to-detector distance	39-45 cm
Angular detector coverage	4.1 sr (40 detectors)
Detector angles	20-160°
Sample env.	RT, cryo



MaNDi instrument Overview



- MaNDi is a diffractometer designed to study protein crystals
- It can collect data from unit cell up to 300Å on edge
- Neutrons are not damaging so most data collection is at room temperature

Thank you!

