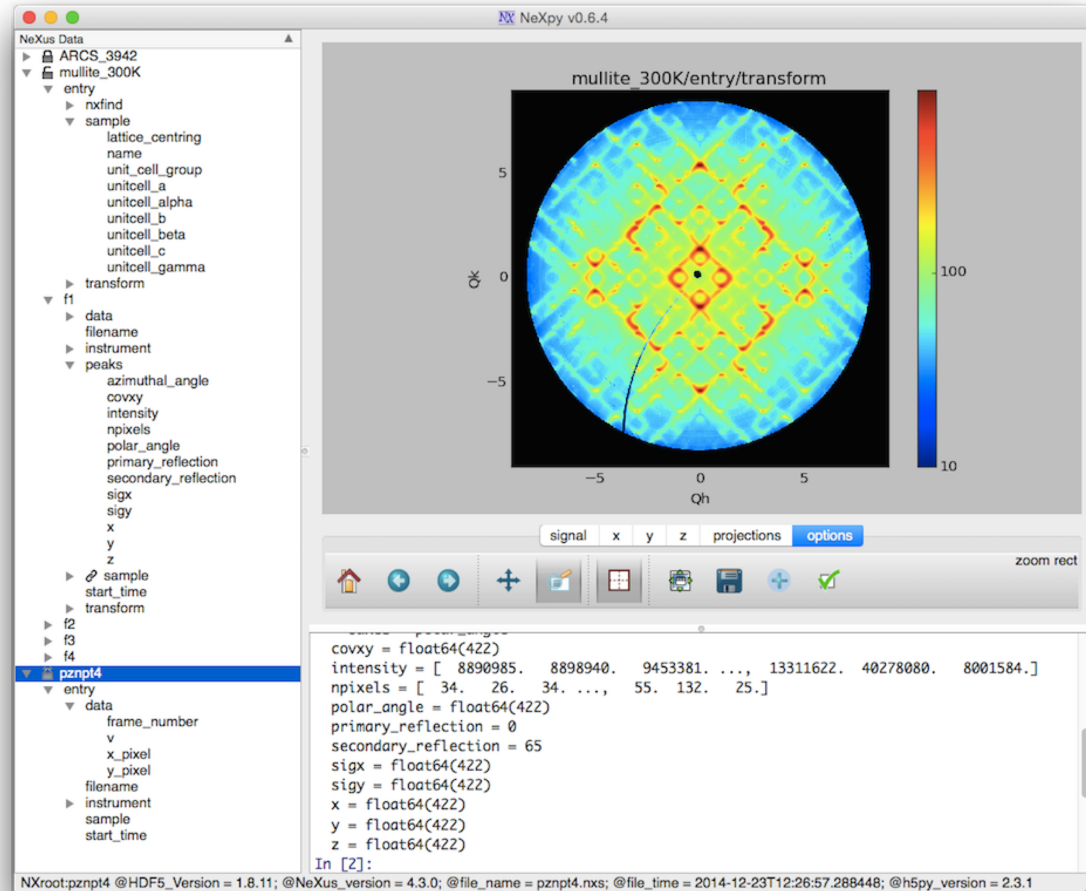
Single Crystal Diffuse Scattering

Ray Osborn

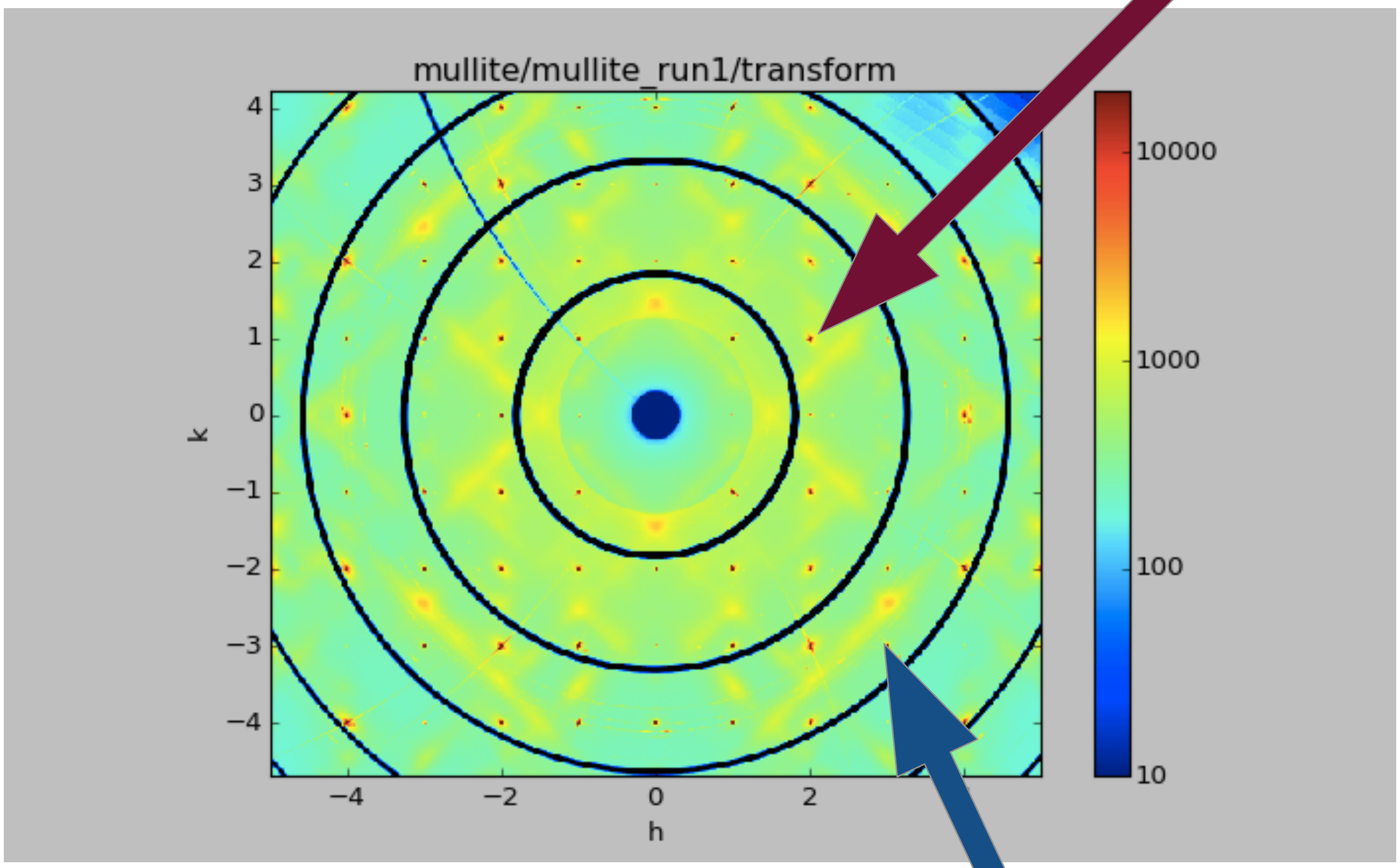
Neutron and X-ray Scattering Group
Materials Science Division
Argonne National Laboratory



Outline

- What is diffuse scattering?
  - What does it look like?
  - What causes it?
  - Who started it?
- What is it good for?
  - A random walk through disordered materials
- How do I model it?
  - A few equations
  - Rules of thumb
- Case Study 1: Diffuse scattering from vacancies in mullite
- Case Study 2: Huang scattering in bilayer manganites
- How do I look at static disorder?
  - Neutrons *vs* X-rays
  - Corelli - Diffuse scattering with elastic discrimination
- Diffuse scattering - the musical

