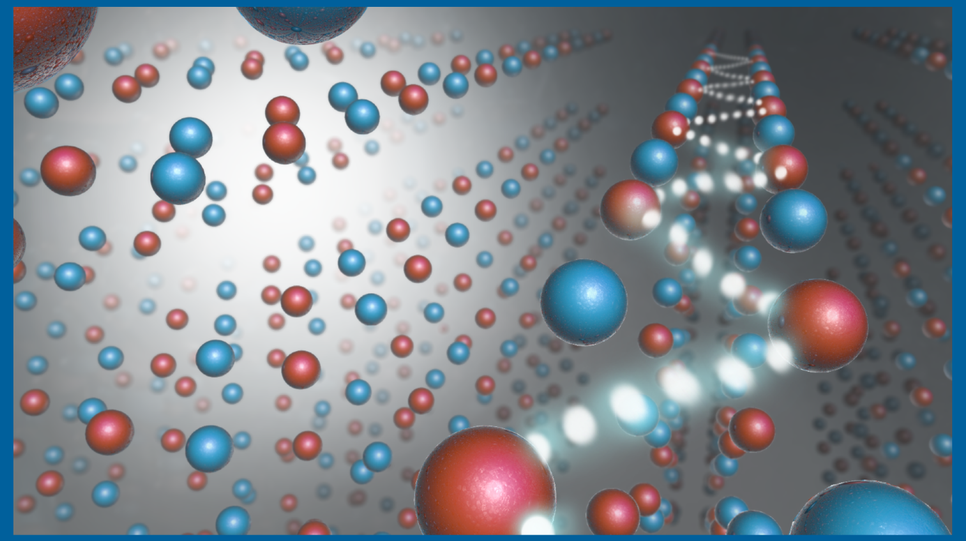
SINGLE CRYSTAL DIFFUSE SCATTERING



RAYMOND OSBORN
Neutron & X-ray Scattering Group
Materials Science Division

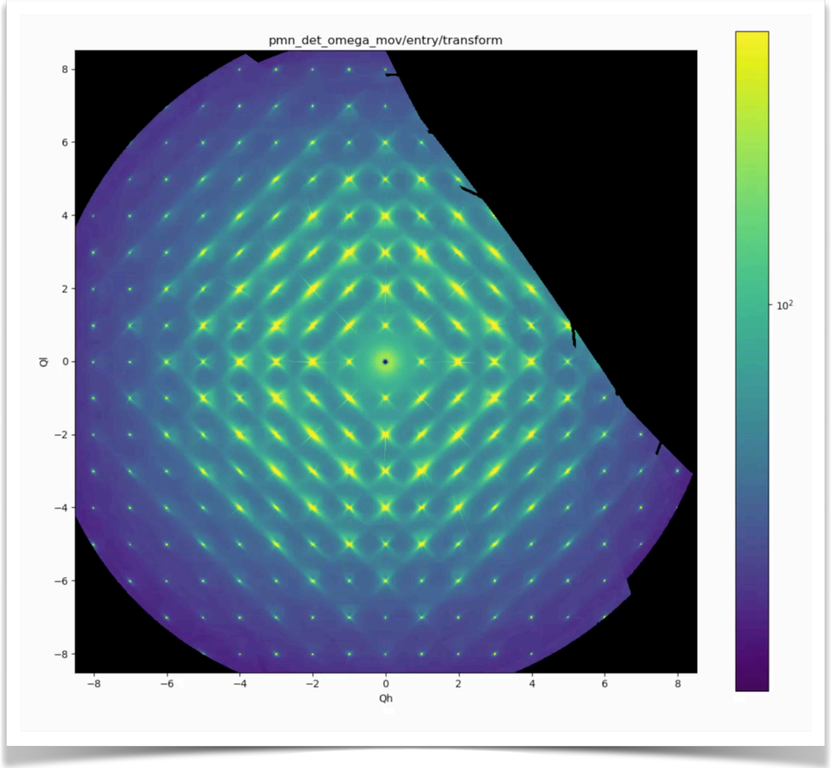
Acknowledgements: Stephan Rosenkranz and Matthew Krogstad

Work supported by the U.S. Department of Energy,
Office of Science, Materials Sciences and Engineering Division.

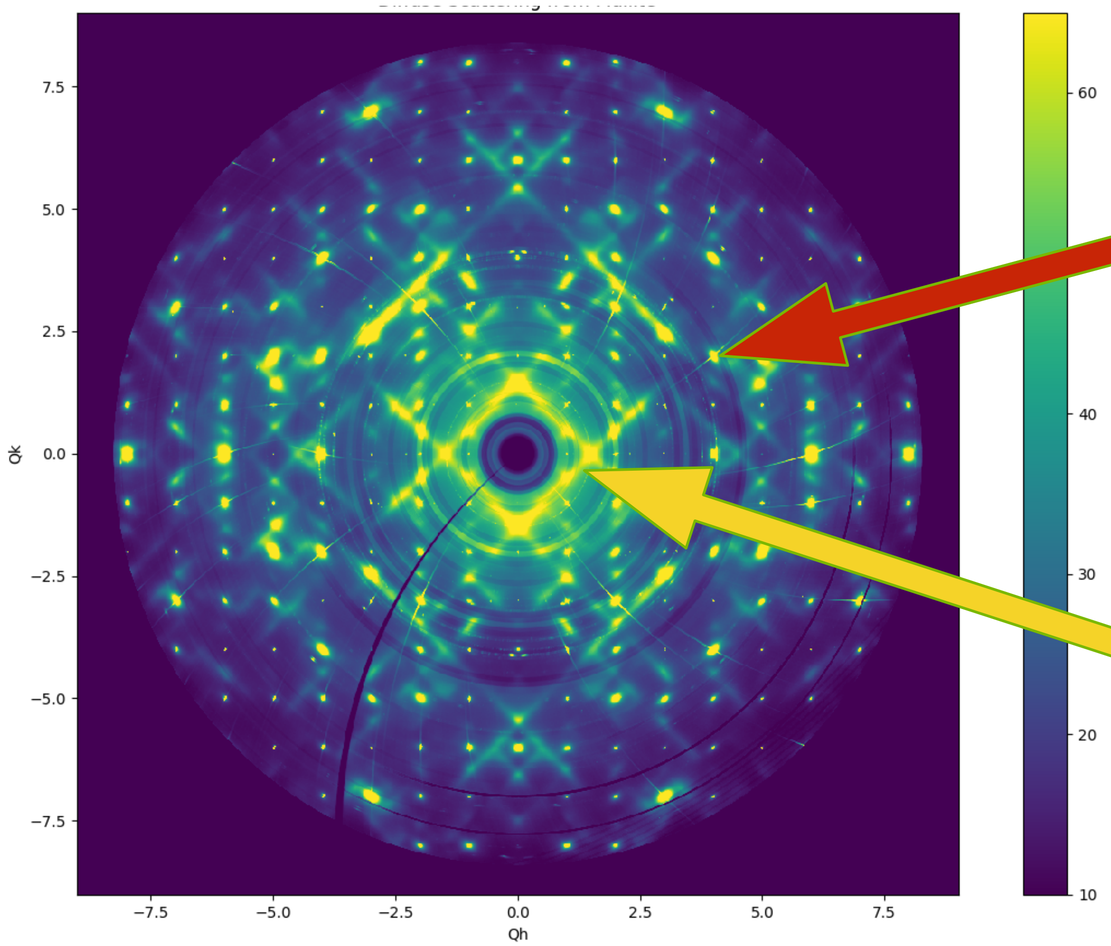
Neutron & X-ray School
August 6, 2024

OUTLINE

- What is diffuse scattering?
  - What causes it?
- What is it good for?
  - A random walk through disordered materials
- How do I model it?
  - A few equations
- How do I measure it?
- Case Study 1: Diffuse scattering from vacancies in mullite
- Case Study 2: 3D-ΔPDF in sodium-intercalated V_2O_5
- How do I look at static disorder?
  - Diffuse scattering with elastic discrimination



WHAT IS DIFFUSE SCATTERING?



Bragg Scattering
Average Structure

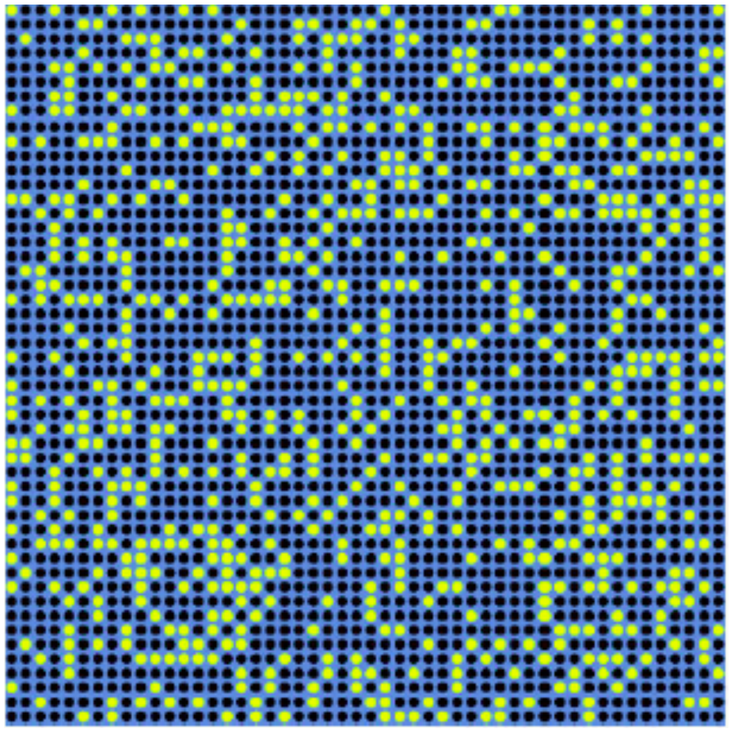
Diffuse Scattering
Deviations from the Average Structure

DIFFUSE SCATTERING

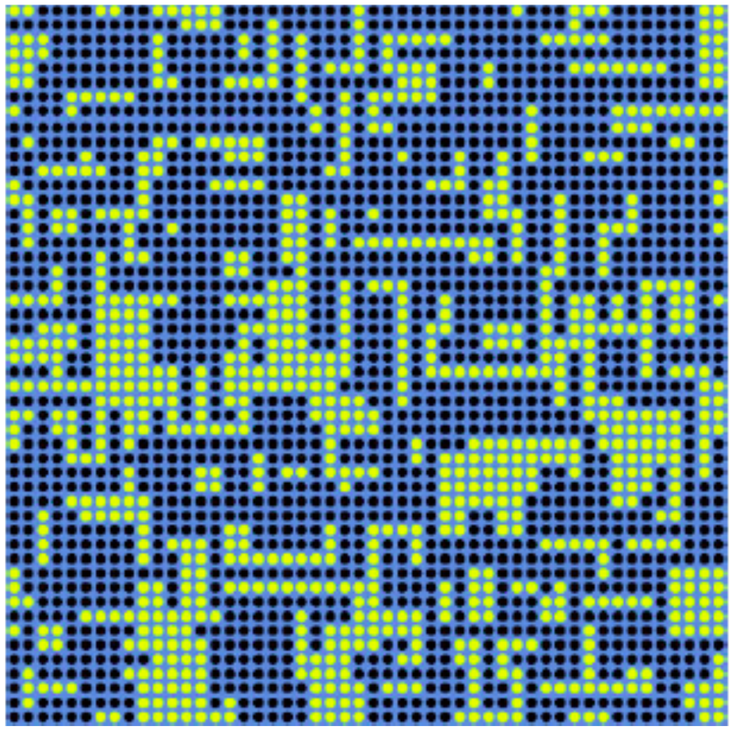
SIMPLE EXAMPLE OF DISORDER

Replace 30% of atoms (blue dots) by vacancies (green dots)

Random Vacancies



Vacancy Clusters

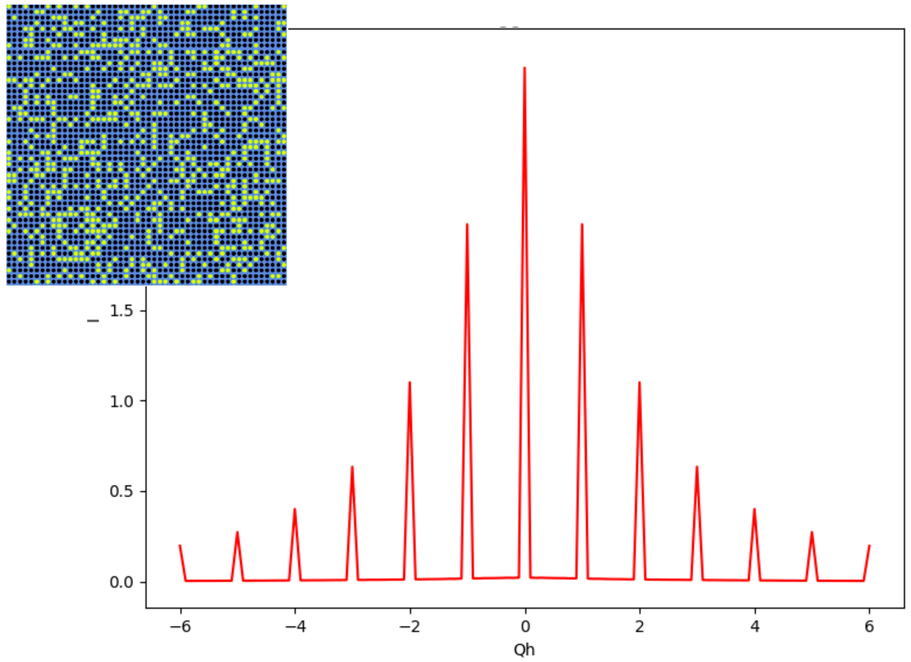


Model due to Thomas Proffen

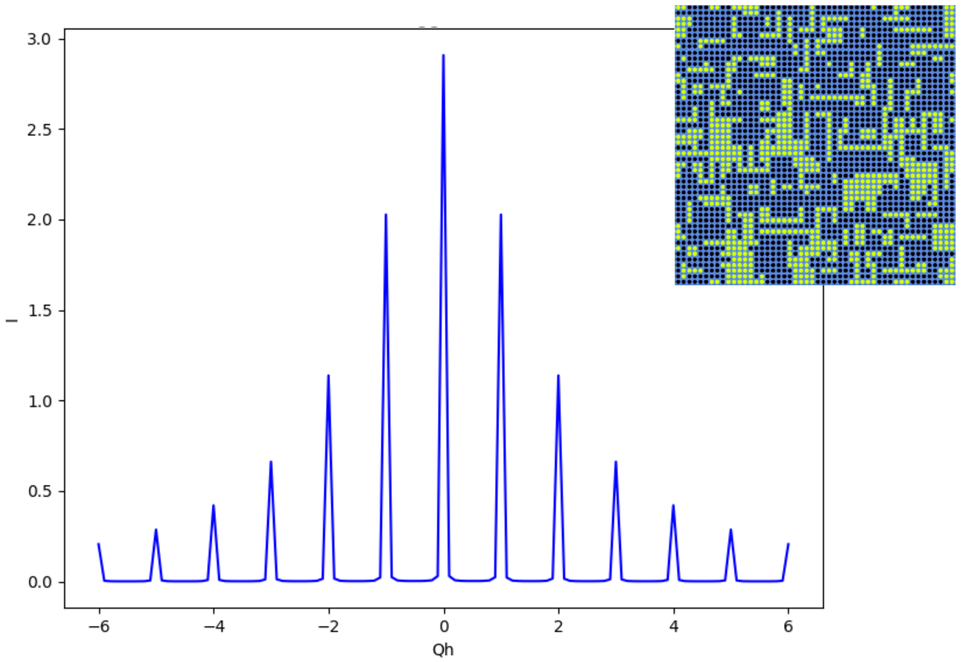
BRAGG SCATTERING

The average occupancy is unchanged ➡ Bragg peaks are identical

Random Vacancies



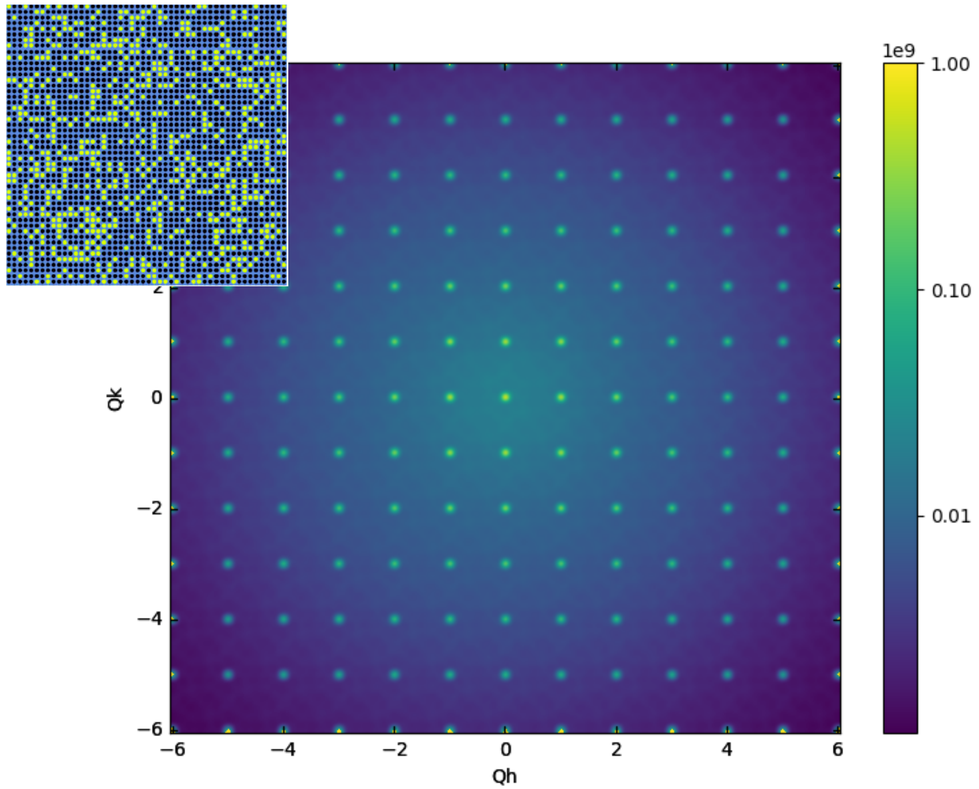
Vacancy Clusters



DIFFUSE SCATTERING

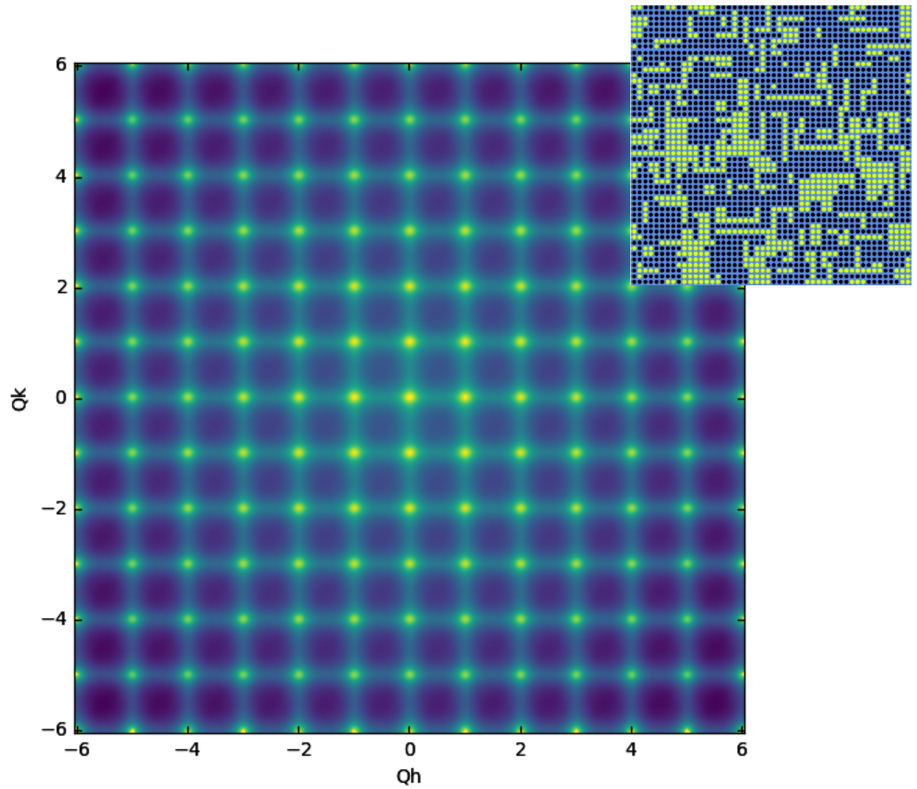
The diffuse scattering is quite different.

Random Vacancies



Laue Monotonic Scattering

Vacancy Clusters

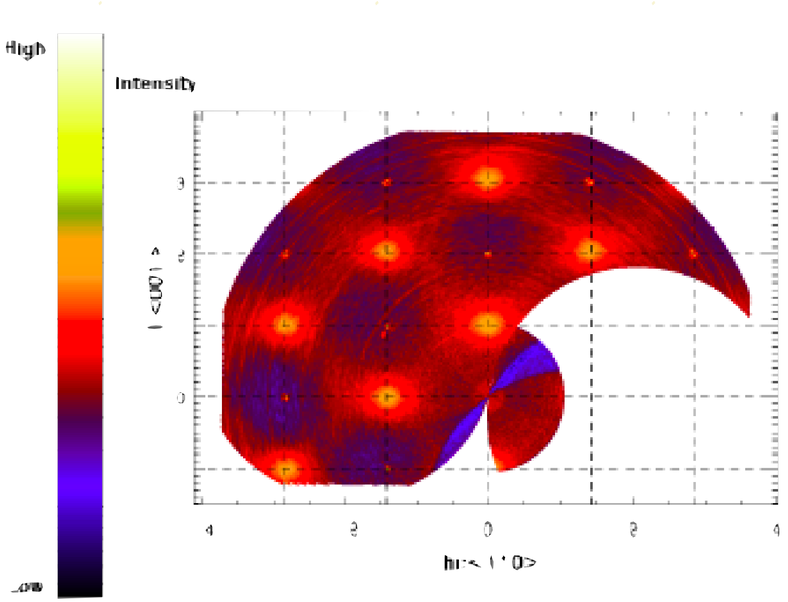


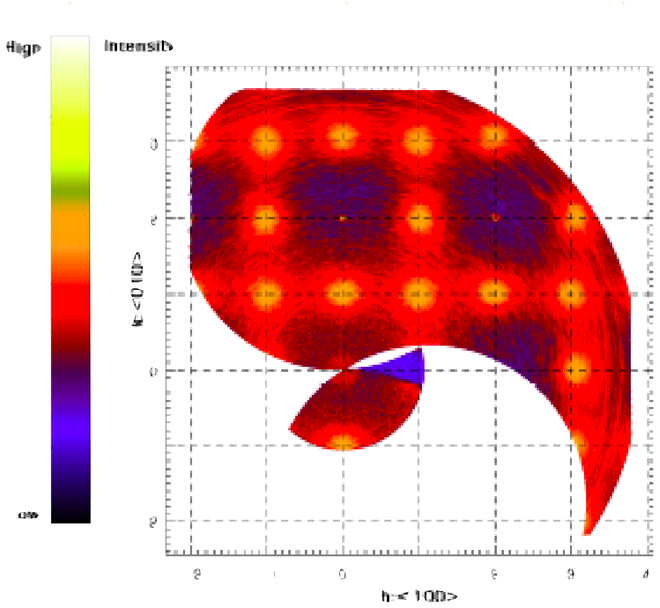
Substitutional Diffuse Scattering

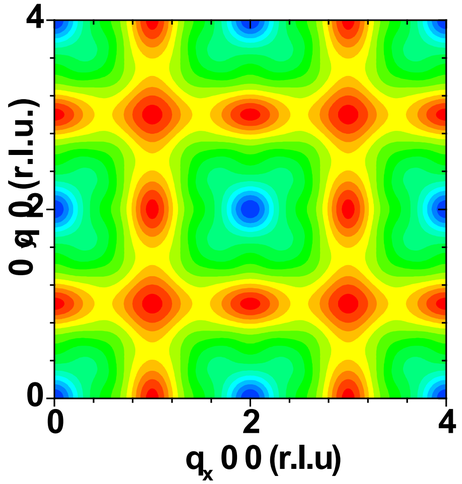
WHAT IS IT GOOD FOR?