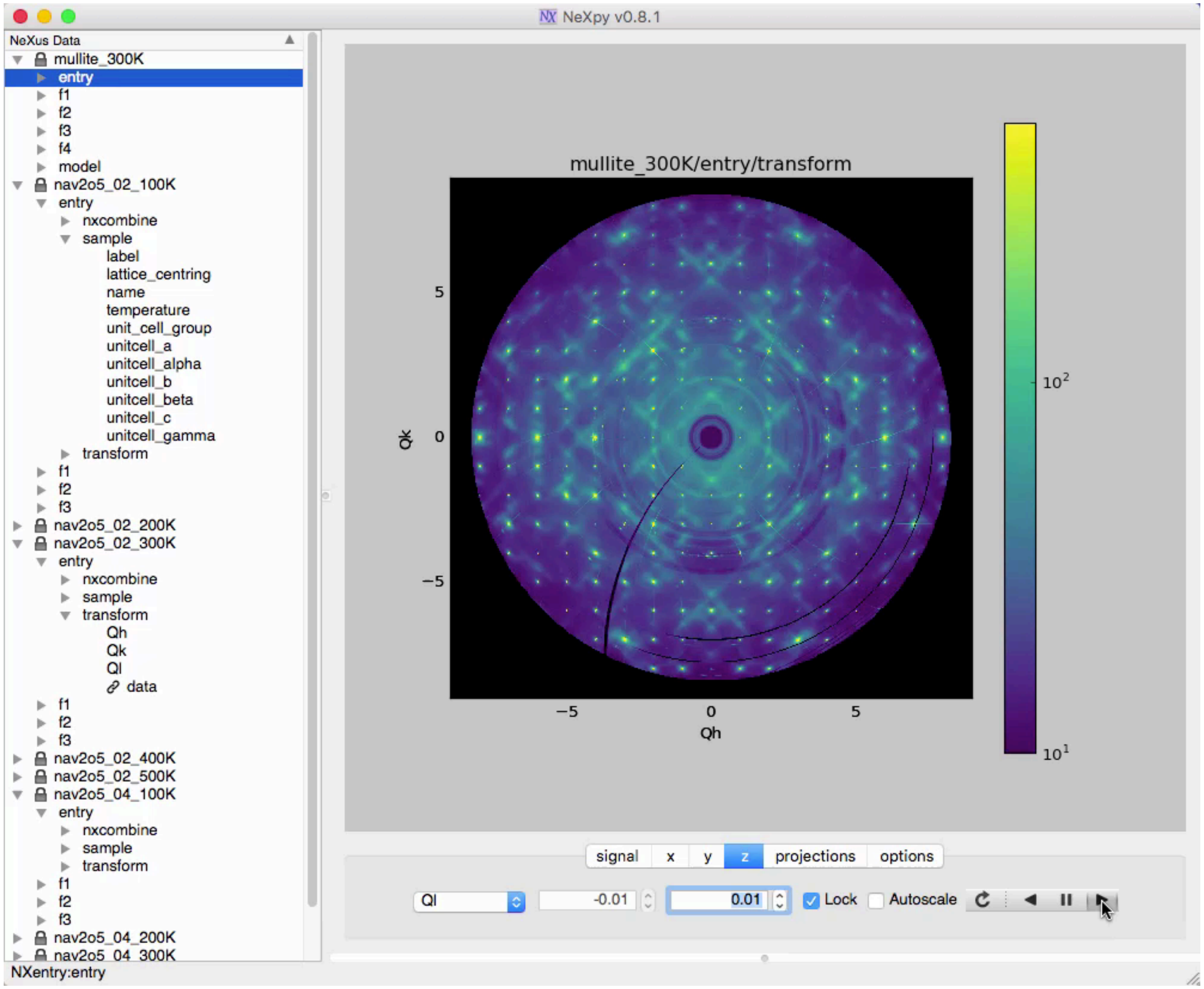
Bragg Scattering *vs* Diffuse Scattering



Bragg Scattering
Average Structure

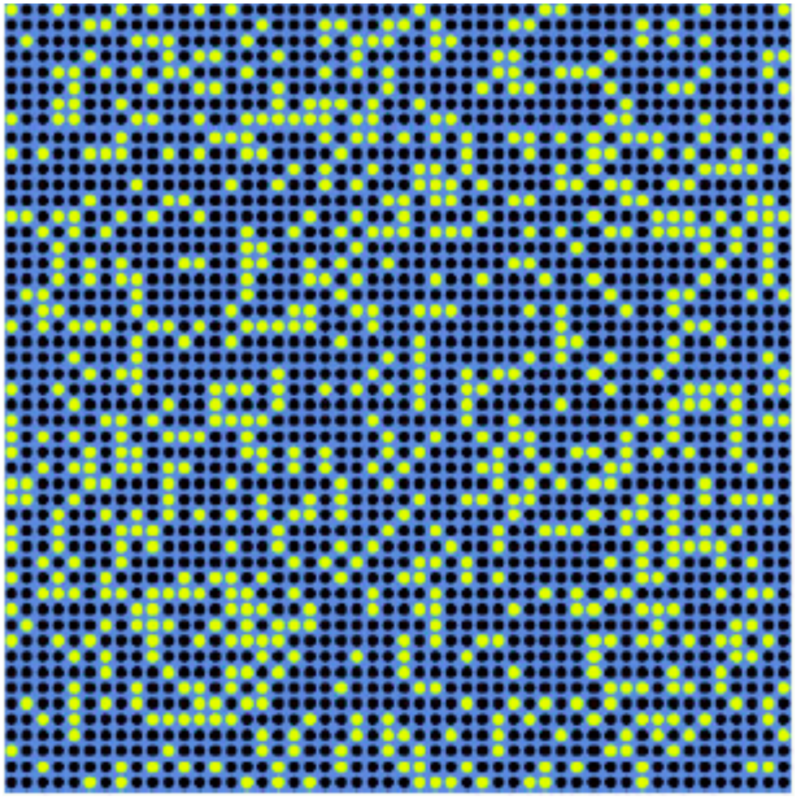
Diffuse Scattering
Deviations from the Average Structure