DIFFUSE SCATTERING FROM METALLIC ALLOYS

Short-range Order in Null Matrix $^{62}Ni_{0.52}Pt_{0.52}$



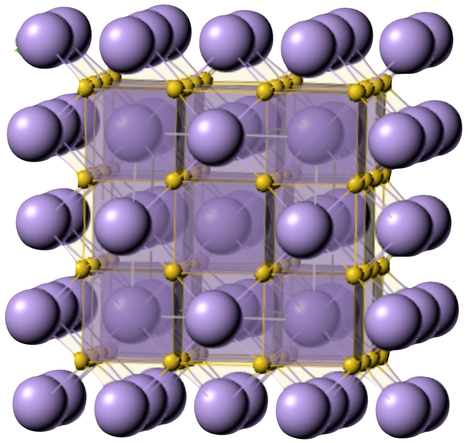




J. A. Rodriguez, *et al*., Phys. Rev. B **74**, 104115

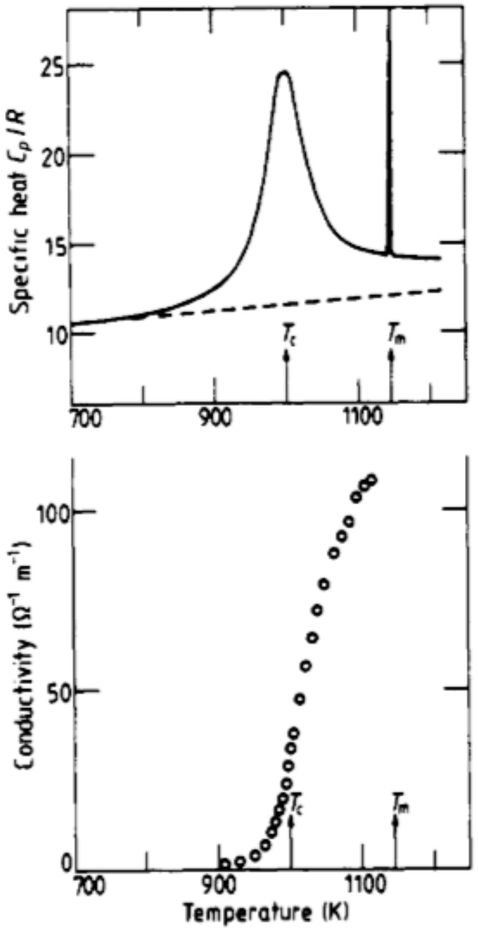
DIFFUSE SCATTERING FROM A FAST-ION CONDUCTOR

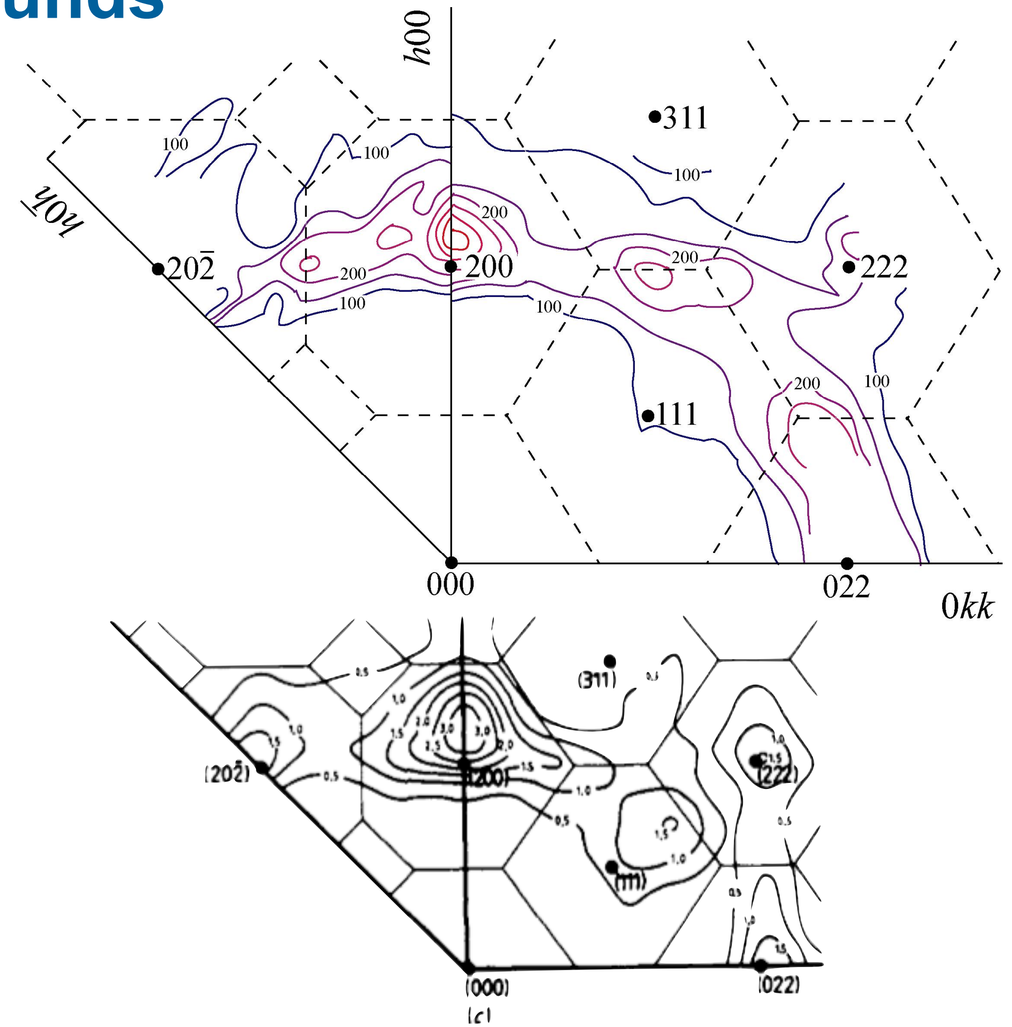
Sublattice Melting in Fluorite Compounds



CaF_2

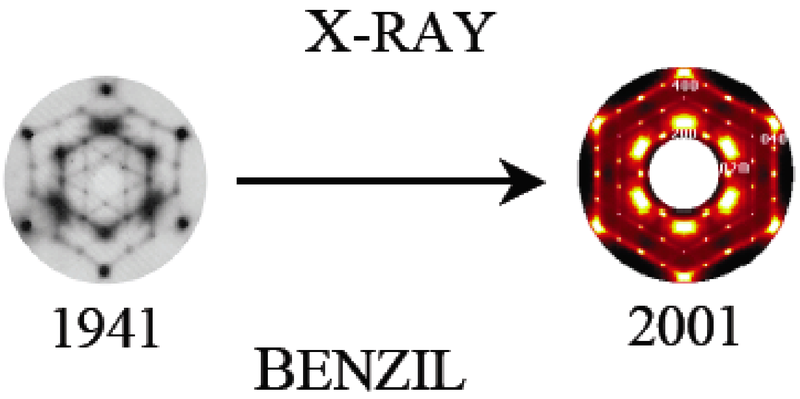
M. T. Hutchings *et al*
J. Phys. C **17**, 3903 (1984)

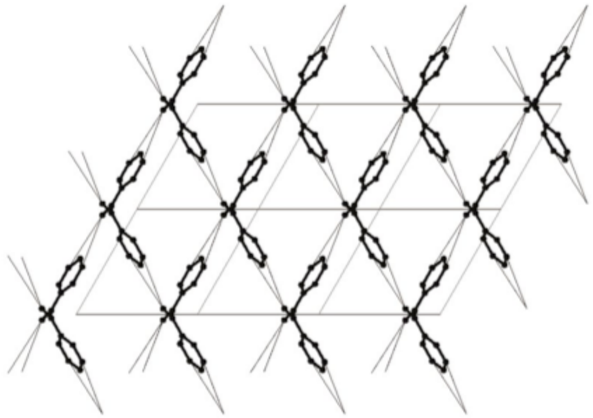


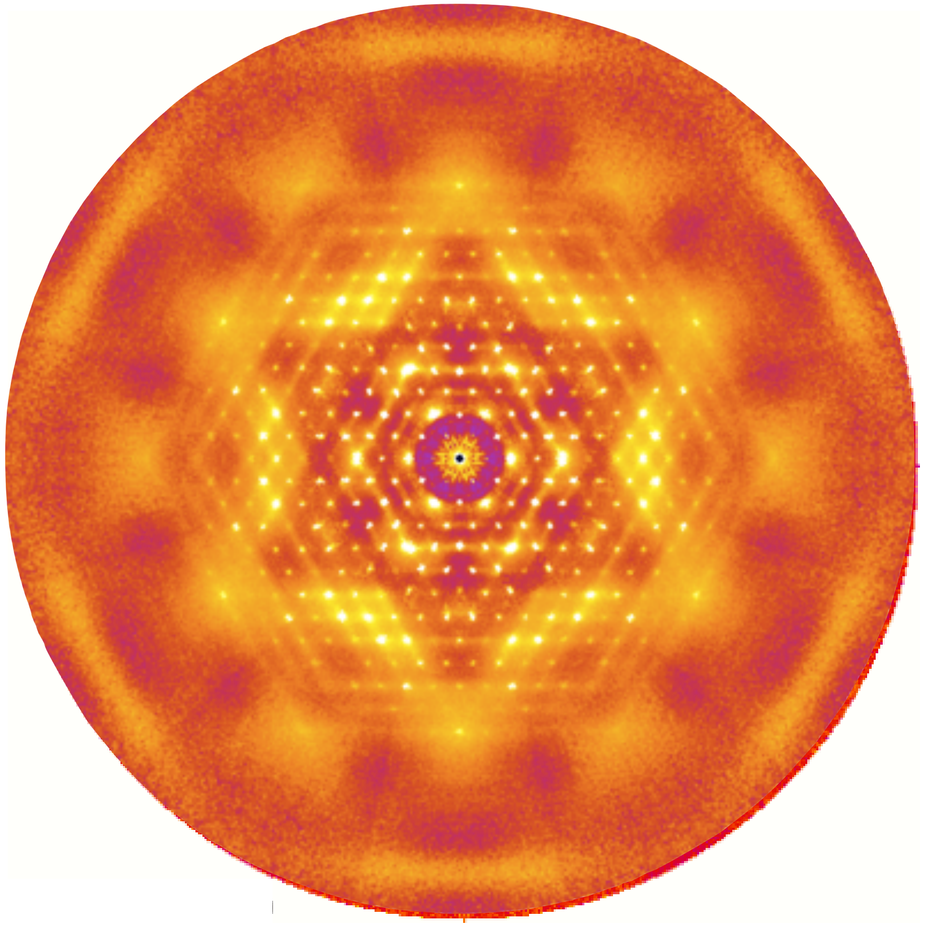


DIFFUSE SCATTERING FROM MOLECULAR SOLIDS

Molecular Flexibility in Benzil

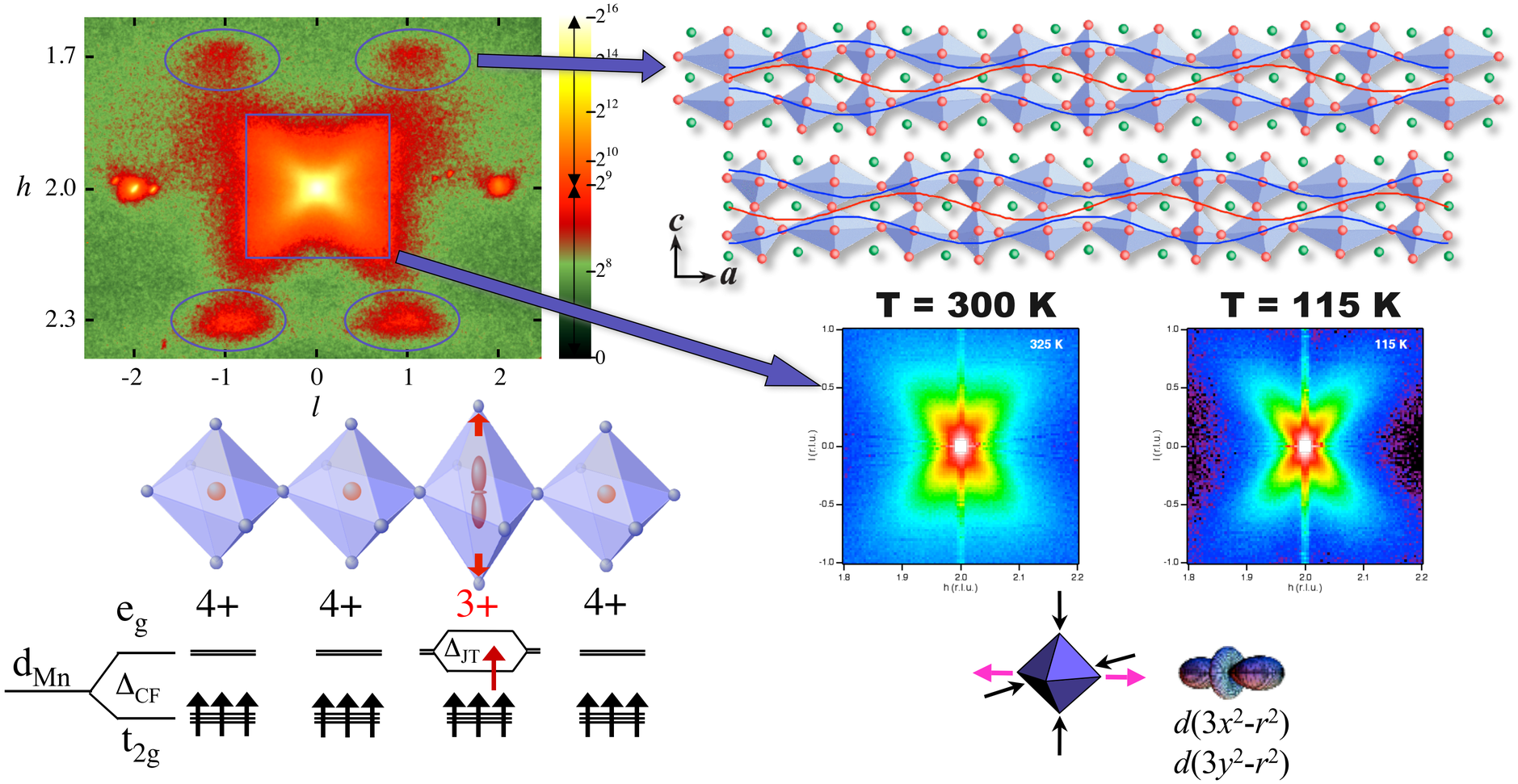






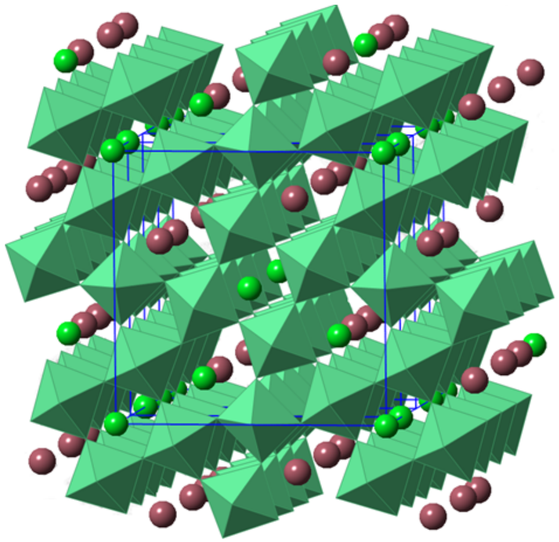
T. R. Welberry *et al* J. Appl. Cryst. **36**, 1400 (2003)

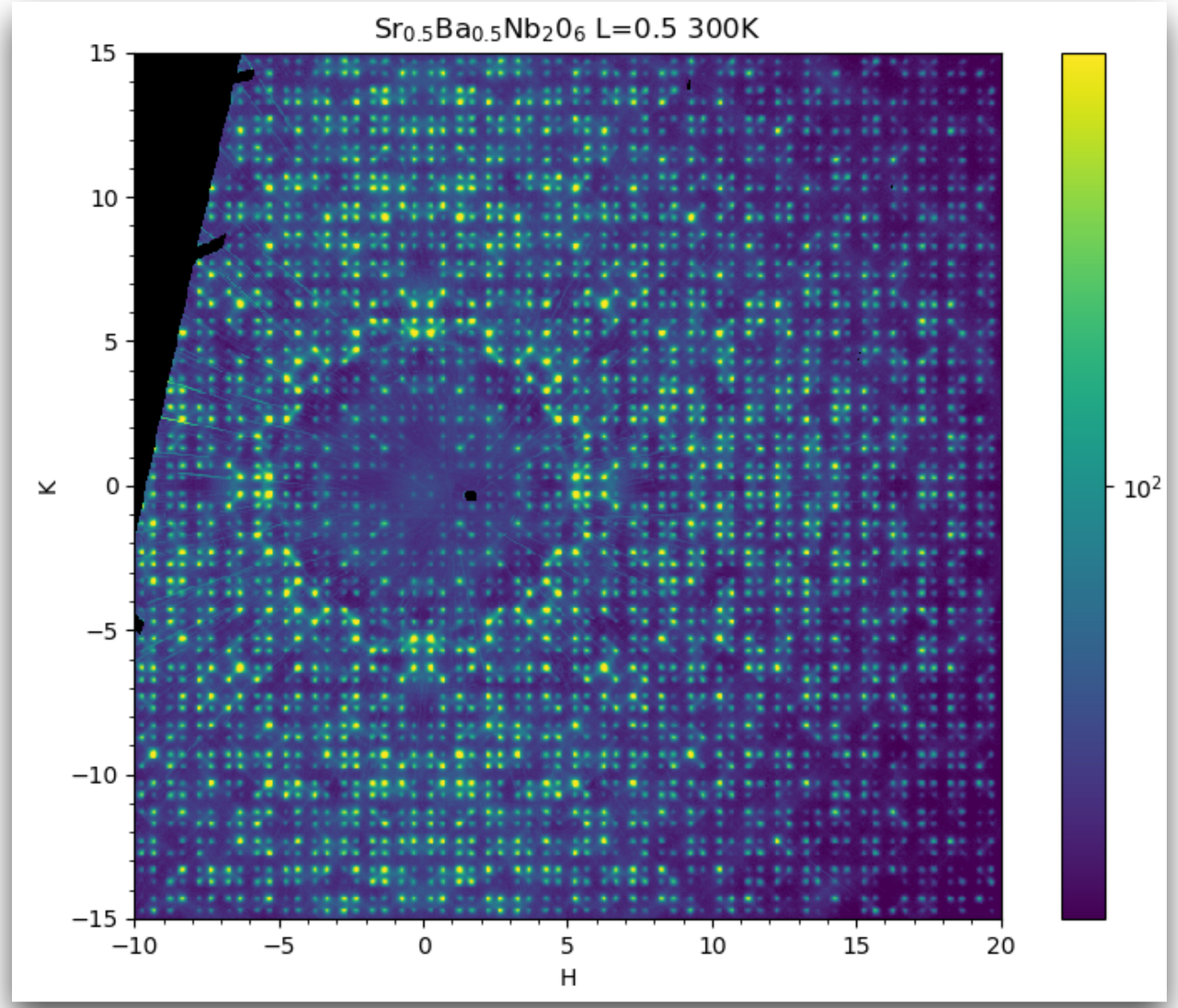
DIFFUSE SCATTERING FROM JAHN-TELLER POLARONS



B. J. Campbell, *et al*., Phys Rev B **65**, 014427 (2002).

INCOMMENSURATE MODULATIONS IN $Sr_{0.5}Ba_{0.5}NbO_6$

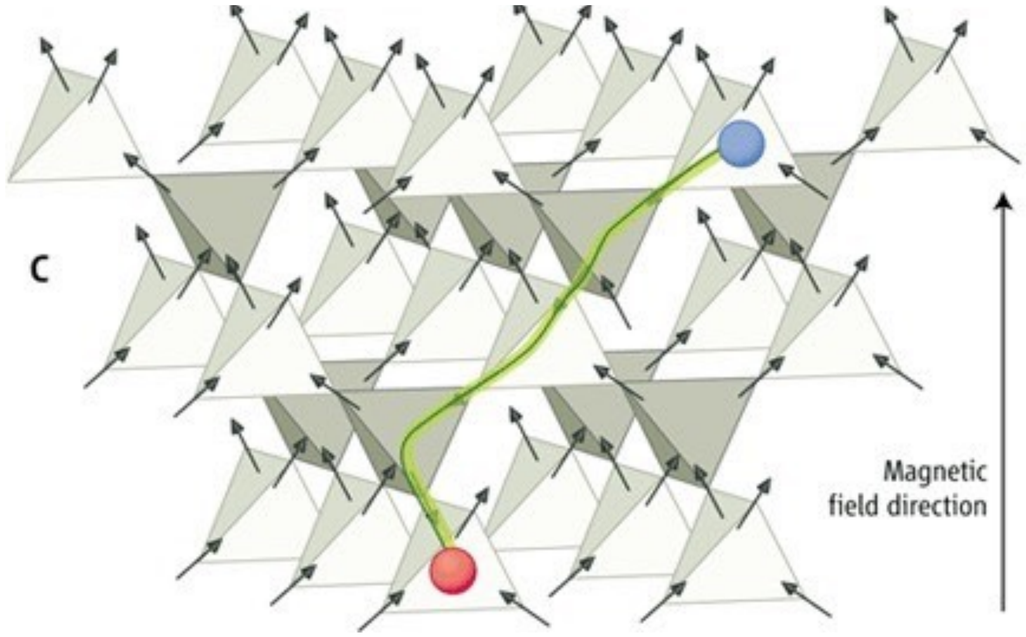


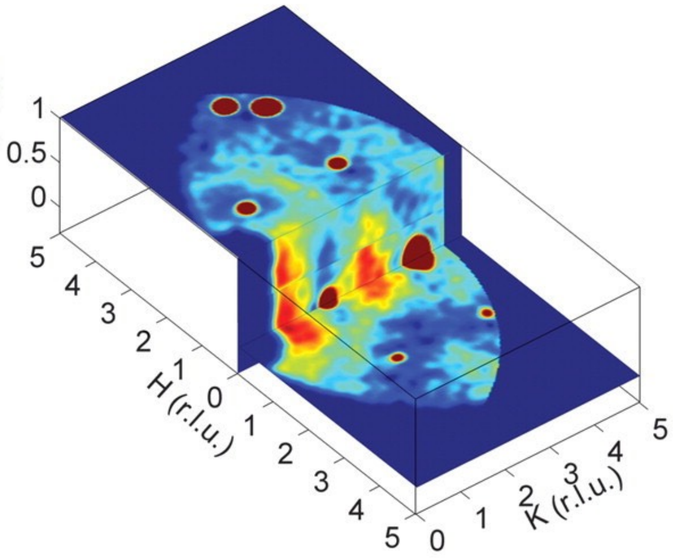


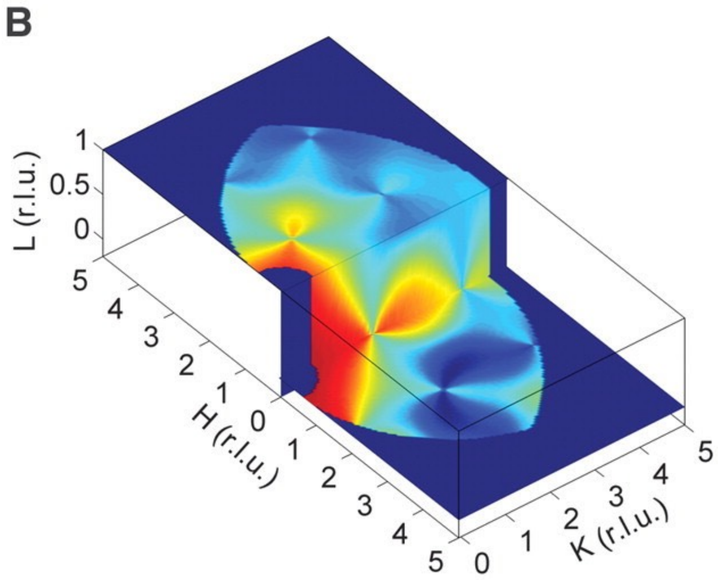
Acknowledgements:
Bixia Wang and Daniel Phelan

MAGNETIC MONOPOLES IN SPIN ICE

Diffuse Magnetic Scattering in $Dy_2Ti_2O_7$





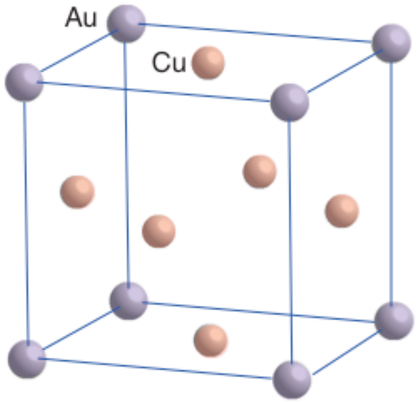


D. J. P. Morris, *et al*., Science **326**, 411 (2009).

HOW DO I MODEL IT?

DIFFUSE SCATTERING THEORY

A Few Equations $I = \sum_i \sum_j b_i b_j \exp(i\mathbf{Q} \cdot \mathbf{r}_{ij})$



J. M. Cowley, J. Appl. Phys. **21**, 24 (1950)

- **Laue Monotonic Diffuse Scattering**

$$I = \bar{b}^2 \sum_{ij} \exp(i\mathbf{Q} \cdot \mathbf{r}_{ij}) + N(\overline{b^2} - \bar{b}^2);\ \bar{b}^2 = (c_A b_A + c_B b_B)^2;\ \overline{b^2} = c_A c_B (b_B - b_A)^2$$

- **Cowley Short-Range Order**

$$I_{diffuse} = N c_A c_B (b_B - b_A)^2 + \textstyle\sum_{ij} \alpha_{ij} c_B c_A (b_B - b_A)^2 \exp(i\mathbf{Q} \cdot \mathbf{r}_{ij});\ \alpha_{ij} = \left(1 - \frac{P_{ij}}{c_j}\right)$$

- **Warren Size Effect**

$$I_{diffuse} = N c_A c_B (b_B - b_A)^2 \left(1 + \sum_{ij} \alpha_{ij} \exp(i\mathbf{Q} \cdot \mathbf{r}_{ij}) + \beta_{ij} \exp(i\mathbf{Q} \cdot \mathbf{r}_{ij})\right);\ \beta_{ij} = f(\epsilon_{AA}^{ij}, \epsilon_{BB}^{ij})$$

- **Borie and Sparks Correlations**

$$I = \sum_i \sum_j b_i b_j \exp\left(i\mathbf{Q} \cdot (\mathbf{R}_i - \mathbf{R}_j)\right) \left[1 + i\mathbf{Q} \cdot (\mathbf{u}_i - \mathbf{u}_j) - \frac{1}{2}\left(\mathbf{Q} \cdot (\mathbf{u}_i - \mathbf{u}_j)\right)^2 + \ldots\right]$$

V. M. Nield and D. A. Keen *Diffuse Neutron Scattering From Crystalline Materials* (2001)
T. R. Welberry *Diffuse X-ray Scattering and Models of Disorder* (2022)

SOME RULES OF THUMB

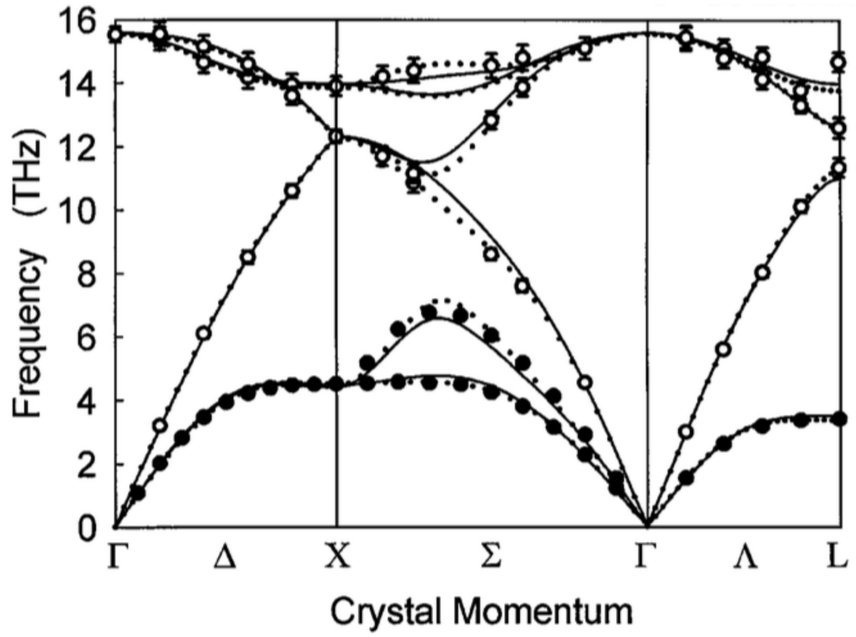
Acknowledgment: Hans Beat Bürgi

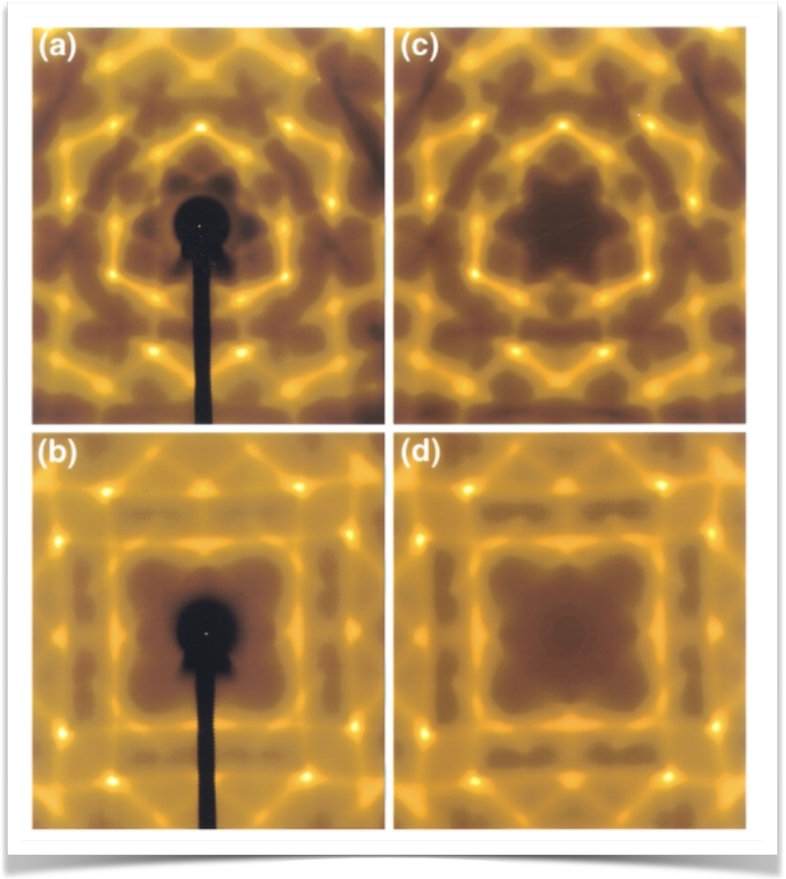
Reciprocal space		Direct space
▪ Sharp Bragg reflections	→	▪ 3D-periodic structure
– no defects		– no defects
▪ Sharp diffuse rods	→	▪ 2D-periodic structure
– no defects		– perpendicular to the streaks
		– disordered in streak directions
▪ Sharp diffuse planes	→	▪ 1D-periodic structure
– no defects		– perpendicular to the planes
		– disordered within the plane
▪ Diffuse clouds	→	▪ 0D-periodic structure
– no defects		– no fully ordered direction

THERMAL DIFFUSE SCATTERING

M. Holt, *et al*, Phys Rev Lett **83**, 3317 (1999).

- Lattice vibrations produce deviations from the average structure even in perfect crystals
- X-ray scattering intensity is given by the integral over all the phonon branches at each Q





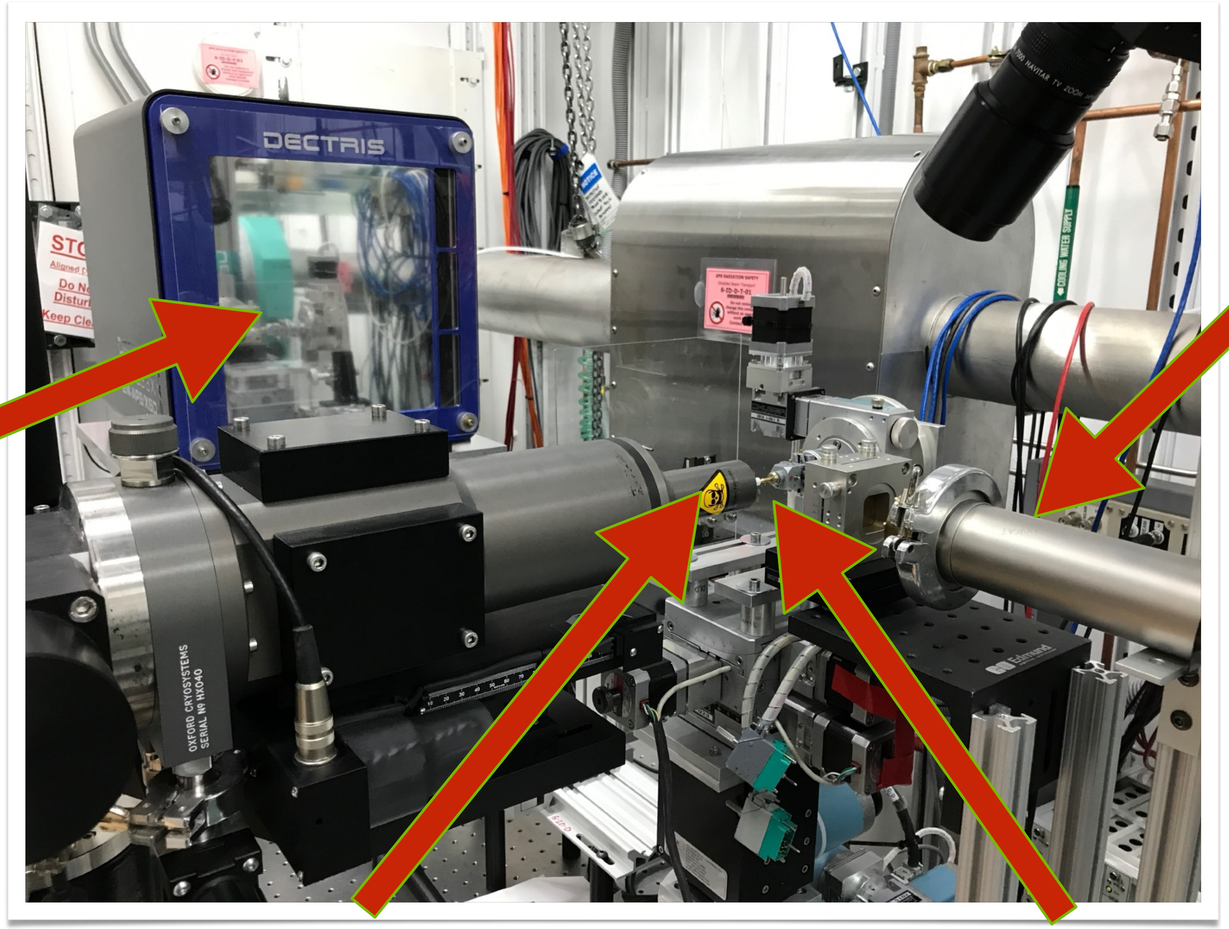
$$I_0 \propto f^2 e^{-2M} \sum_{j=1}^{6} \frac{|\mathbf{q} \cdot \hat{\mathbf{e}}_j|^2}{\omega_j} \coth\left(\frac{\hbar\omega_j}{2k_B T}\right).$$

HOW DO I MEASURE IT?

MEASURING X-RAY DIFFUSE SCATTERING

Continuous Rotation Method

Sector 6 - APS



Incident Beam

Detector

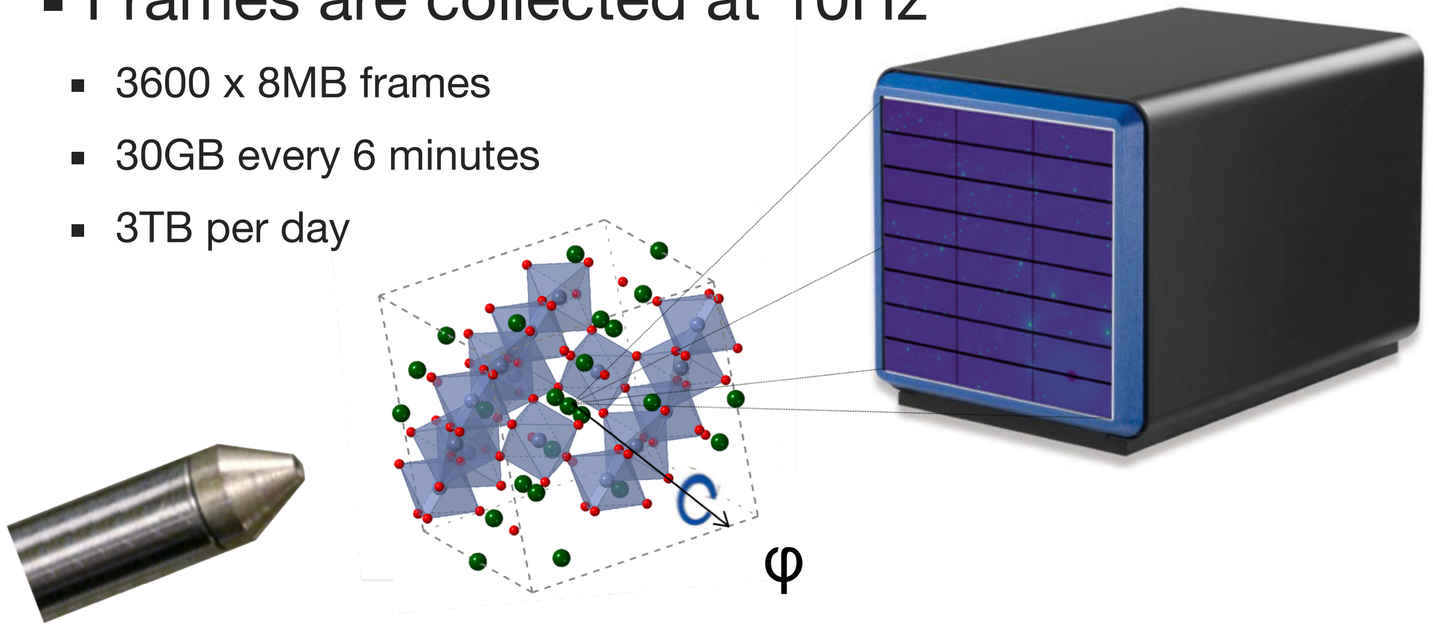
Cryocooler

Sample

X-RAY SCATTERING GEOMETRY

Continuous Rotation Method

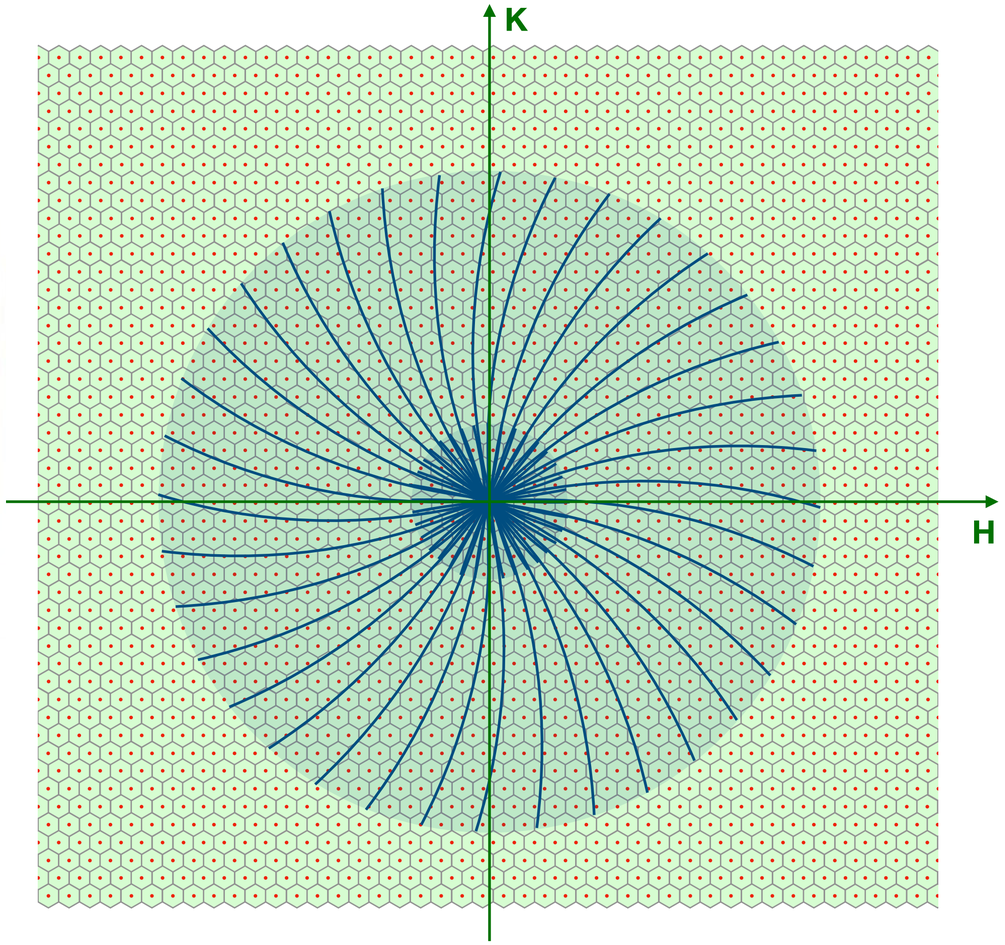
- The sample is continuously rotated at $1°s^{-1}$
- Frames are collected at 10Hz
  - 3600 x 8MB frames
  - 30GB every 6 minutes
  - 3TB per day



Incident Beam

Sample

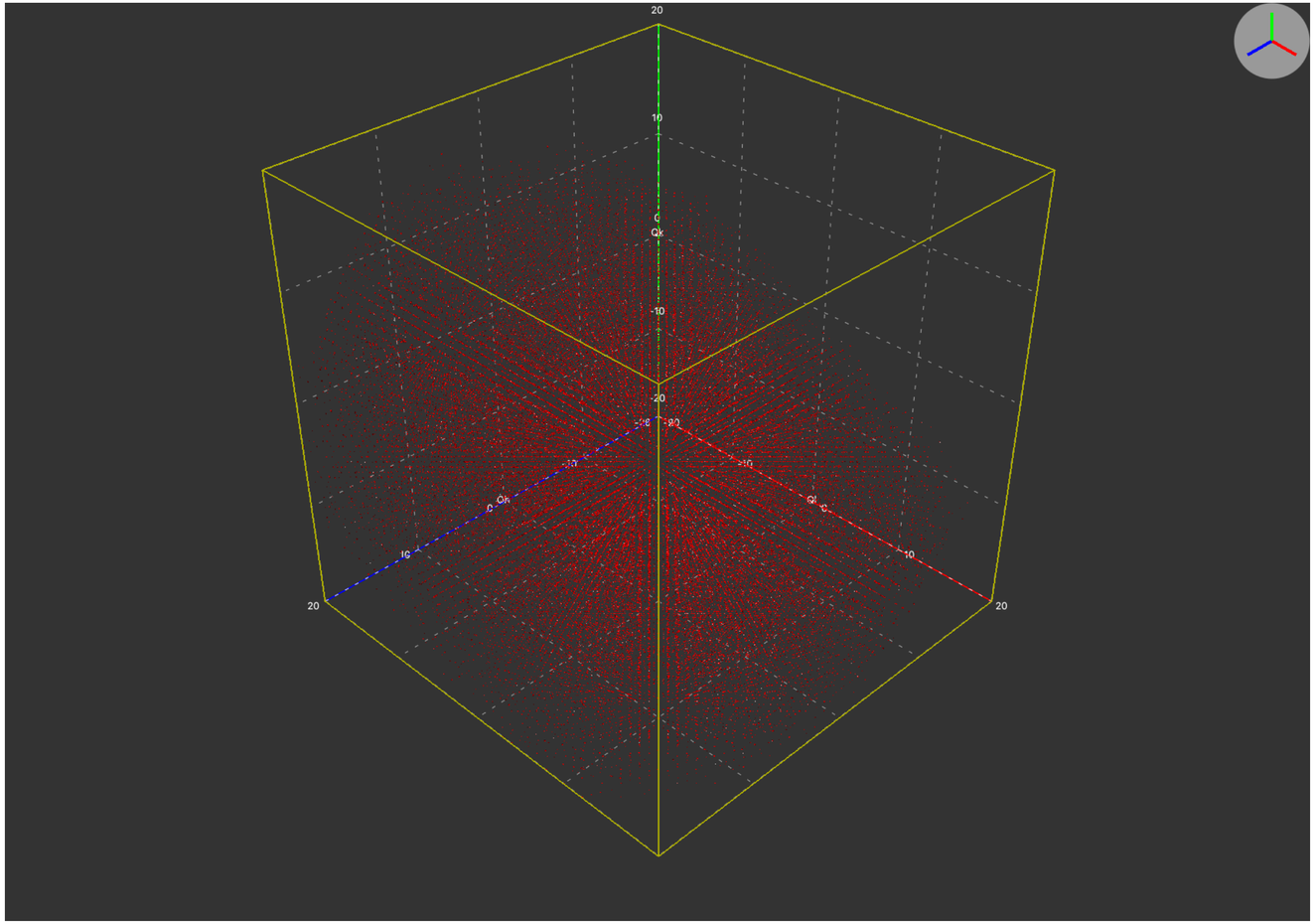
Pilatus 2M CdTe Detector



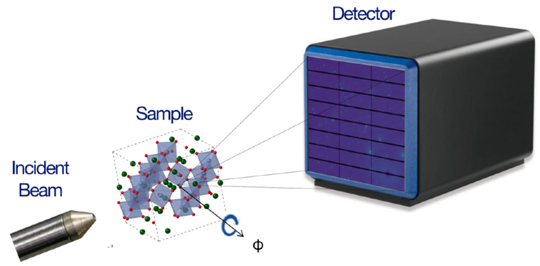
Reciprocal Space

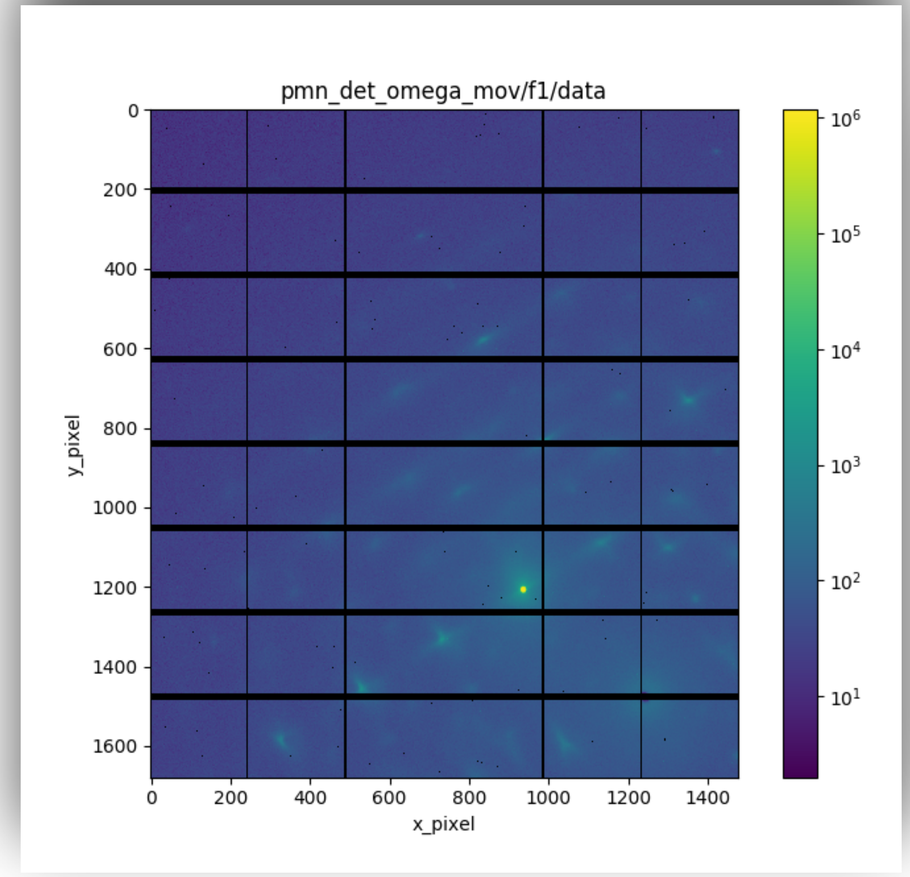
Q-RANGE IN ROTATION METHOD ON SECTOR 6

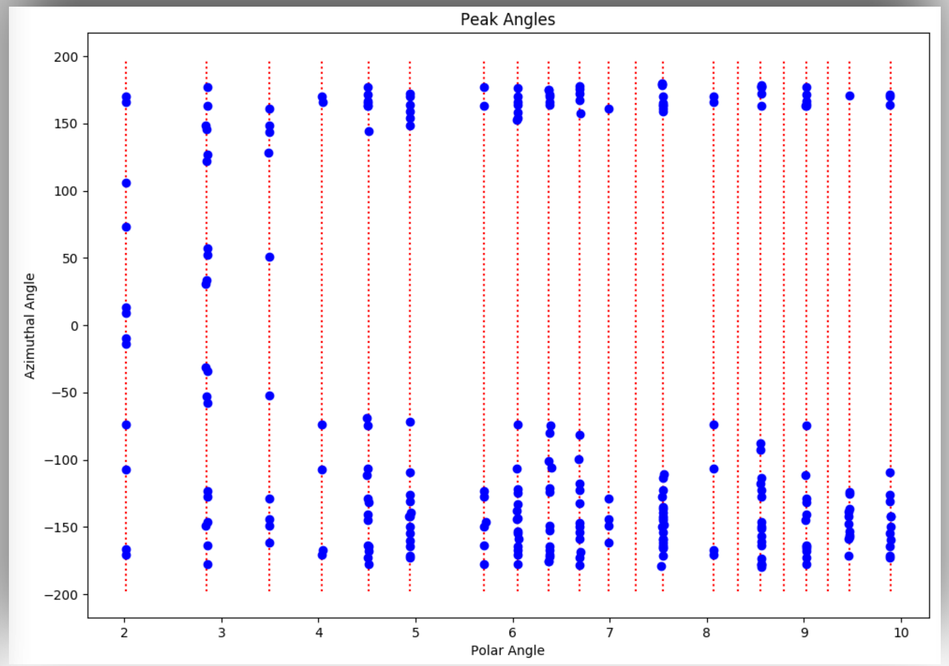
- With the following parameters, we cover -15Å^{-1}<**Q**<15Å^{-1}
  - E_i ~ 87 keV
  - λ ~ 0.14 Å
  - Detector distance ~650 mm
  - Pilatus 2M CdTe: 1679x1475 pixels
  - Pixel size ~170 µm
- This Q-range includes thousands of Brillouin zones.
  - *e.g.*, for *a* ~ 10 Å, ~60,000 Bragg peaks