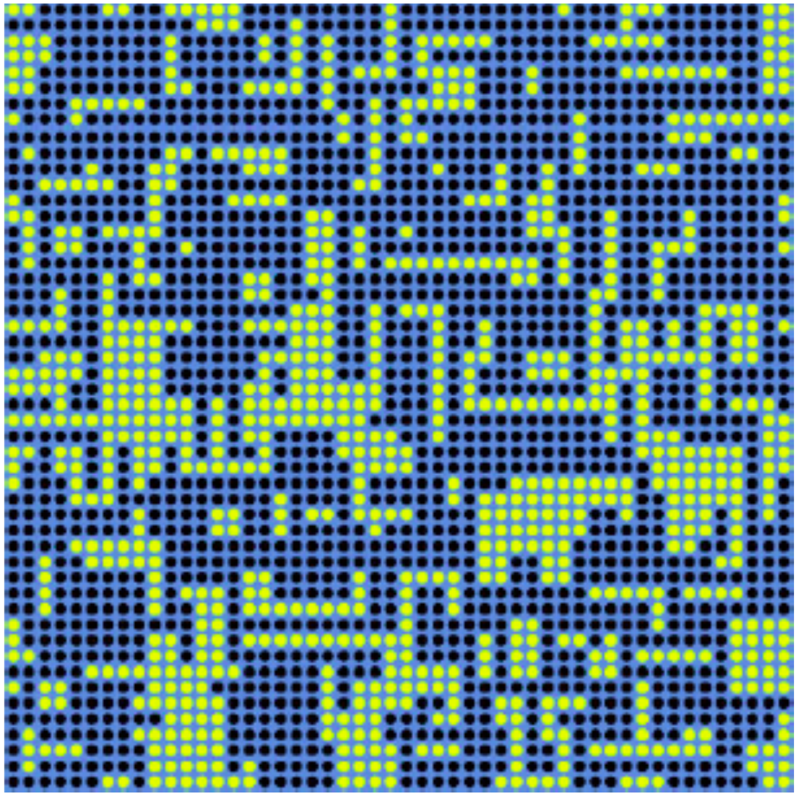
Single Crystal Diffuse Scattering in 3D



Simple Example of Disorder

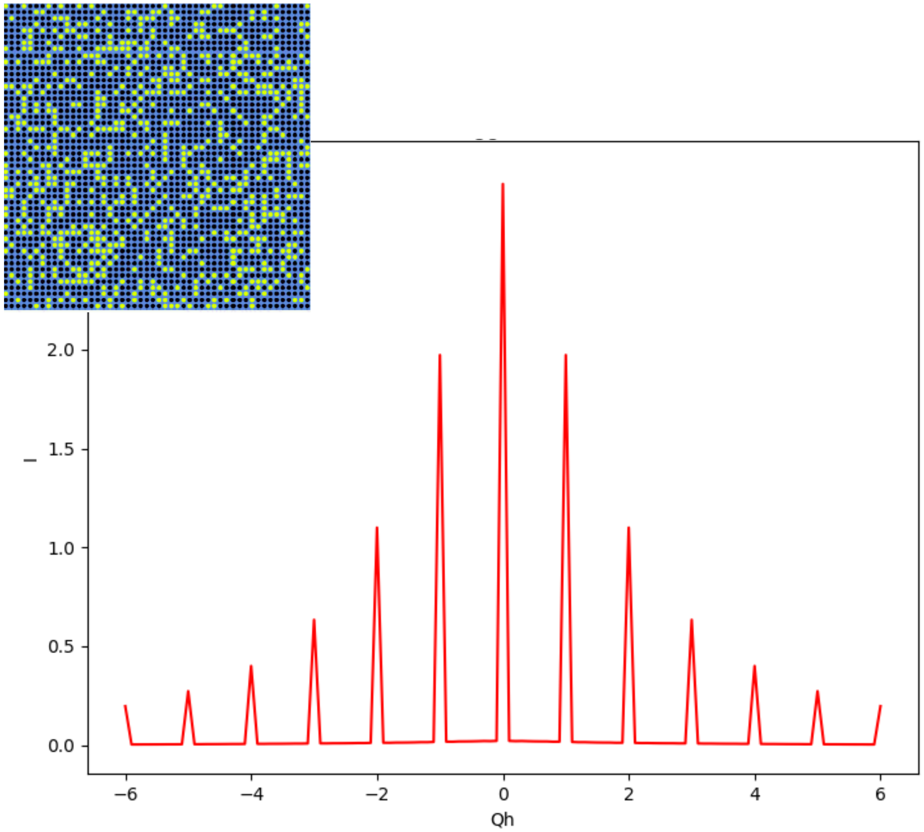
- In these examples, 30% of atoms (blue dots) have been replaced by vacancies (green dots)
  - Left-Hand-Side: random substitution
  - Right-Hand-Side: high probability of vacancy clusters
    - Thanks to Thomas Proffen