EXPERIMENT WORKFLOW







pmn_det_omega_mov_mask/f1 Peak Table

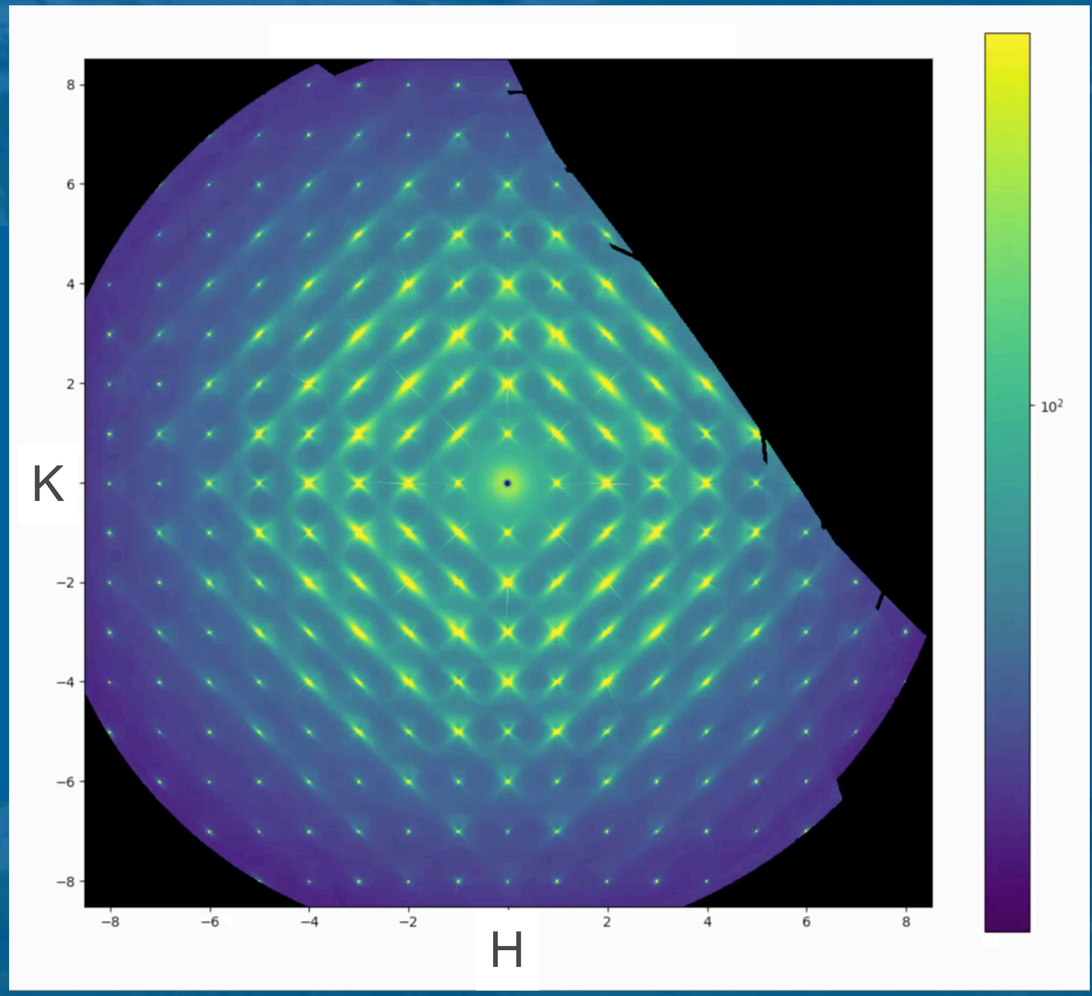
Primary 0 Secondary 1 Orient

i	x	y	z	ola ▲	Azi	Intensity	H	K	L	Diff
195	1214	1638	1574	2.01	-10.00	2.44e+07	-0.00	0.00	-1.00	0.000
291	1280	1637	2447	2.01	13.15	1.8e+07	1.00	-0.00	0.00	0.000
403	1269	1639	3371	2.01	9.14	2.12e+07	-0.00	0.00	1.00	0.001
76	1203	1636	652	2.01	-13.70	3.89e+06	-1.00	-0.00	-0.00	0.001
336	1083	1522	2824	2.01	-73.81	2.35e+08	0.00	1.00	0.00	0.001
116	1401	1523	960	2.01	73.36	1.99e+08	-0.00	-1.00	0.00	0.000
342	1402	1428	2894	2.01	106.43	2.37e+08	-0.00	-1.00	0.00	0.000
126	1083	1426	1030	2.02	-107.25	2.36e+08	0.00	1.00	0.00	0.000
78	1282	1313	672	2.02	166.43	1.95e+07	1.00	0.00	-0.00	0.001
406	1215	1311	3391	2.02	-170.57	2.74e+07	-0.00	0.00	-1.00	0.001
196	1271	1311	1595	2.02	170.31	1.49e+07	-0.00	0.00	1.00	0.001
296	1204	1313	2468	2.03	-166.77	1.99e+07	-1.00	0.00	-0.00	0.001
84	1362	1676	718	2.83	30.83	3.35e+07	-0.99	-1.00	0.00	0.003
302	1120	1675	2530	2.83	-31.44	3.53e+07	0.99	1.00	-0.00	0.002
306	1364	1275	2563	2.84	148.77	4.44e+07	-0.99	-1.00	0.00	0.002
90	1122	1274	751	2.84	-149.17	2.49e+07	0.99	1.00	-0.00	0.003
181	1373	1670	1443	2.84	33.83	8.12e+07	0.00	-1.00	-1.00	0.000
215	1055	1616	1732	2.84	-53.13	1.23e+08	0.00	1.00	-1.00	0.001
274	1440	1602	2288	2.85	57.29	1.25e+08	1.00	-1.00	0.00	0.001
421	1429	1618	3506	2.85	52.51	1.32e+08	0.00	-1.00	1.00	0.001
391	1109	1669	3256	2.85	-34.45	6.54e+07	-0.00	1.00	1.00	0.000
58	1043	1601	518	2.85	-57.74	1.13e+08	-1.00	1.00	0.00	0.001
64	1441	1349	571	2.85	122.40	1.08e+08	1.00	-1.00	0.00	0.000
394	1375	1281	3290	2.85	145.75	8.31e+07	-0.00	-1.00	-1.00	0.000
220	1430	1333	1779	2.86	127.17	1.31e+08	-0.00	-1.00	1.00	0.001
427	1056	1331	3553	2.86	-127.69	9.27e+07	-0.00	1.00	-1.00	0.001
186	1112	1279	1477	2.86	-146.36	8.88e+07	0.00	1.00	1.00	0.000
23	1254	1240	232	2.86	177.08	2.57e+07	1.00	0.00	-1.00	0.000
280	1045	1346	2341	2.86	-123.16	1.37e+08	-1.00	1.00	0.00	0.001

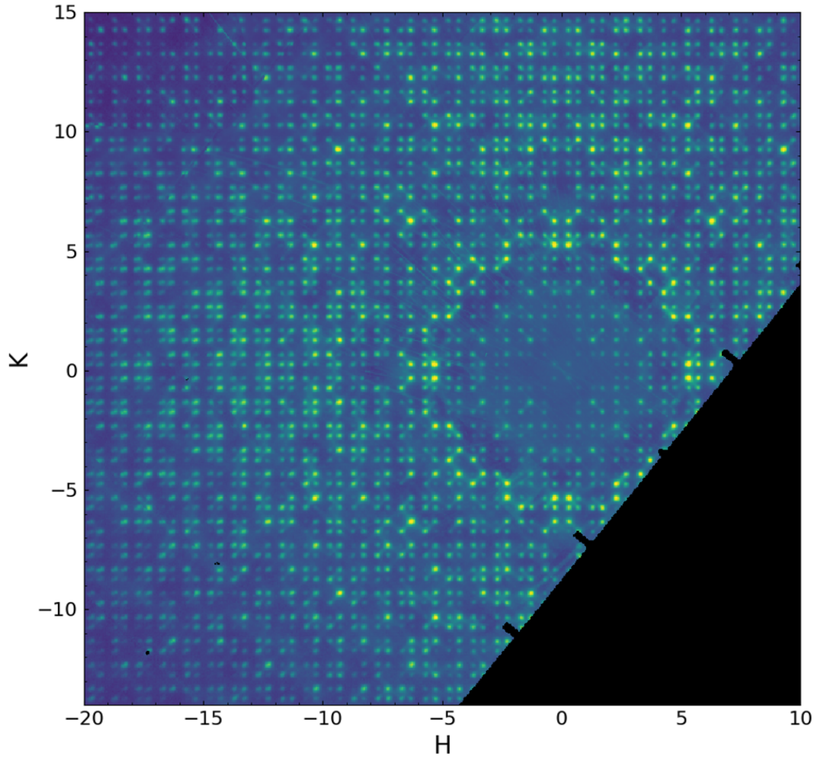
Score: 0.0007 Threshold 0.05 Save Orientation Close Window

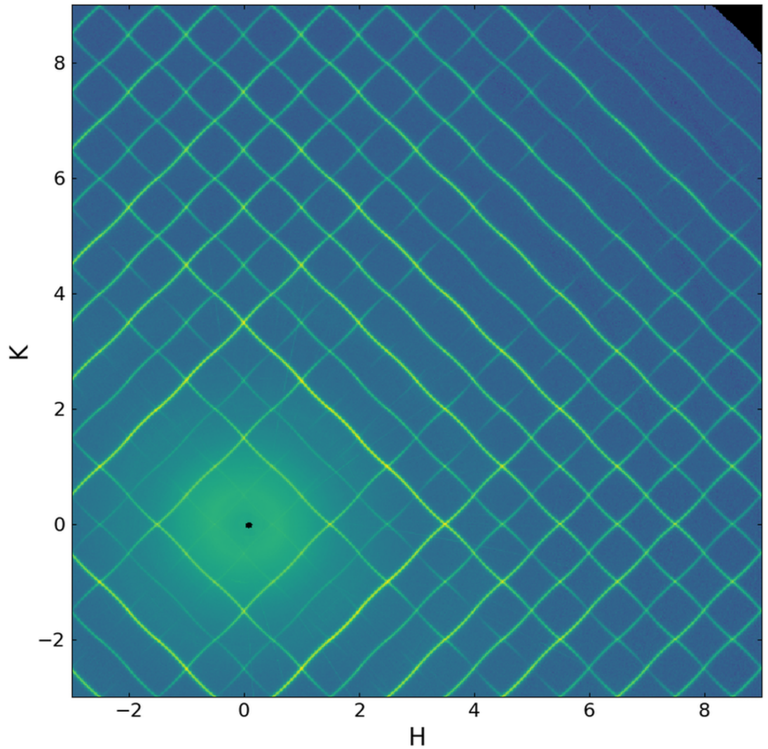
DIFFUSE SCATTERING IN 3D
THE RELAXOR $PbMg_{1/3}Nb_{2/3}O_3$

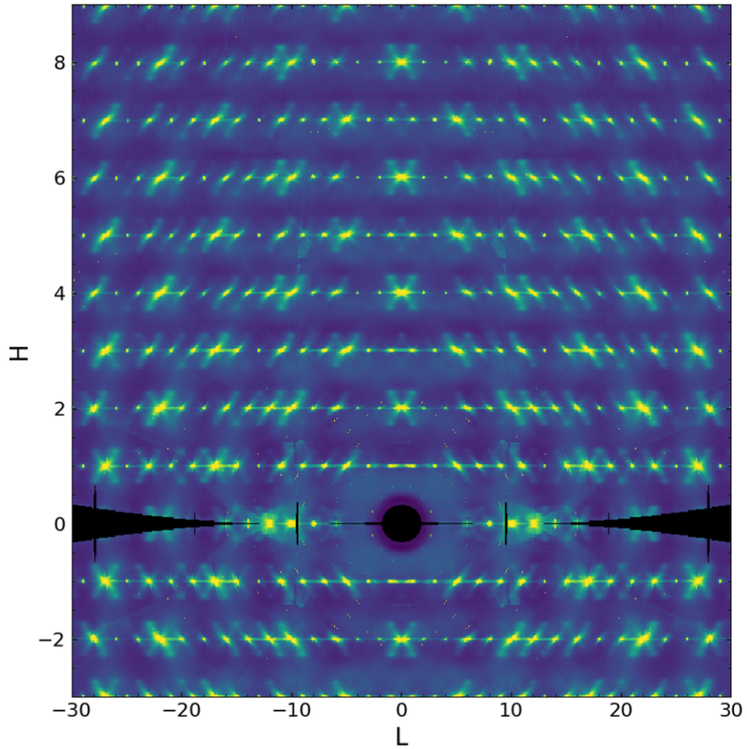
M. J. Krogstad, *et al*, Nature Materials **48**, 1 (2018).



DIFFUSE GALLERY







CASE STUDY 1: MULLITE

MULLITE - A CASE STUDY

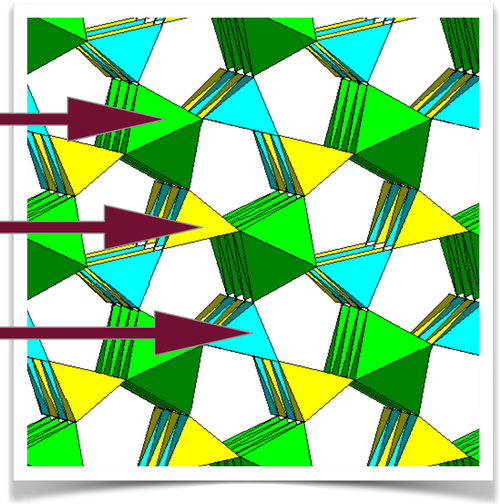
B. D. Butler, T. R. Welberry, & R. L. Withers, Phys Chem Minerals **20**, 323 (1993)

- Mullite is a ceramic that is formed by adding O^{2+} vacancies to Sillimanite
  - Sillimanite has alternating AlO_4 and SiO_4 tetrahedra
  - Mullite has excess Al^{3+} occupying Si^{2+} sites for charge balance
- This results in strong vacancy-vacancy correlations

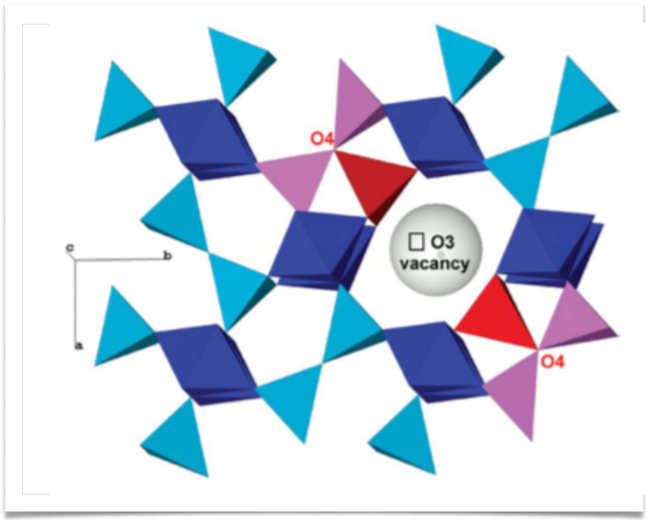
AlO_6 Octahedra

SiO_4 Tetrahedra

AlO_4 Tetrahedra



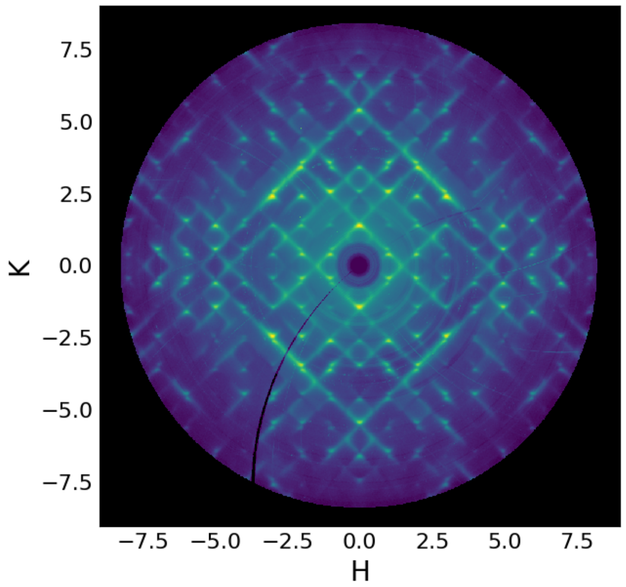
Sillimanite: Al_2SiO_5



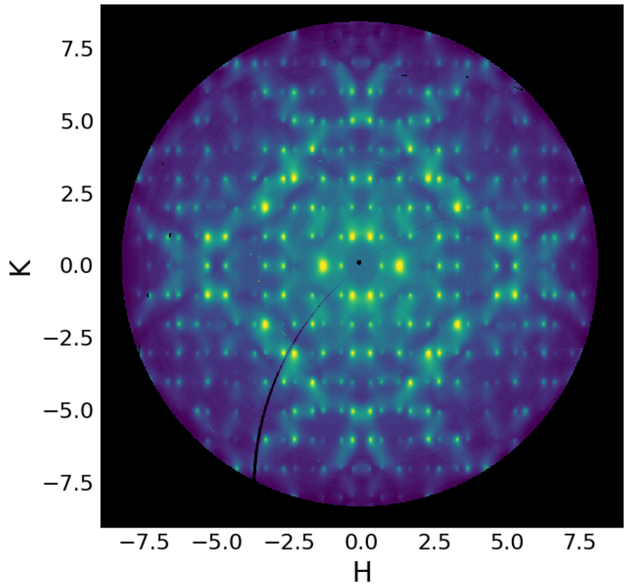
Mullite: $Al_2(Al_{2+2x}Si_{2-2x})O_{10-x}$

3D DIFFUSE SCATTERING IN MULLITE

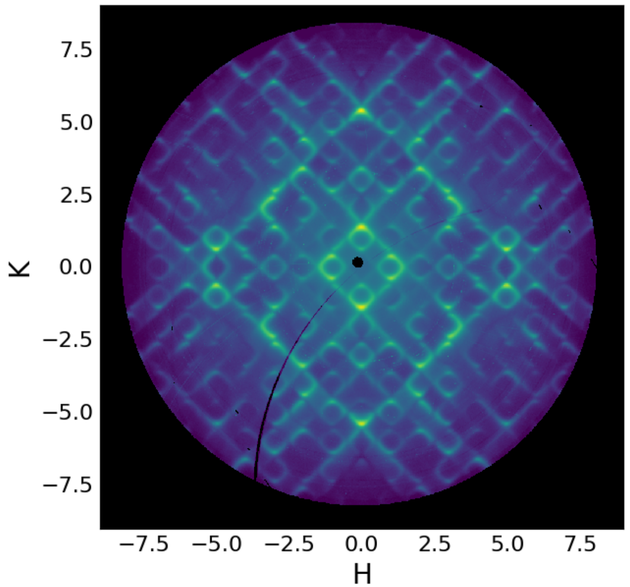
- There is strong diffuse scattering throughout reciprocal space
- The shape of the diffuse scattering is strongly dependent on the value of L



L=0.16



L=0.5

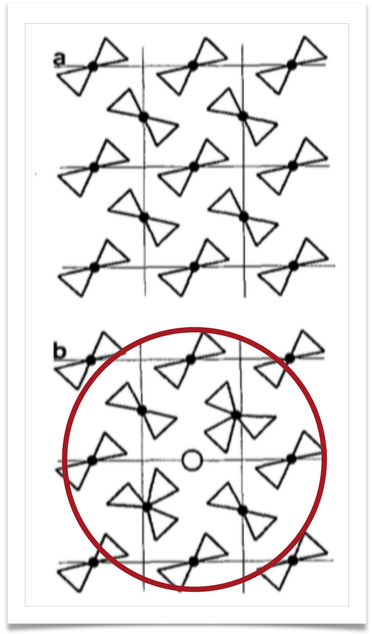


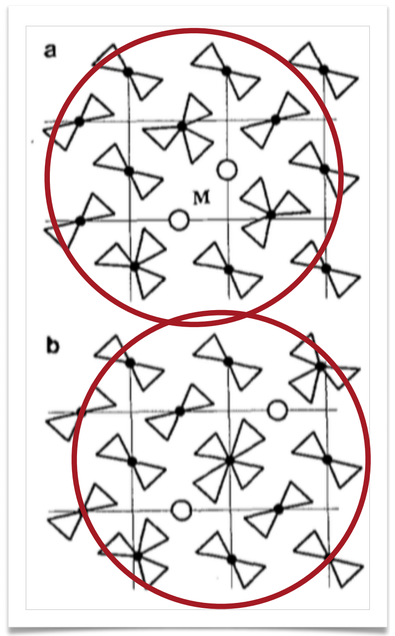
L=0.75

MONTE CARLO ANALYSIS

B. D. Butler, T. R. Welberry, & R. L. Withers,
Phys Chem Minerals **20**, 323 (1993)

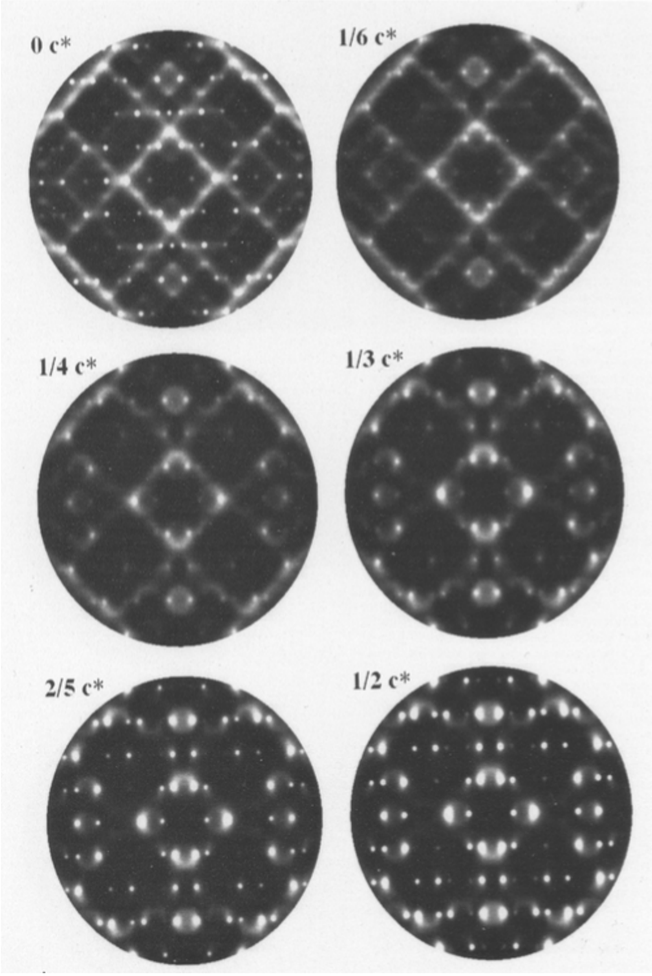
- In a classic analysis, Richard Welberry and colleagues developed a set of interaction energies to model mullite disorder
- Interaction energies were initialized:
  - insights from chemical intuition
  - insights from the measured diffuse scattering
- The diffuse scattering was calculated using a Monte Carlo algorithm to generate vacancy distributions first in 2D slices and then in 3D

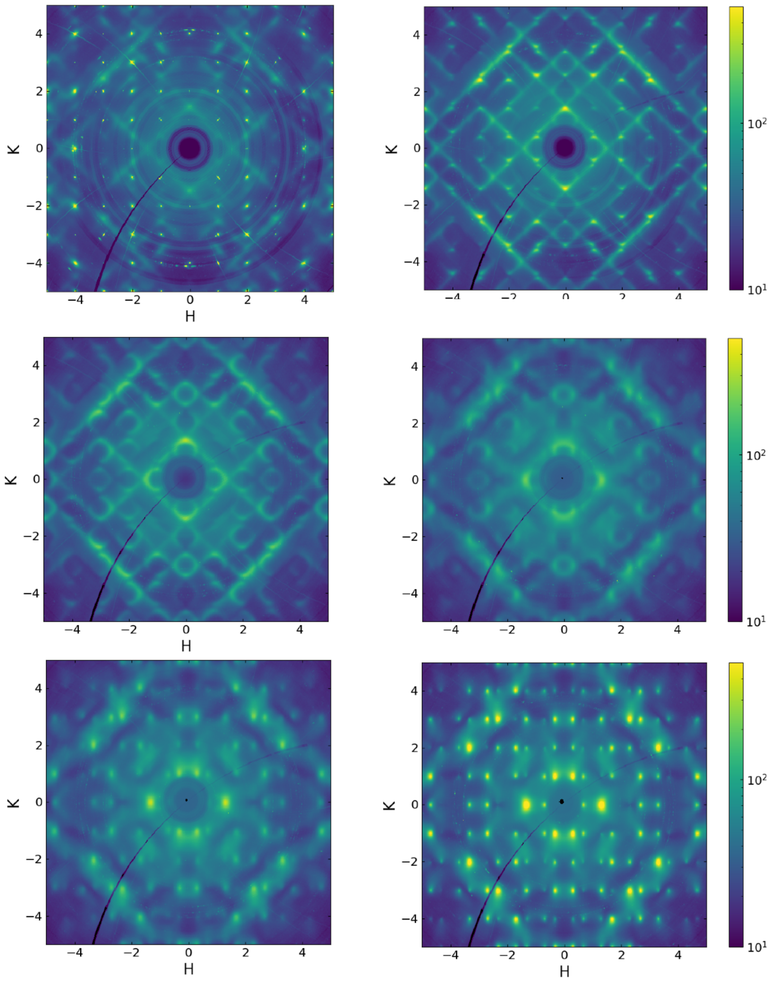




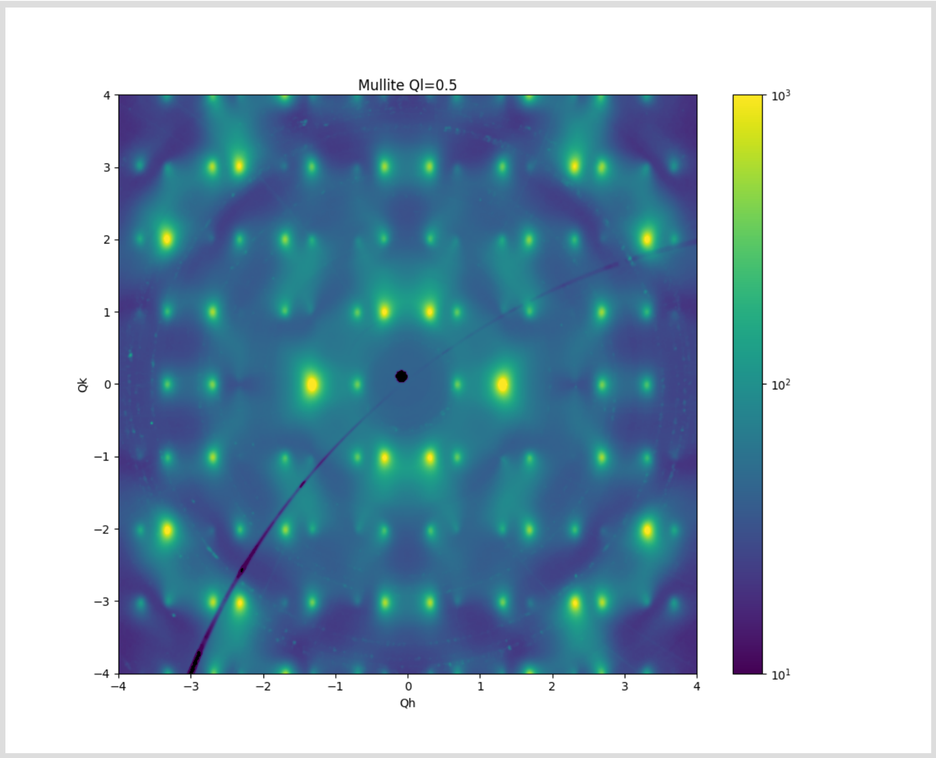
Interatomic vector	α_{lmn}	Interatomic vector	α_{lmn}
$\frac{1}{2}\langle 1\,1\,0\rangle$	−0.24	$\langle 0\,2\,0\rangle$	+0.13
$[1\,1\,0]$	−0.23	$\frac{1}{2}\langle 3\,1\,0\rangle$	+0.22
$[1\,-1\,0]$	−0.05	$\frac{1}{2}\langle 1\,3\,0\rangle$	−0.01
$\langle 1\,0\,0\rangle$	−0.06	$\langle 1\,0\,1\rangle$	+0.07
$\langle 0\,1\,0\rangle$	+0.22	$\langle 0\,1\,1\rangle$	−0.12
$\langle 0\,0\,1\rangle$	−0.03	$\frac{1}{2}\langle 3\,3\,0\rangle$	+0.17
$\frac{1}{2}[1\,-1\,2]$	+0.12	$\langle 1\,1\,1\rangle$	−0.01
$\frac{1}{2}[1\,1\,2]$	+0.12	$\frac{1}{2}\langle 3\,1\,2\rangle$	−0.11
$\langle 2\,0\,0\rangle$	−0.12	$\frac{1}{2}\langle 3\,3\,2\rangle$	−0.07

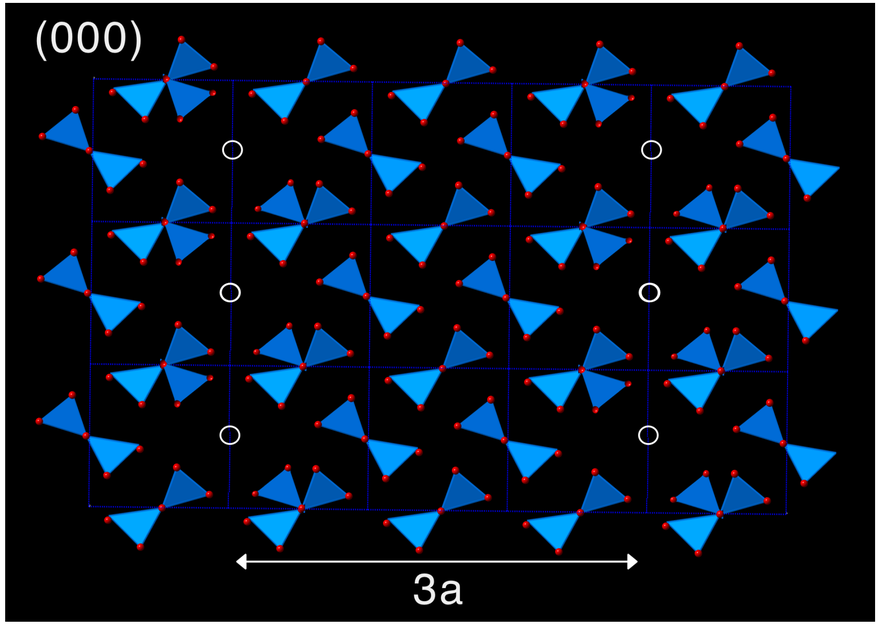
MONTE CARLO ANALYSIS RESULTS





VACANCY ORDERING IN MULLITE

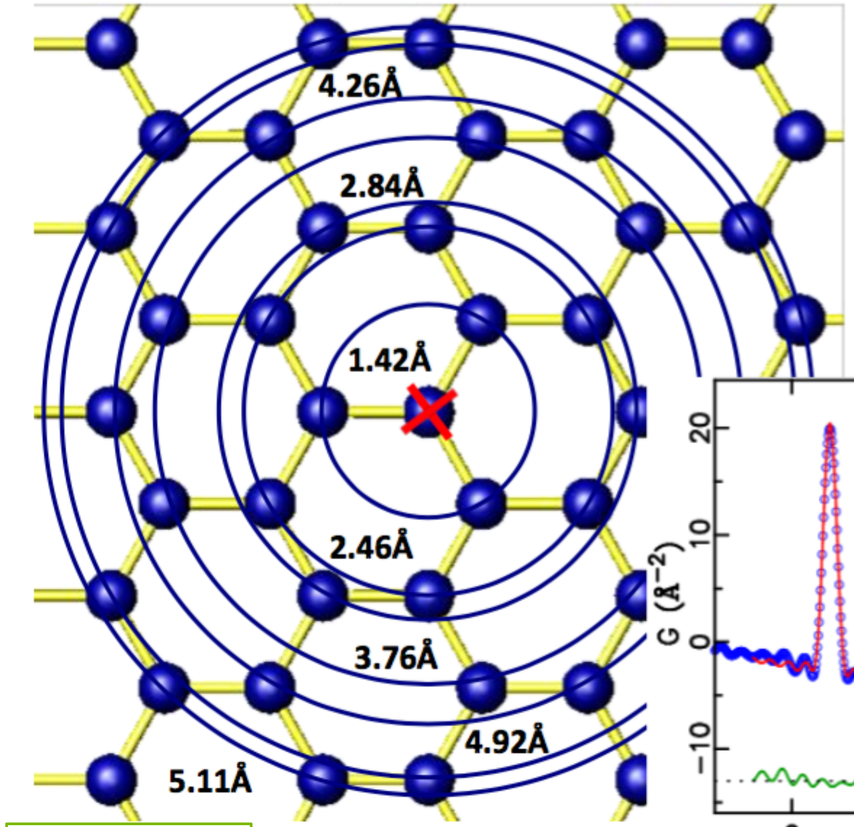




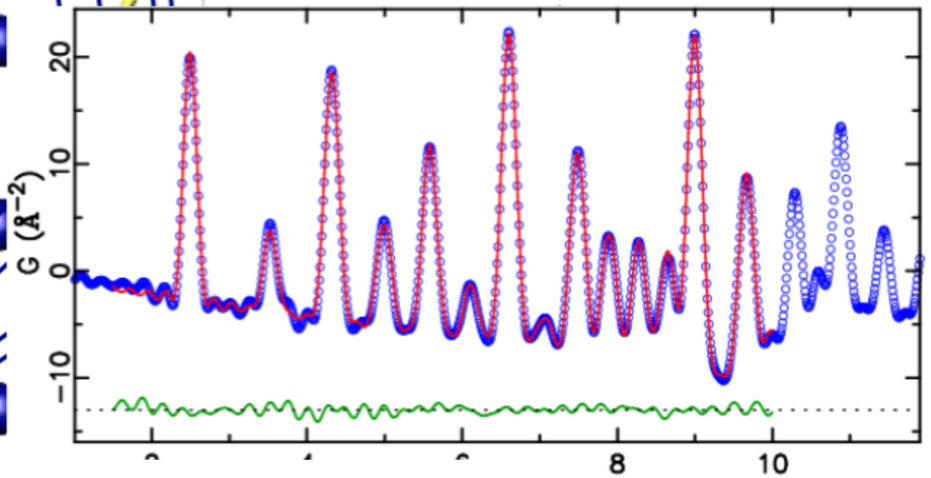
$$\mathbf{q} = \pm\frac{1}{2}\mathbf{c}^* \pm \frac{1}{3}\mathbf{a}^*$$

CASE STUDY 2: SODIUM-INTERCALATED V_2O_5 3D-ΔPDF

PAIR DISTRIBUTION FUNCTION ANALYSIS



Radial atomic **p**air **d**istribution **f**unction (PDF) gives the interatomic distance distribution, or "probability" of finding atomic pairs distance *r* apart



$$G(r) = 4\pi r[\rho(r) - \rho_o] = (2/\pi) \int_{Q=Q_{min}}^{Q_{max}} Q[S(Q) - 1]\sin(Qr)dQ$$

Emil Bozin (ADD 2013)

THREE-DIMENSIONAL PAIR DISTRIBUTION FUNCTIONS

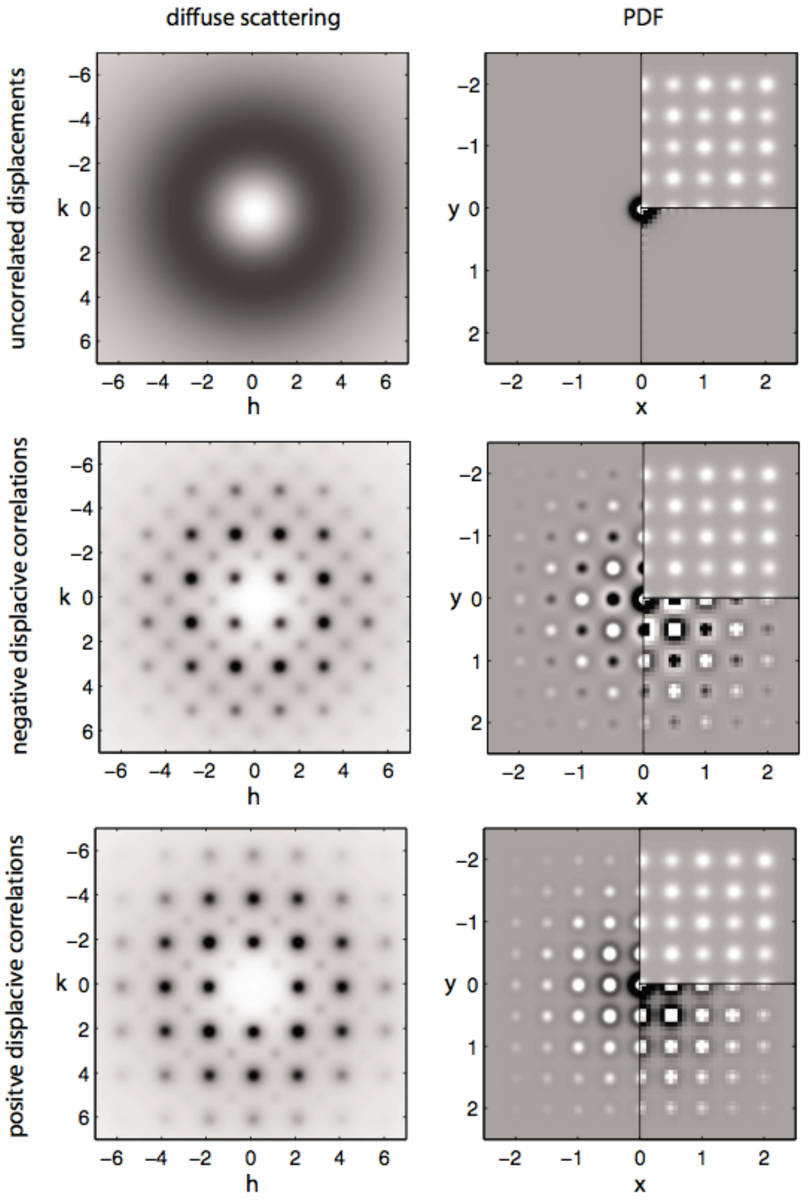
238 Z. Kristallogr. **2012**, *227*, 238–247 / **DOI** 10.1524/zkri.2012.1504

The three-dimensional pair distribution function analysis of disordered single crystals: basic concepts

Thomas Weber* and Arkadiy Simonov

Laboratory of Crystallography, ETH Zurich Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland

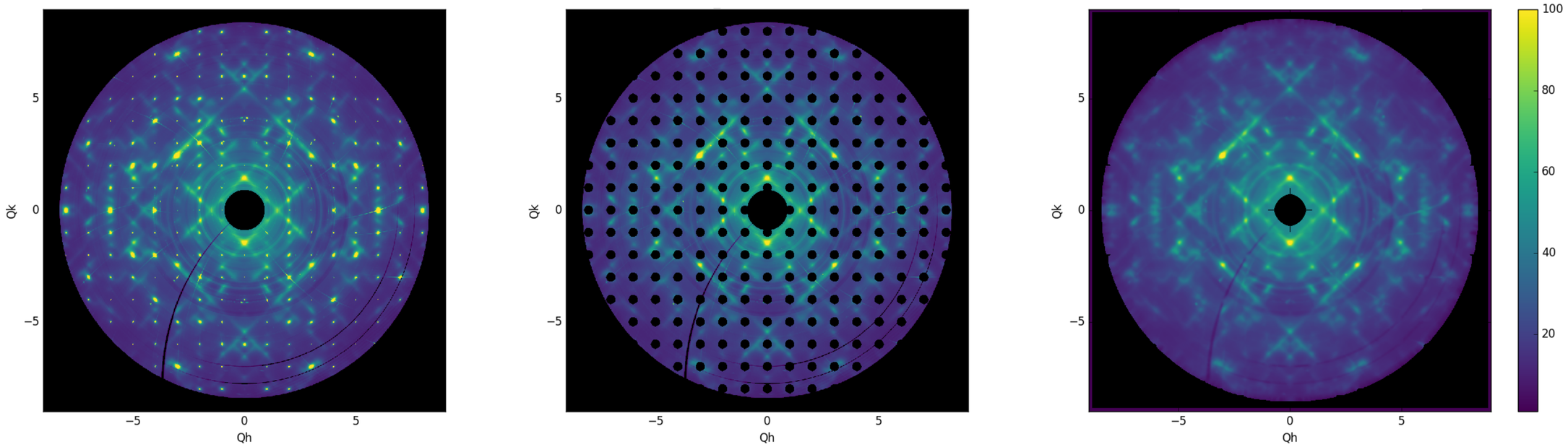
- The 3D PDF technique was pioneered by Thomas Weber and colleagues at ETH
  - Philippe Schaub, Walter Steurer, Arkadiy Simonov
  - See *Yell* - A. Simonov, *et al*, J Appl Cryst **47**, 1146 (2014).
- The ability to measure three-dimensional S(**Q**) over a large volume of reciprocal space provides the 3D analog of PDF measurements.
  - Total PDFs if Bragg peaks and diffuse scattering can be measured simultaneously
  - ΔPDFs if the Bragg peaks are eliminated
- This allows a model-independent view of the measurements in real space.



“PUNCH AND FILL”

$$I = \sum_i \sum_j b_i b_j \exp(i\mathbf{Q} \cdot \mathbf{r}_{ij})$$

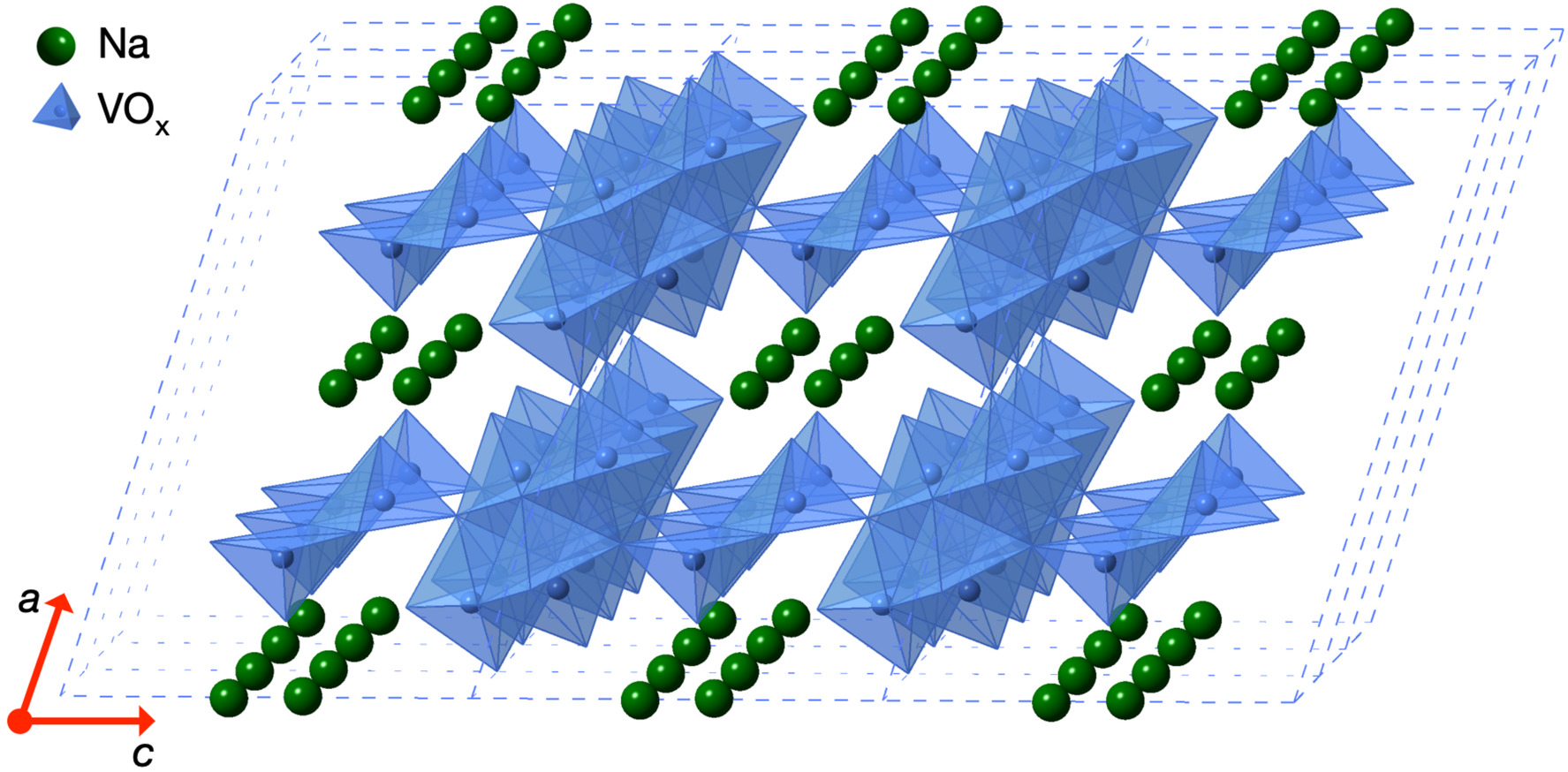
$$P_{tot}(\mathbf{r}) = FT\left[I(\mathbf{Q})\right] = FT\left[|\bar{F}(\mathbf{Q})|^2\right] + FT\left[|\Delta F(\mathbf{Q})|^2\right] = P_{hkl}(\mathbf{r}) + \Delta P(\mathbf{r})$$



Symmetrize Punch Fill

A. Simonov, T. Weber, and W. Steurer, Journal of Applied Crystallography **47**, 1146 (2014).

SODIUM-INTERCALATED V_2O_5

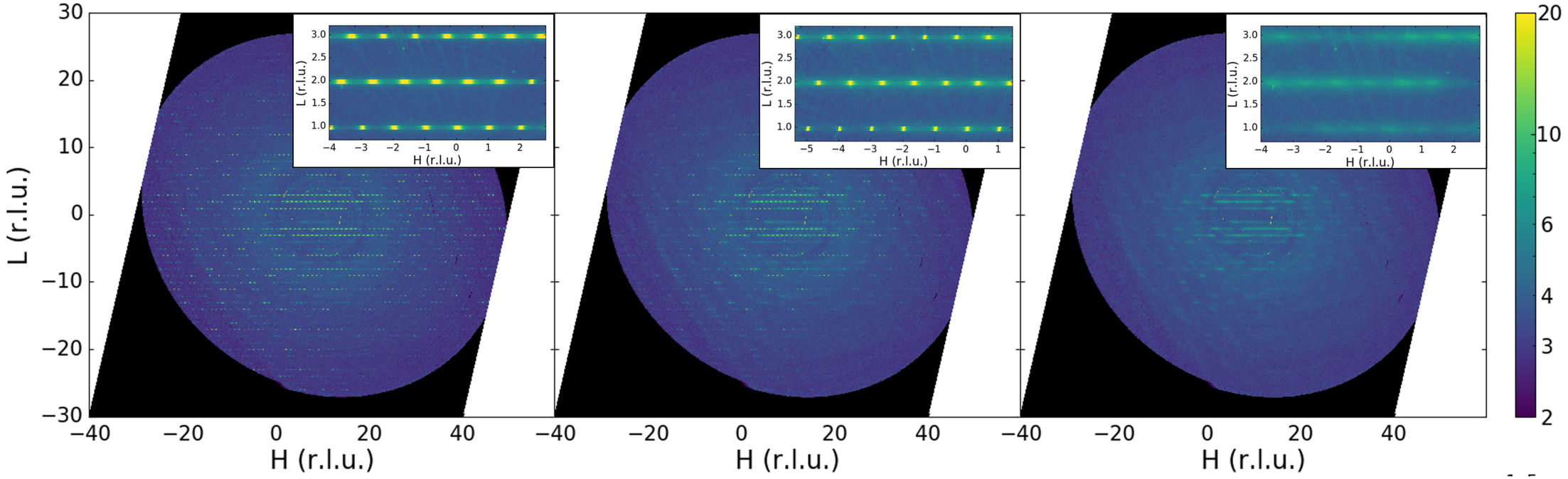


M. J. Krogstad, S. Rosenkranz, J. M. Wozniak, G. Jennings, J. P. C. Ruff, J. T. Vaughey, and R. Osborn
Nature Materials **19**, 63 (2020).