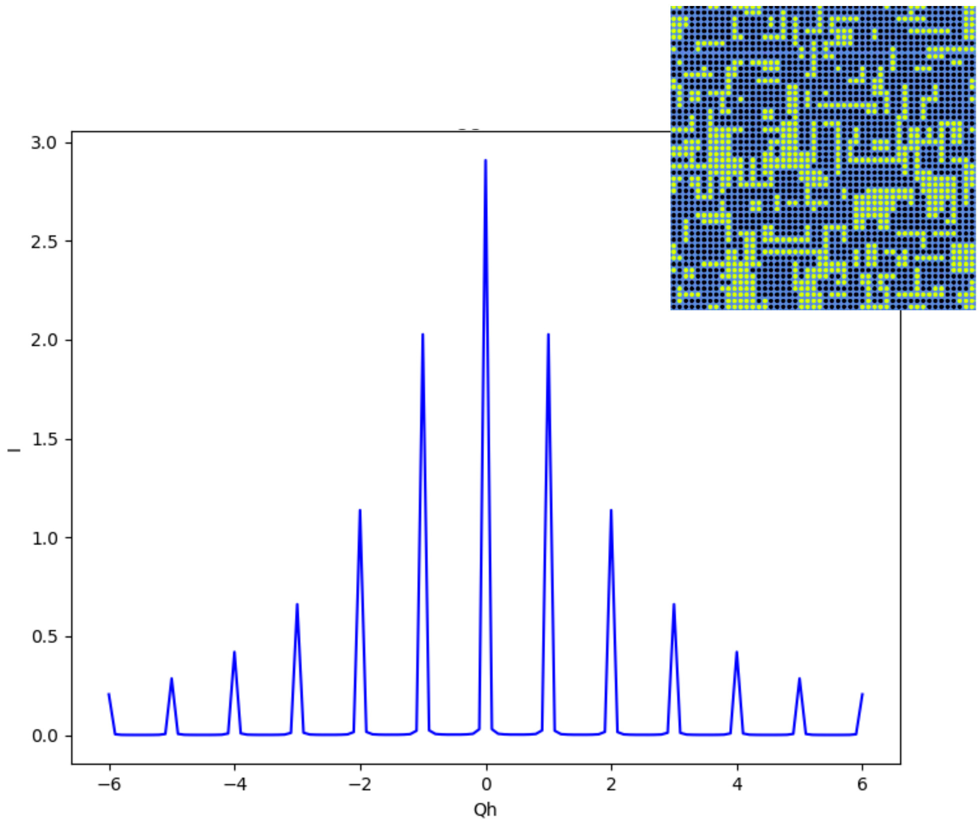




Bragg Scattering

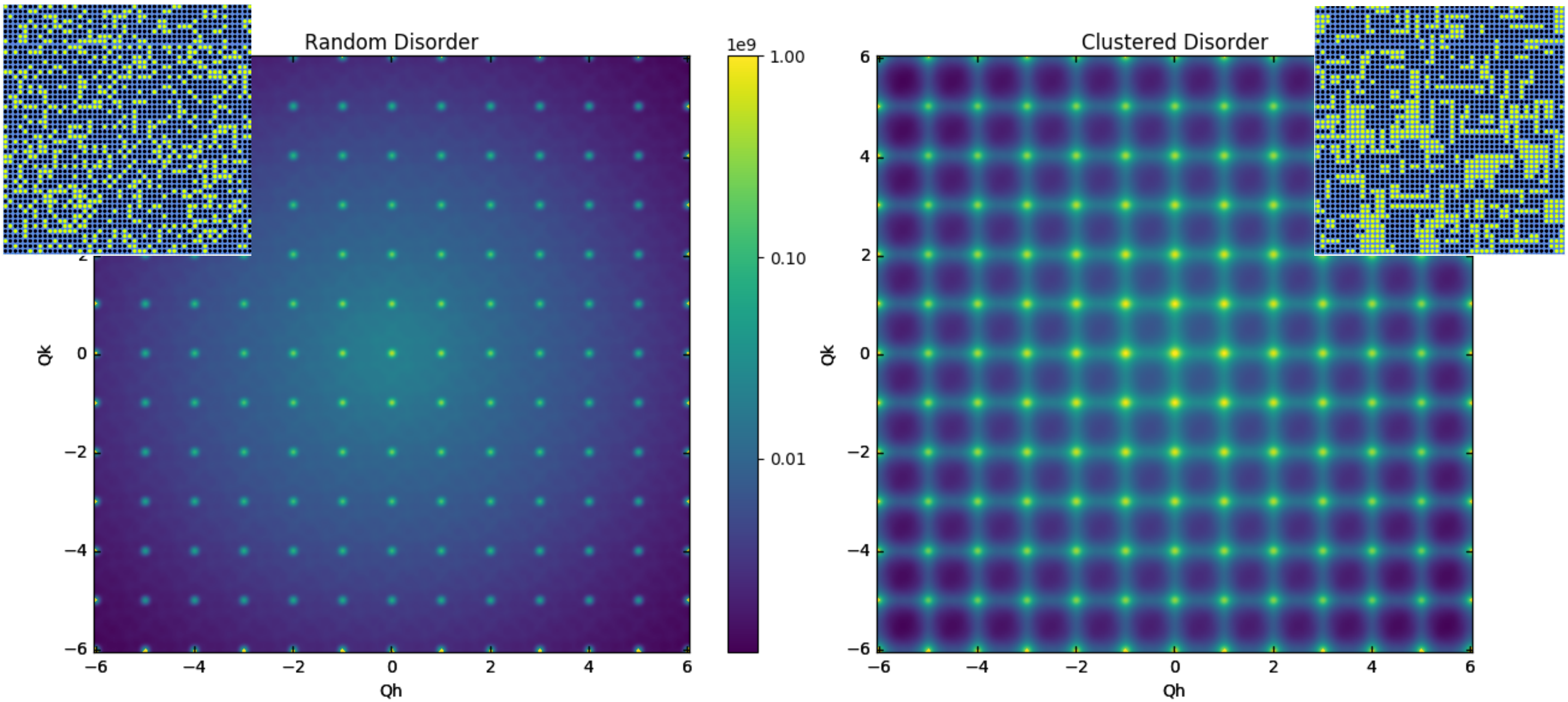
- Bragg scattering is determined by the average structure.
  - Since the average vacancy occupation is identical, both examples have identical Bragg peaks



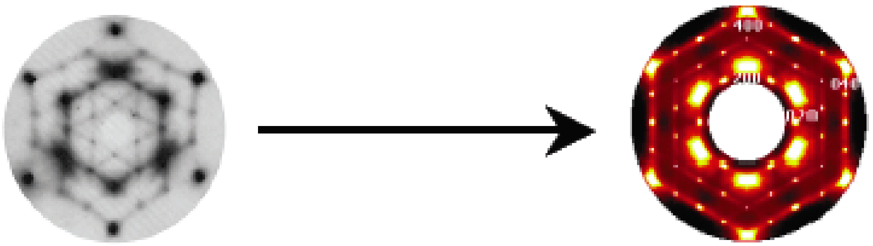


Diffuse Scattering

- The diffuse scattering is quite different in the two examples
  - Random vacancy distributions lead to a constant background (Laue monotonic scattering)
  - Vacancy clusters produce rods of diffuse scattering connecting the Bragg peaks



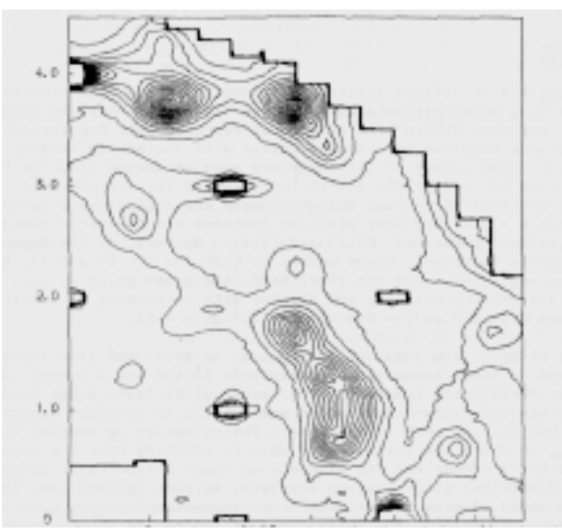
An Ultra-Short History of Advances in Diffuse Scattering