SUBLATTICE MELTING IN $Na_{0.45}V_2O_5$

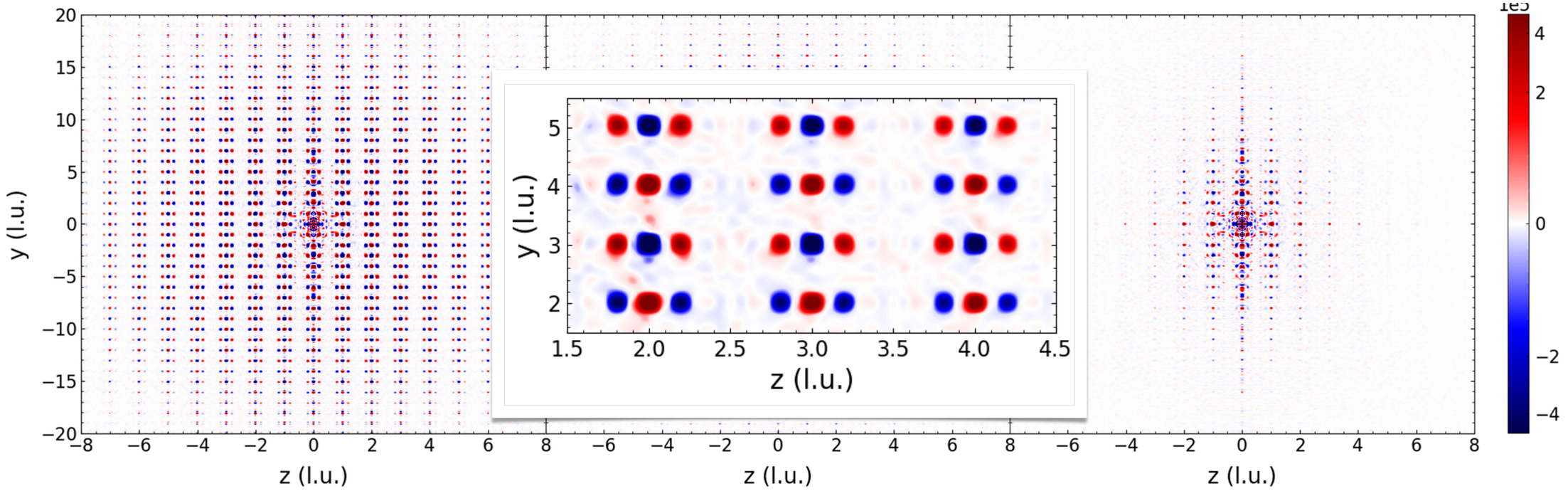
Order-Disorder Transition in the Half-Filled Sodium Sublattice

K=0.5



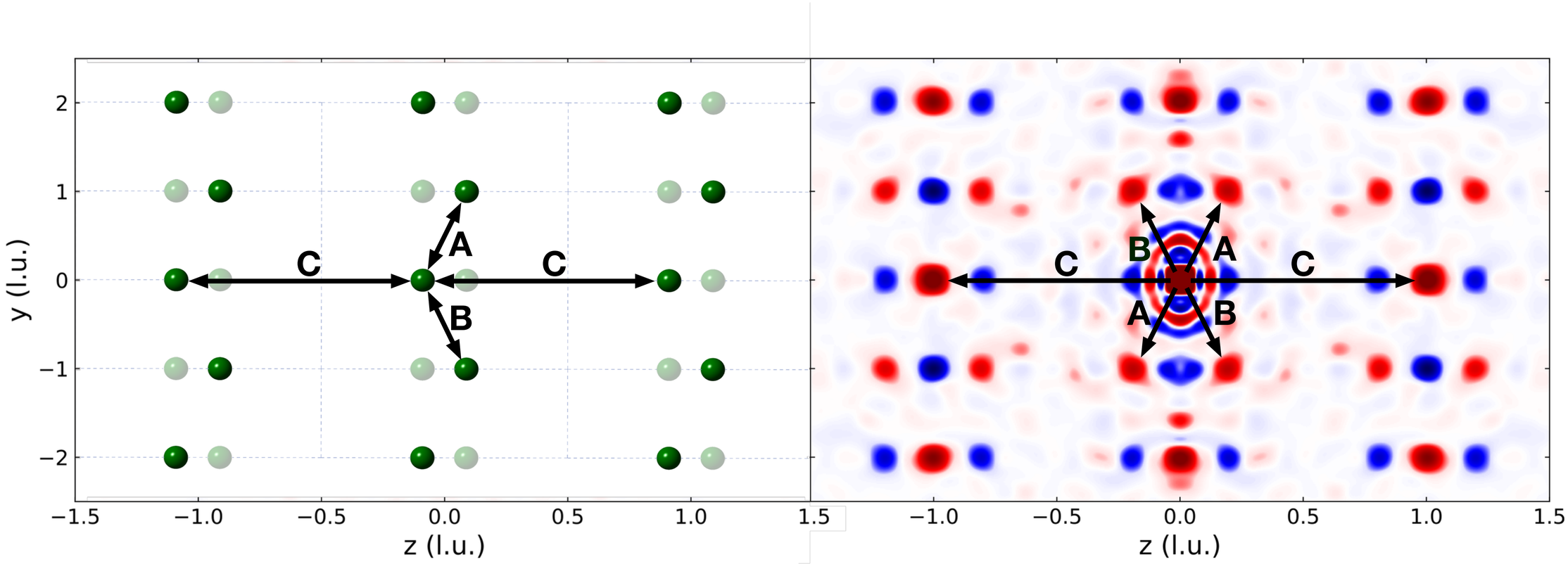
50K 200K 250K

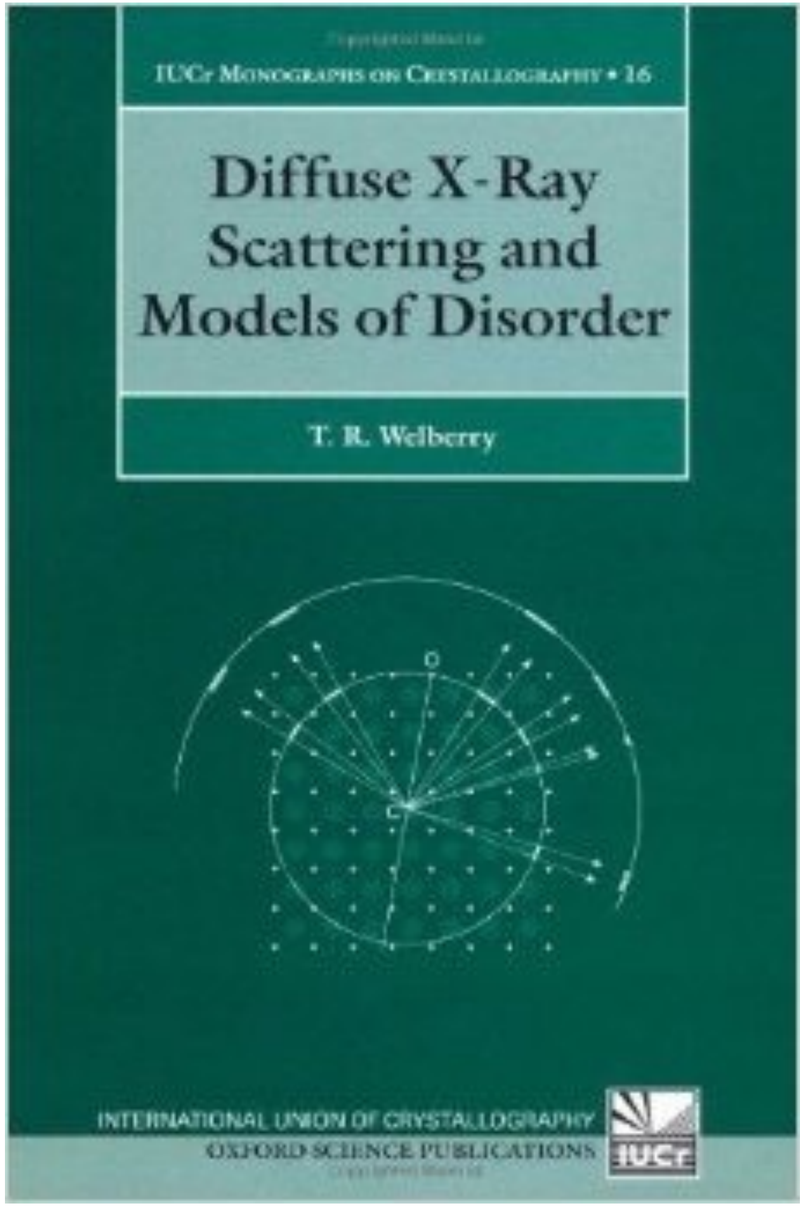
3D-ΔPDF ANALYSIS OF $Na_{0.45}V_2O_5$



50K 200K 250K

REAL SPACE *vs* 3D–ΔPDF





24.3.3 *Ordering of Na within the two-leg ladders.*

Fig. 24.10(a) shows a small region near the origin of the x = 0 plane of the ΔPDF map obtained from the 50K X-ray data. The strong white origin peak indicates perfect positive correlation for an atom with itself. Other white peaks also indicate a positive correlation between an atom at the origin with another at a position given by the vectors A, B or C (and the reverse vectors -A, -B and -C). Conversely the dark peaks indicate strong negative correlations. It is quite straightforward to deduce from the observed pattern of white and dark peaks that the local arrangement of the Na ions must follow a pattern like that shown in Fig. 24.10(b), where the occupancy of the two Na sites on each rung of the two-leg ladders tends to alternate between (Na□†) and (□Na) producing a zig-zag chain of occupied sites. Neighbouring ladders at $z = \pm 1.0$ have the same occupancy pattern which is in phase with the ladder at $z = 0$.

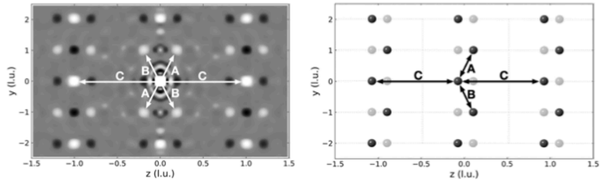


Fig. 24.10 A comparison of (a) the ΔPDF peak intensities at 50K in the $x = 0$ plane of $Na_{0.45}V_2O_5$ with (b) the derived real-space model of sodium ions. Data used in this figure are reproduced with kind permission of Dr Ray Osborn.

24.3.4 *ΔPDF peak intensities in the $z = 0$ plane.*

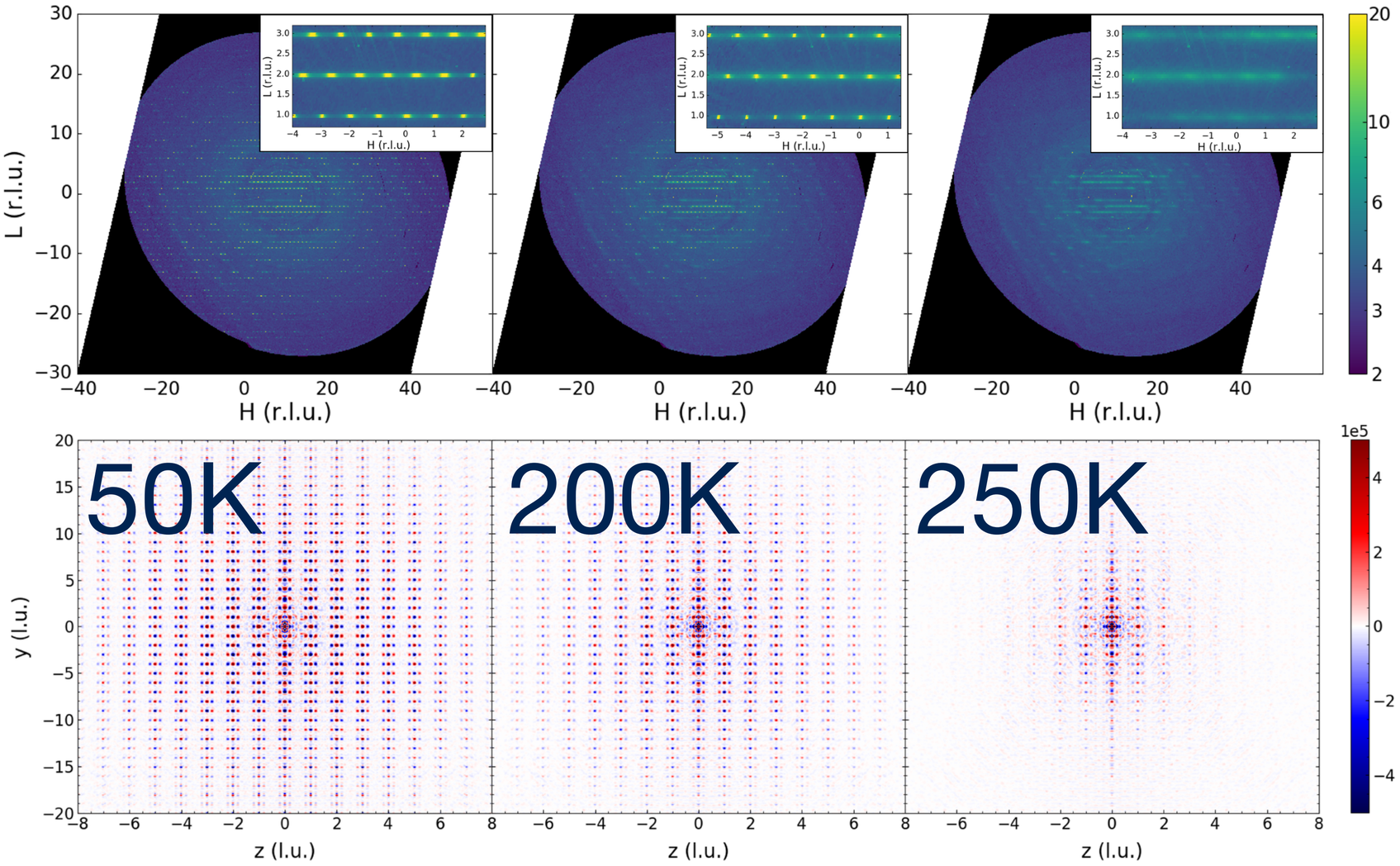
Fig. 24.12 shows the $z = 0$ plane of the ΔPDF map observed at three different temperatures. Fig. 24.11(b) shows an enlargement of part of Fig. 24.11(a) where white arrows (labelled A –F) have been used to identify different interatomic vectors. The same set of vectors is shown in Fig. 24.11(e) which is a plot of the $z = 0$ plane of the average structure. The maps are dominated by the same alternating correlations of Na occupancy along the ladder direction parallel to y. Similarly neighbouring chains at $x = \pm 1$ are instep with that at $x = 0$ for temperatures 50K and 150K but at 250K these correlations have been lost.

Although the maps are dominated by the correlations in the Na ladders there are numerous weaker peaks that correspond to correlations between the ladder Na_1 ions and the interstitial Na_2 ions. These correspond to vectors A, B, C and E in Fig. 24.11(e) and involve one Na_1 and one Na_2 ion. These peaks are clearly evident in the 50K map, somewhat less evident at 150K and even less evident at 250K. They are weak relative to those involving Na_1 ions alone simply because of the low occupancy of the Na_2 sites.

†here □ is used to represent a vacant site

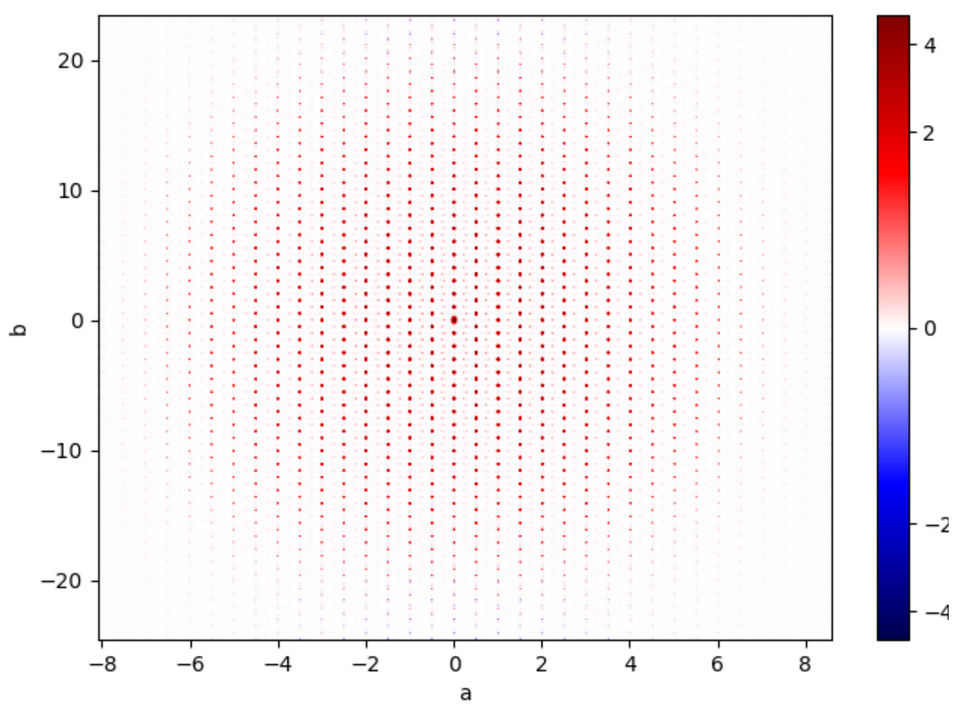
ORDER-DISORDER TRANSITION VIEWED IN REAL SPACE

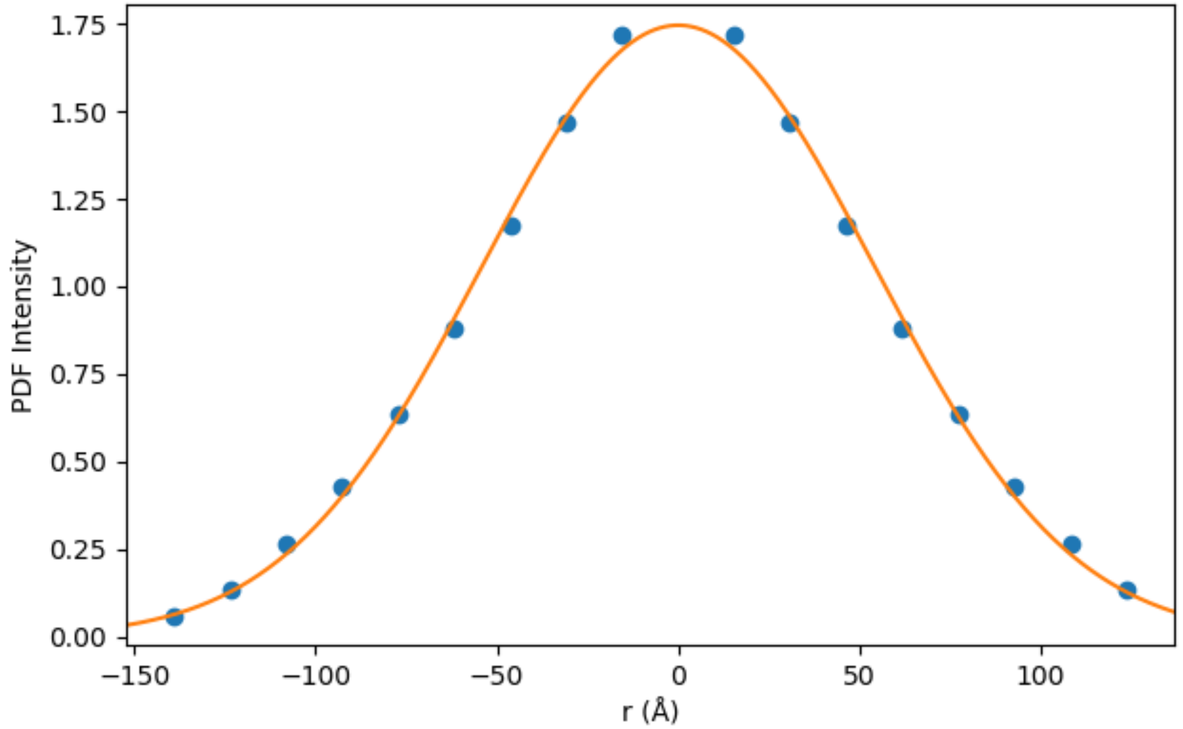
$Na_{0.45}V_2O_5$



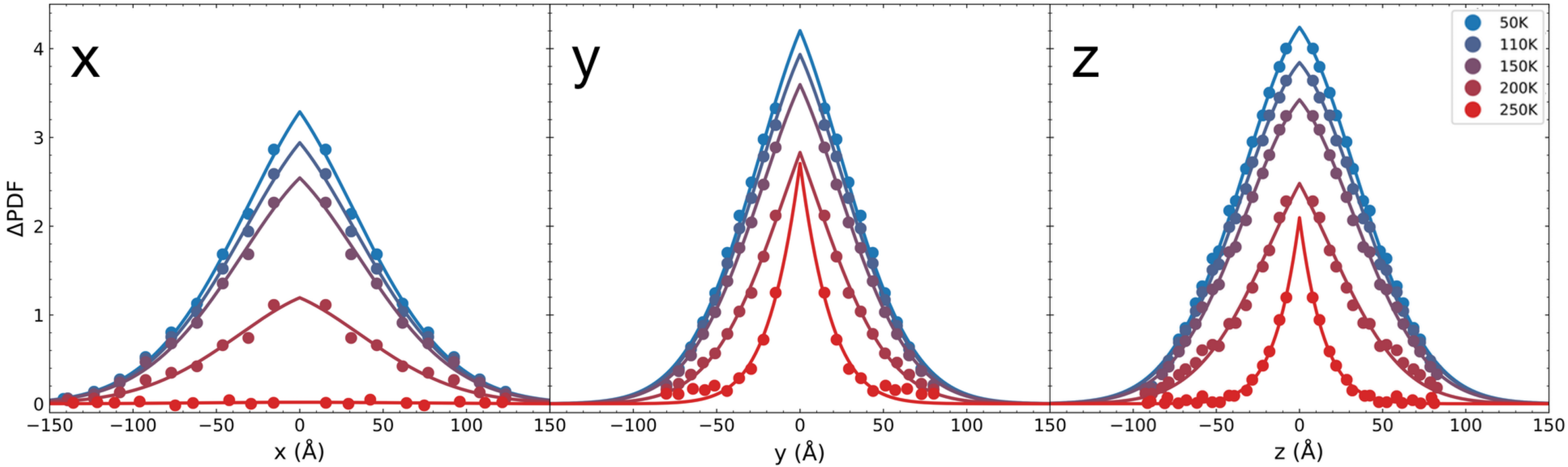
EFFECT OF Q-RESOLUTION

- Finite Q-resolution ➡ Gaussian envelope in real space.
- The width can be determined from the total PDF
  - *i.e.*, the transform of the long-range crystal structure.



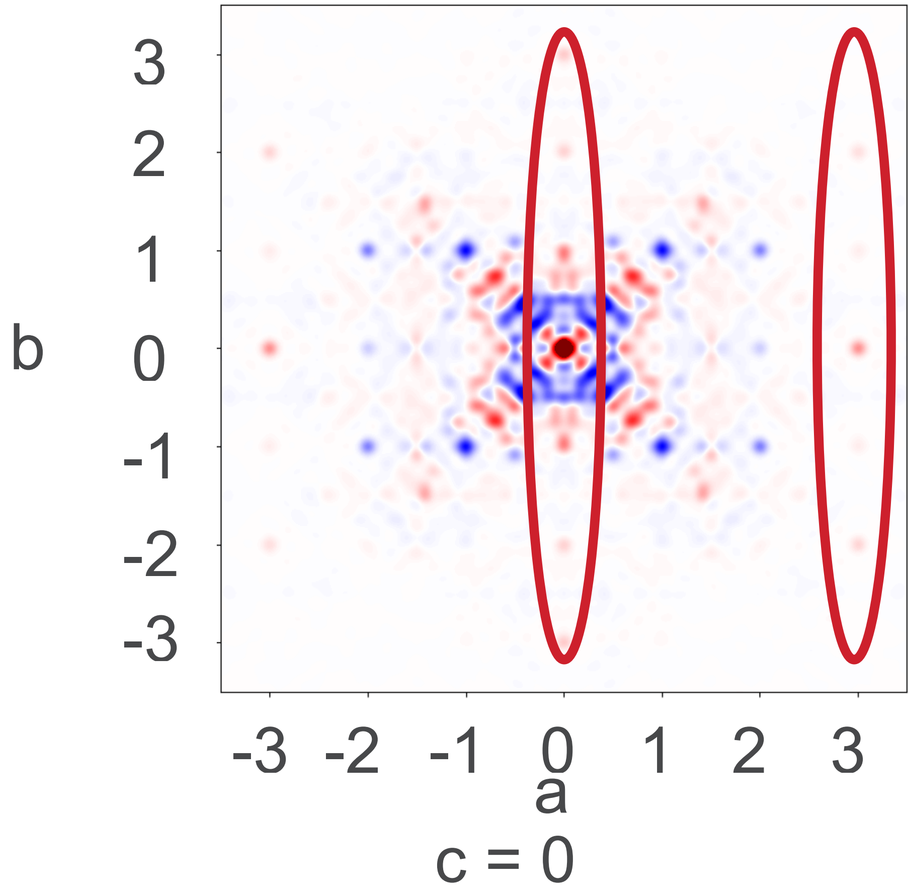


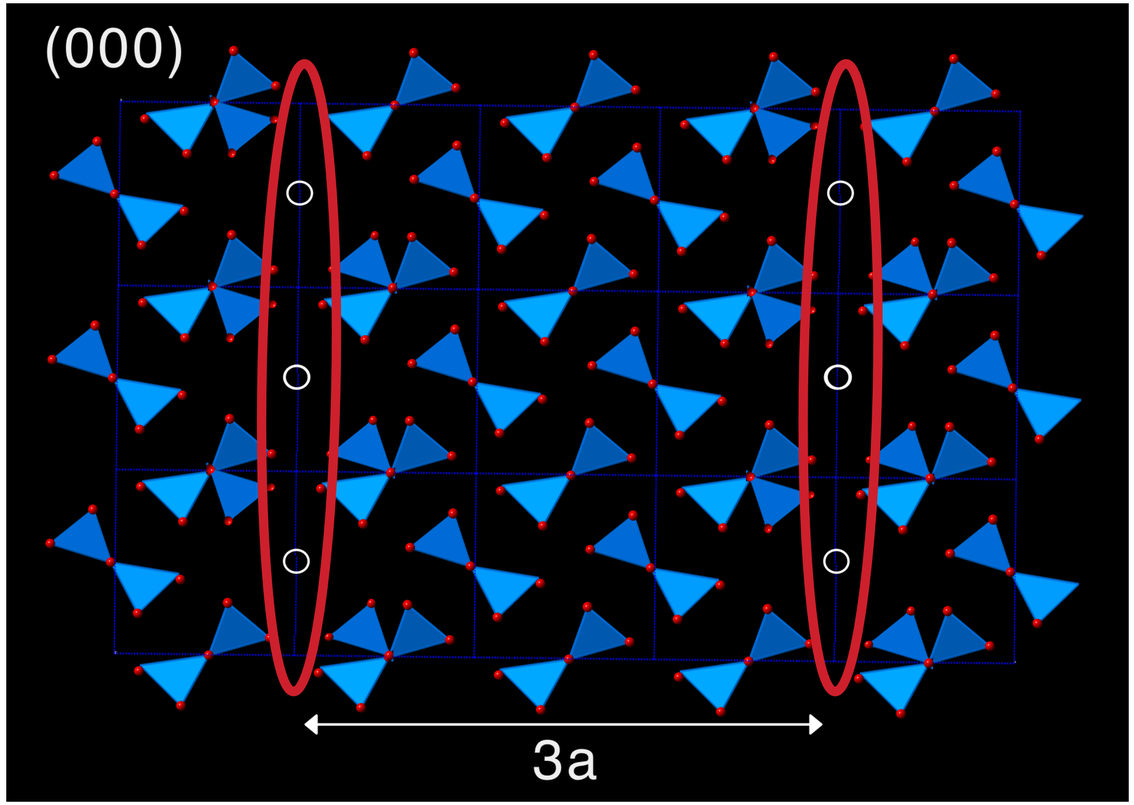
FITTING CORRELATION LENGTHS IN REAL SPACE



$$f(\mathbf{r}) = A \times G(\mathbf{r}) \times \exp(-|\mathbf{r}|/\xi)$$

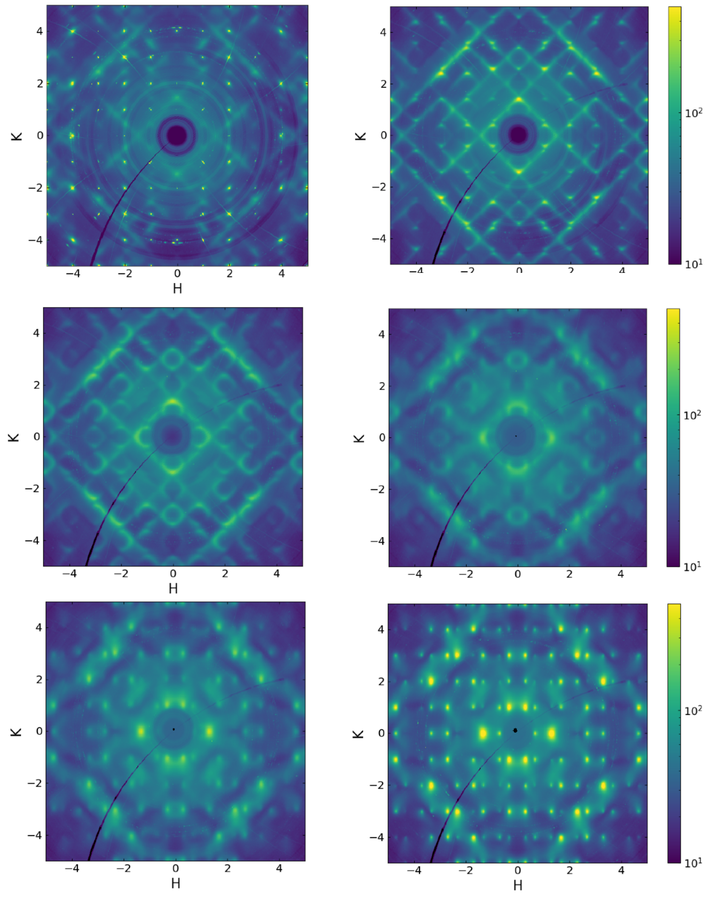
BACK TO MULLITE





THE NATURE OF STRUCTURAL SOLUTIONS

B. D. Butler, T. R. Welberry, & R. L. Withers
Phys Chem Minerals **20**, 323 (1993)



Interatomic vector	α_{lmn}	Interatomic vector	α_{lmn}
$\frac{1}{2}\langle 1\,1\,0\rangle$	−0.24	$\langle 0\,2\,0\rangle$	+0.13
$[1\,1\,0]$	−0.23	$\frac{1}{2}\langle 3\,1\,0\rangle$	+0.22
$[1\,-1\,0]$	−0.05	$\frac{1}{2}\langle 1\,3\,0\rangle$	−0.01
$\langle 1\,0\,0\rangle$	−0.06	$\langle 1\,0\,1\rangle$	+0.07
$\langle 0\,1\,0\rangle$	+0.22	$\langle 0\,1\,1\rangle$	−0.12
$\langle 0\,0\,1\rangle$	−0.03	$\frac{1}{2}\langle 3\,3\,0\rangle$	+0.17
$\frac{1}{2}[1\,-1\,2]$	+0.12	$\langle 1\,1\,1\rangle$	−0.01
$\frac{1}{2}[1\,1\,2]$	+0.12	$\frac{1}{2}\langle 3\,1\,2\rangle$	−0.11
$\langle 2\,0\,0\rangle$	−0.12	$\frac{1}{2}\langle 3\,3\,2\rangle$	−0.07

$$I_{diffuse} = Nc_Ac_B(b_B - b_A)^2 + \sum_{ij}\alpha_{ij}c_Bc_A(b_B - b_A)^2\exp(i\mathbf{Q}\cdot\mathbf{r}_{ij}); \quad \alpha_{ij} = \left(1 - \frac{P_{ij}}{c_j}\right)$$

"It is now possible to interpret the short-range order in the crystal structure without a detailed simulation of the disorder, which has in the past often required the optimization of a sometimes large number of model parameters fitted over a substantial volume of reciprocal space. In fact, the ΔPDF magnitudes directly determined from the reciprocal space data are simply related to the Warren-Cowley SRO parameters that have frequently been used to parametrize diffuse scattering models." *Richard Welberry*

HOW DO I LOOK AT STATIC DISORDER?

COMPARISON OF ELASTIC SCATTERING AND THE STATIC APPROXIMATION

$$G(\mathbf{r},t) = \frac{1}{N}\left\langle \sum_{i=1}^{N}\sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t) + \mathbf{r}_j(0))\right\rangle$$

$$S(\mathbf{Q},\omega) = \frac{1}{N}\frac{1}{2\pi\hbar}\int_{\infty}^{\infty} e^{-i\omega t}dt \int G(\mathbf{r},t)e^{-i\mathbf{Q}\cdot\mathbf{r}}d\mathbf{r} \qquad \hbar\delta(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}d(\hbar\omega)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh}^{static} = b_{coh}^2 N \int G(\vec{r},0)e^{i\vec{Q}.\vec{r}}d\vec{r}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh}^{elastic} = b_{coh}^2 N \int G(\vec{r},\infty)e^{i\vec{Q}.\vec{r}}d\vec{r}$$

CROSS CORRELATION CHOPPER

S. Rosenkranz and R. Osborn, PRAMANA- Journal of Physics, **71**, 705 (2008).

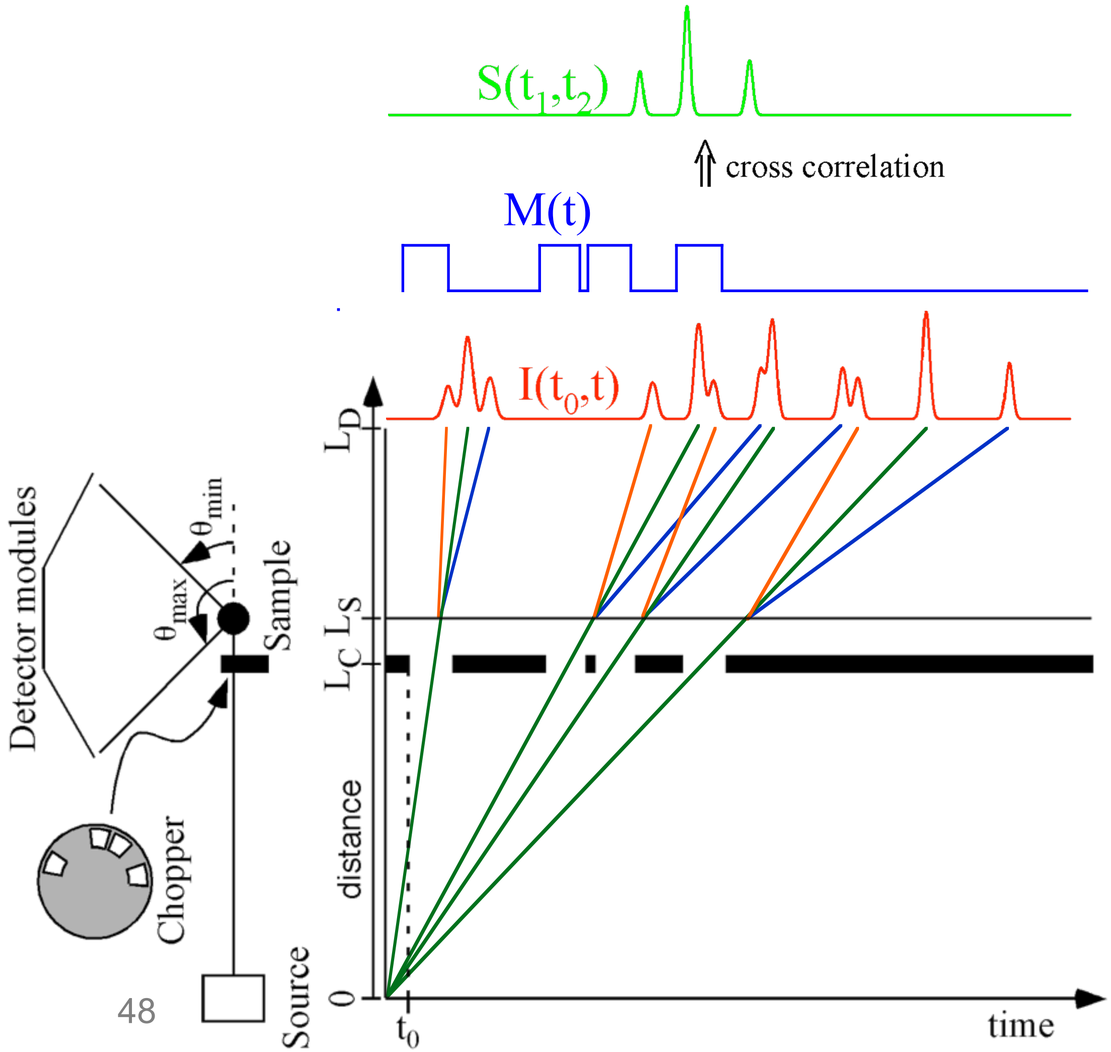
TOF Laue Diffractometer
- highly efficient data collection
- wide dynamic range in Q

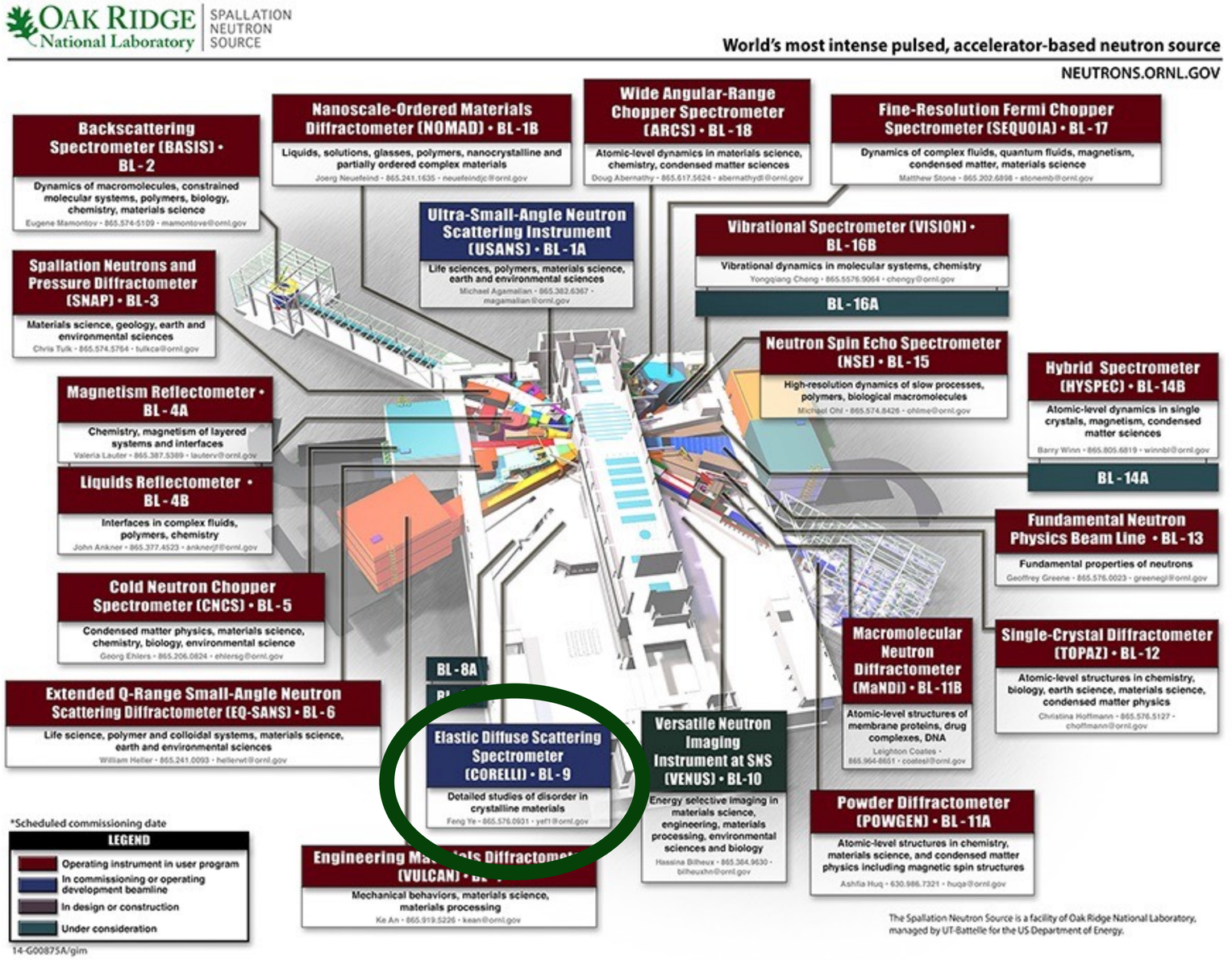
Statistical Chopper
- elastic energy discrimination
- optimum use of white beam

Elastic scattering: $\hbar\omega = 0$

Inelastic scattering: $\hbar\omega = +E_0$

$\hbar\omega = -E_0$

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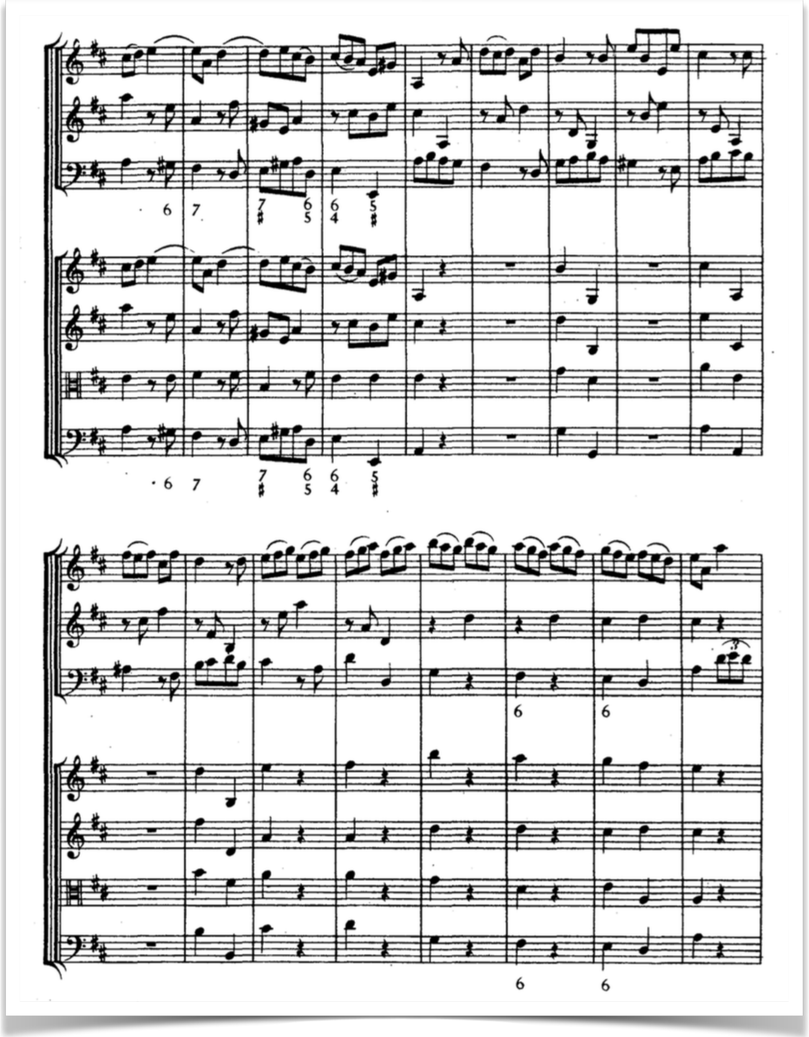
In design or construction
Under consideration
14-G00875A/gim
The Spallation Neutron Source is a facility of Oak Ridge National Laboratory, managed by UT-Battelle for the US Department of Energy.

Arcangelo Corelli (1653-1713)

Arcangelo Corelli was the greatest violinist of his age and an influential composer who became known as the "Father of the Concerto Grosso". This musical form contrasts music from a small ensemble of solo musicians with the full orchestra. Similarly, the properties of many materials are enriched by the interactions between both short and long-range ordering motifs that the *Corelli* instrument is designed to explore.

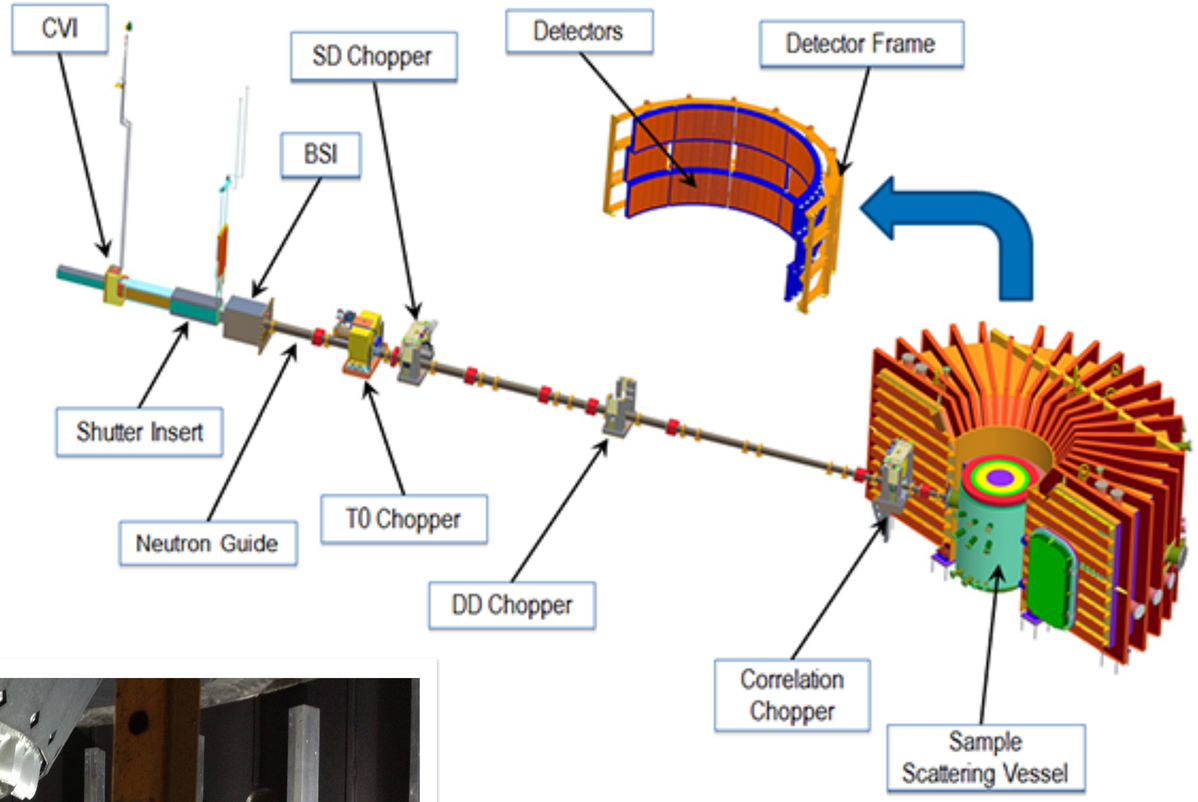


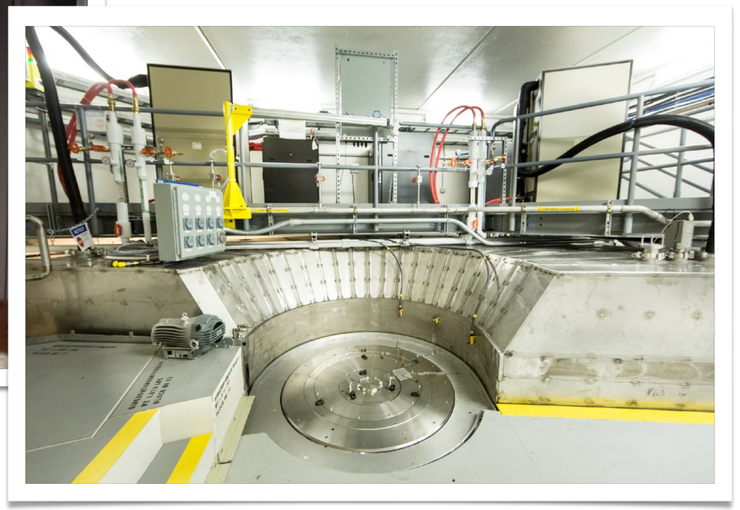
CORELLI

Instrument Scientists

Feng Ye

Arianna Minelli





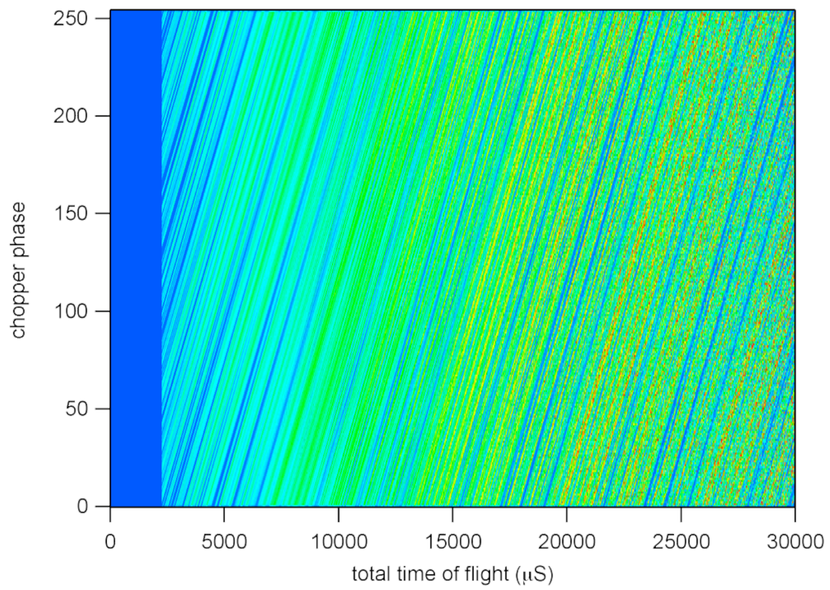
Instrument Proposers

Stephan Rosenkranz

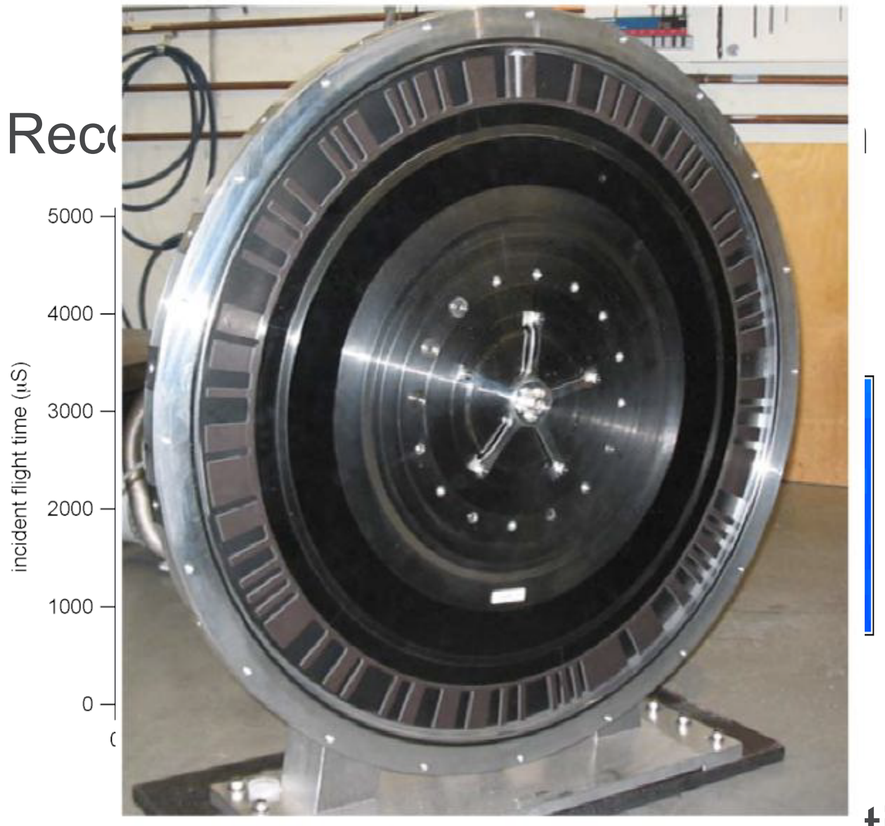
Ray Osborn

CROSS CORRELATION IN ACTION

Raw Data



Cross Correlation

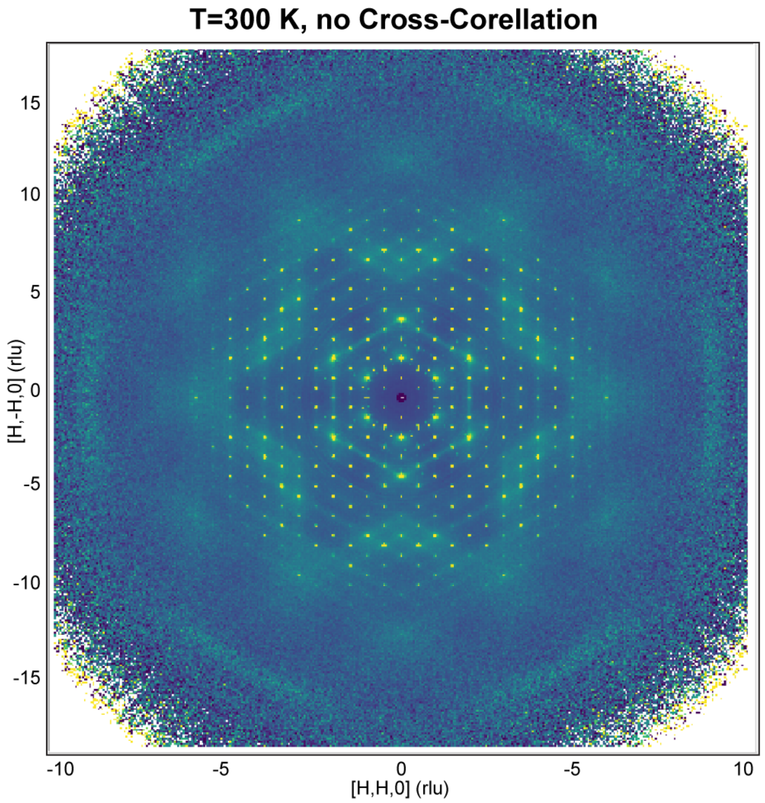


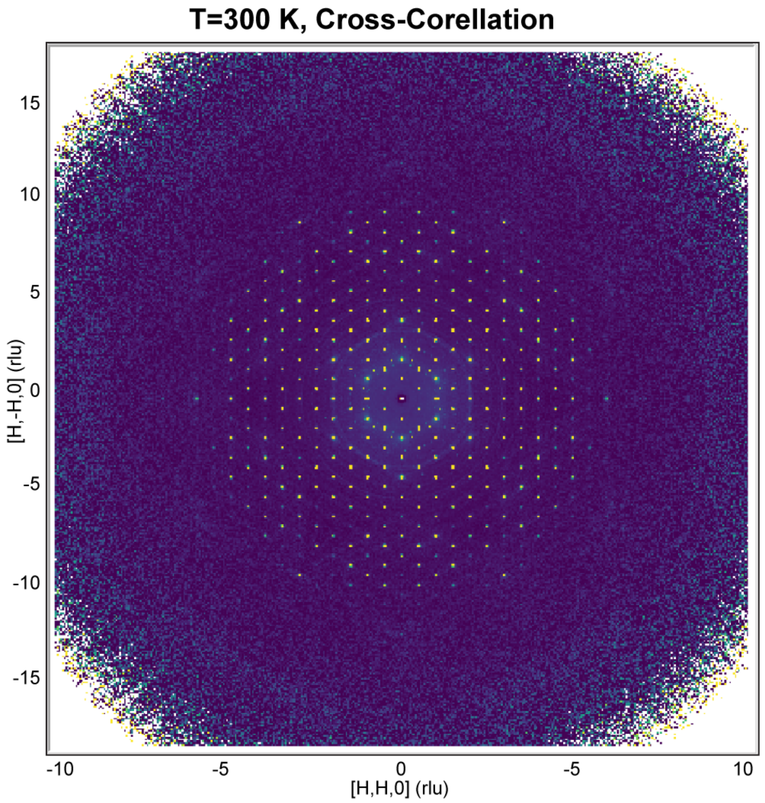
elastic

inelastic

ELASTIC DISCRIMINATION WITH CROSS CORRELATION

Benzil $C_{14}H_{10}O_2$

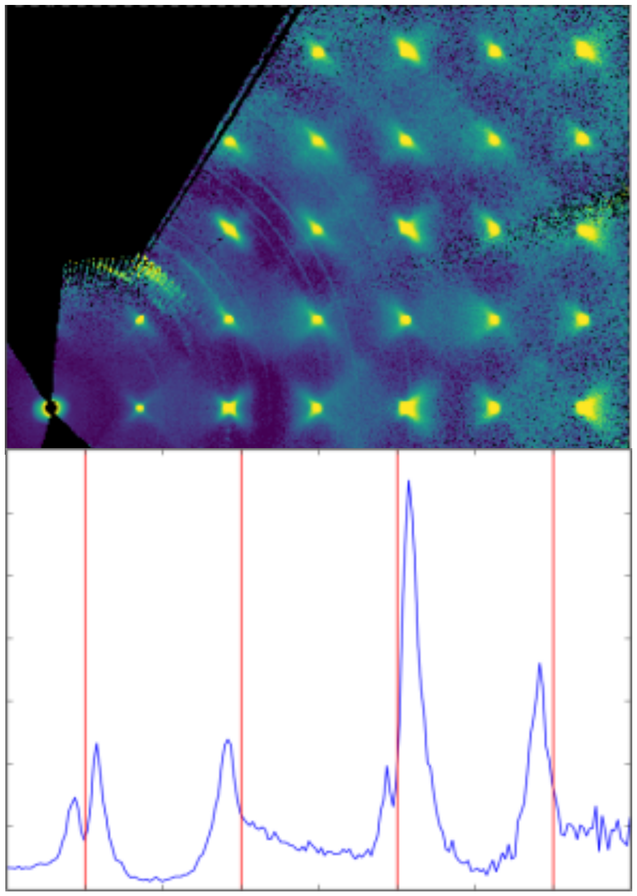




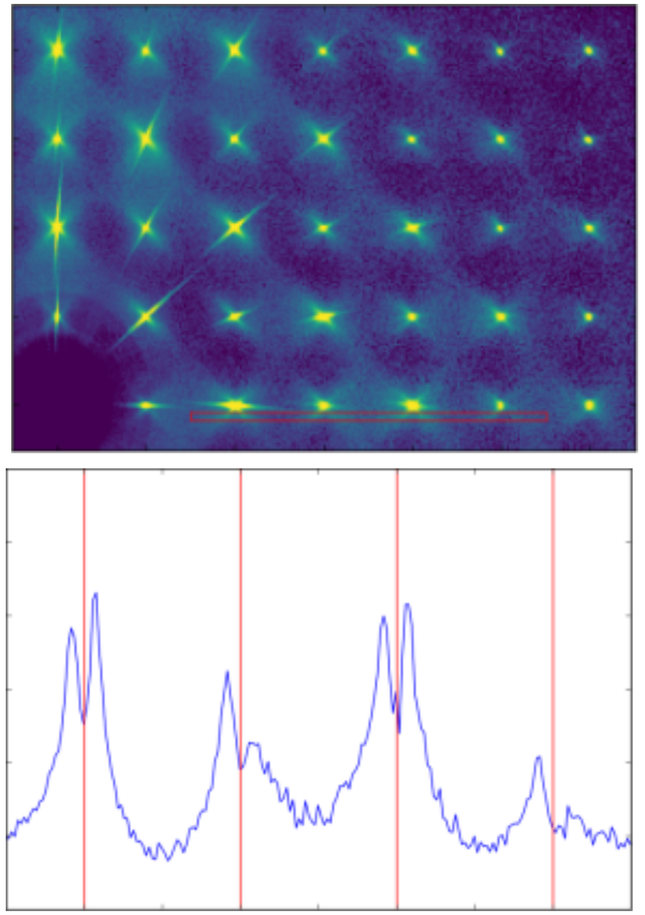
T. R. Welberry and R. Whitfield, Quantum Beam Science **2**, 2 (2018)

COMPLEMENTARITY OF NEUTRONS AND X-RAYS

$Pb(Mg_{1/3}Nb_{2/3})O_3$-30%$PbTiO_3$ — M. J. Krogstad, *et al.*, Nat Mater **48**, 1 (2018).



Corelli Neutrons



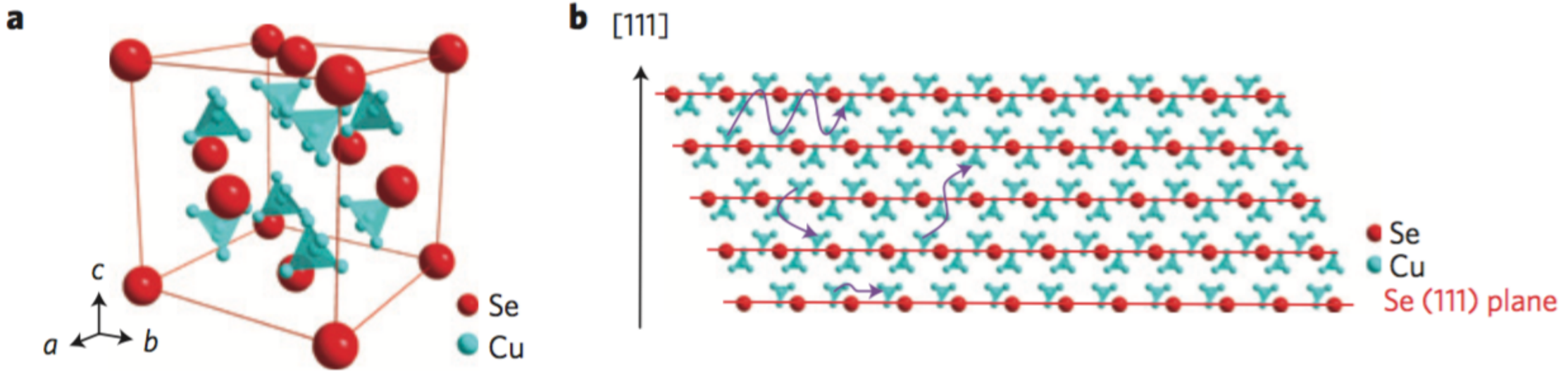
CHESS 55keV X-rays

SUBLATTICE MELTING IN SUPERIONIC $Cu_{1.8}Se$

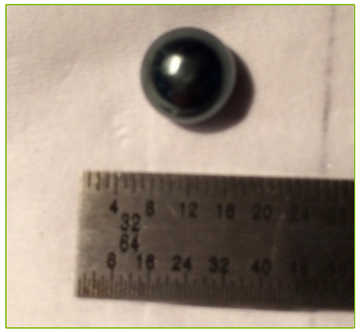
LETTERS
PUBLISHED ONLINE: 11 MARCH 2012 | DOI: 10.1038/NMAT3273
nature materials

Copper ion liquid-like thermoelectrics

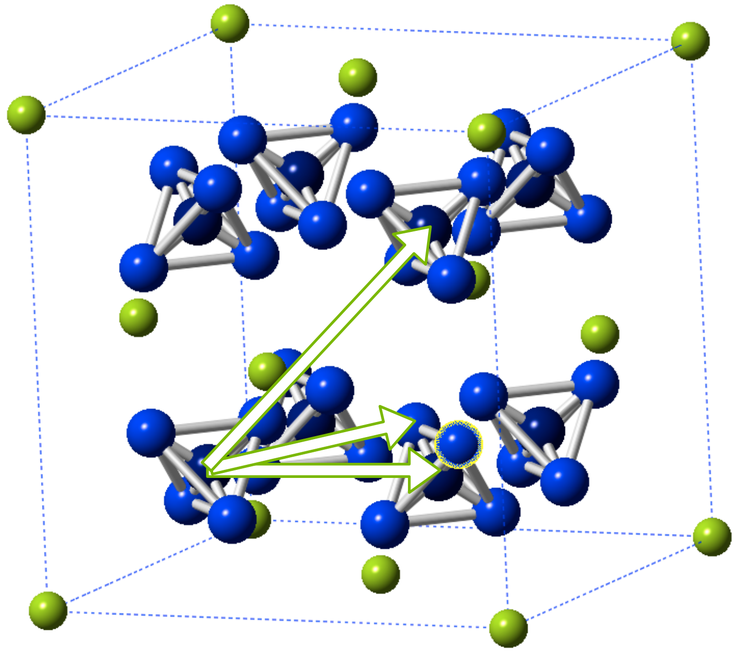
Huili Liu[1,2], Xun Shi[1,3]*, Fangfang Xu[3], Linlin Zhang[3], Wenqing Zhang[3], Lidong Chen[1]*, Qiang Li[4], Ctirad Uher[5], Tristan Day[6] and G. Jeffrey Snyder[6]

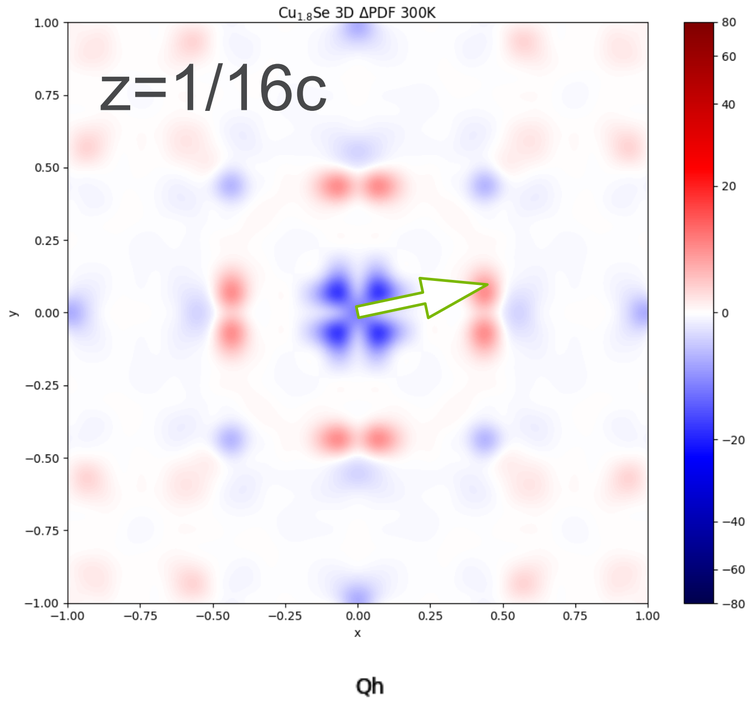


3D-ΔPDF ON CORELLI



Alex Rettie

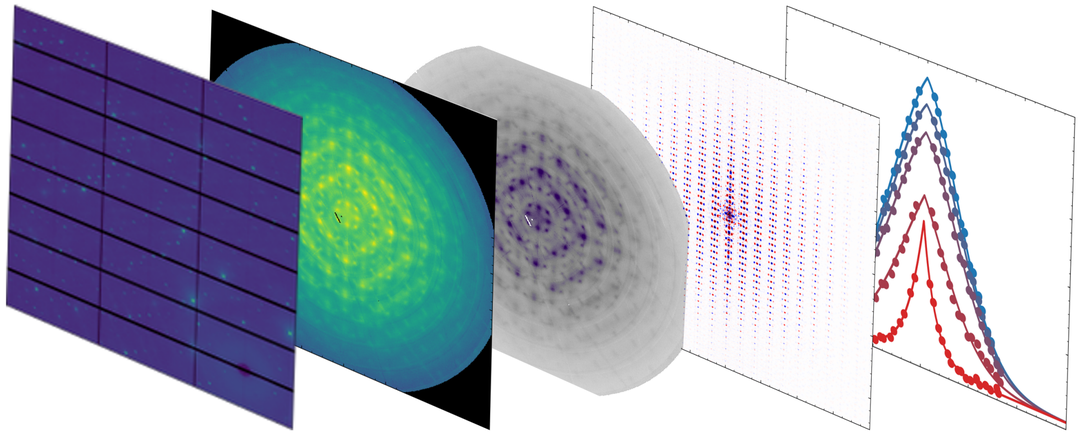




Symmetrized Corelli Data

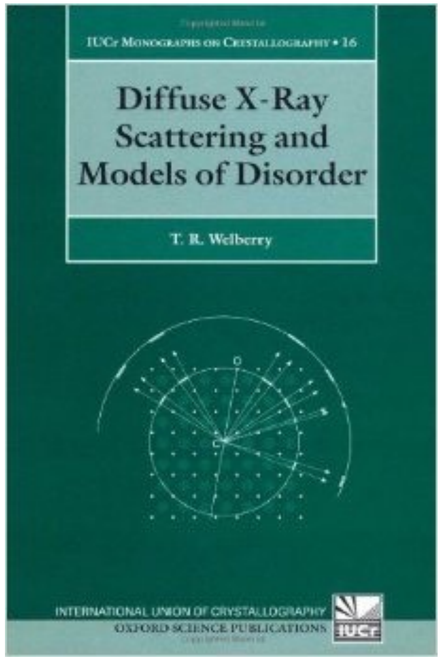
THE FUTURE

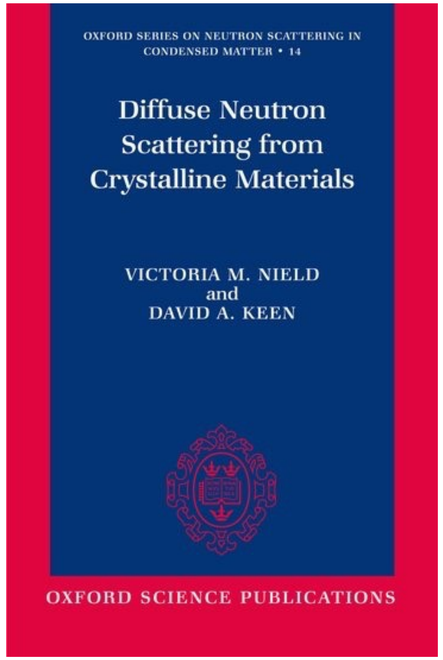
- Advances in instrumentation have transformed our ability to measure single crystal total scattering over large volumes of reciprocal space.
  - High-Energy X-rays
  - Time-of-Flight Neutrons
- This is enabling new ways of analyzing the data:
  1. Unsupervised machine learning
  2. *ab initio* computational modeling
  3. 3D-ΔPDF - real-space pair distributions
- The results give unique insight into disordered materials
  - Bridging the gap between diffraction and imaging

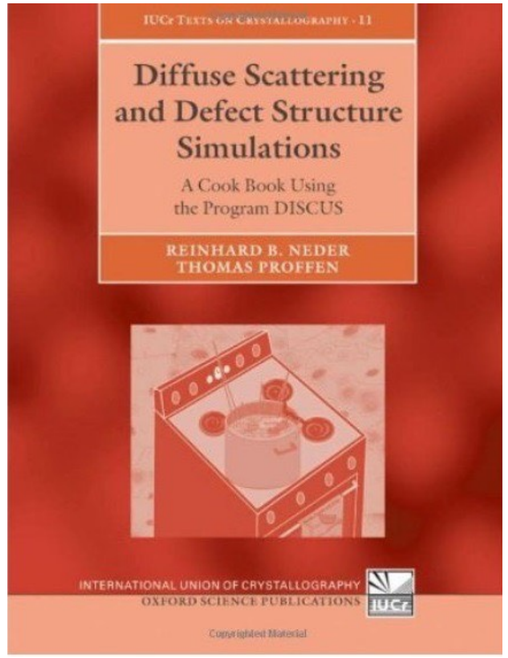


A FEW REFERENCES

- T. R. Welberry & B. Butler, Chem Rev **95**, 2369–2403 (1995).
- F. Frey, Acta Cryst B **51**, 592–603 (1995).
- T. R. Welberry & D. J. Goossens, Acta Cryst A **64**, 23–32 (2007).
- D. A. Keen & A. L. Goodwin, Nature News **521**, 303–309 (2015).







FEEDBACK

Single Crystal Diffuse Scattering - Raymond Osborn

- Lecture, Tuesday, August 6 - 11:10am to 12:10pm
- https://forms.office.com/g/NRAfaeWR71