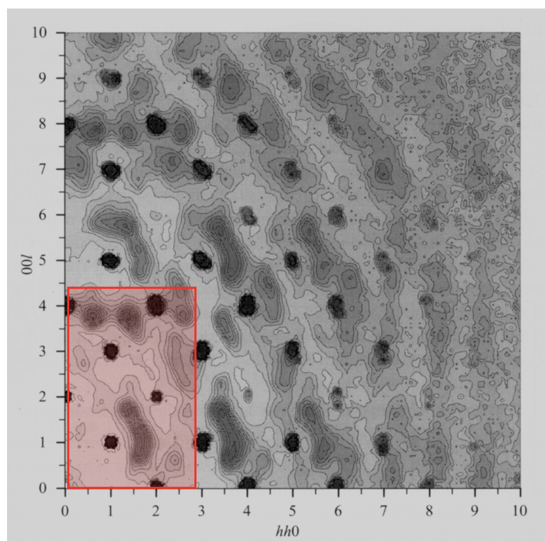


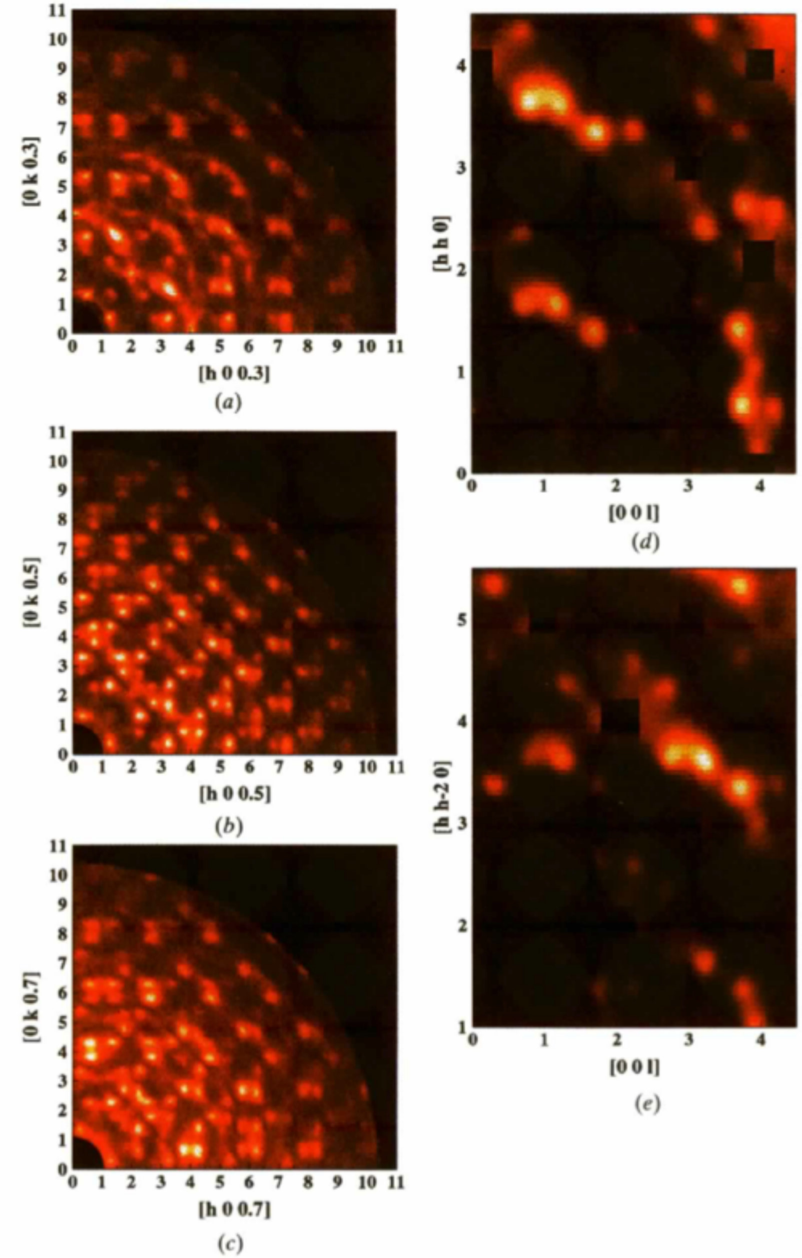
1941 2001

BENZIL

Yttria-Stabilized Zirconia





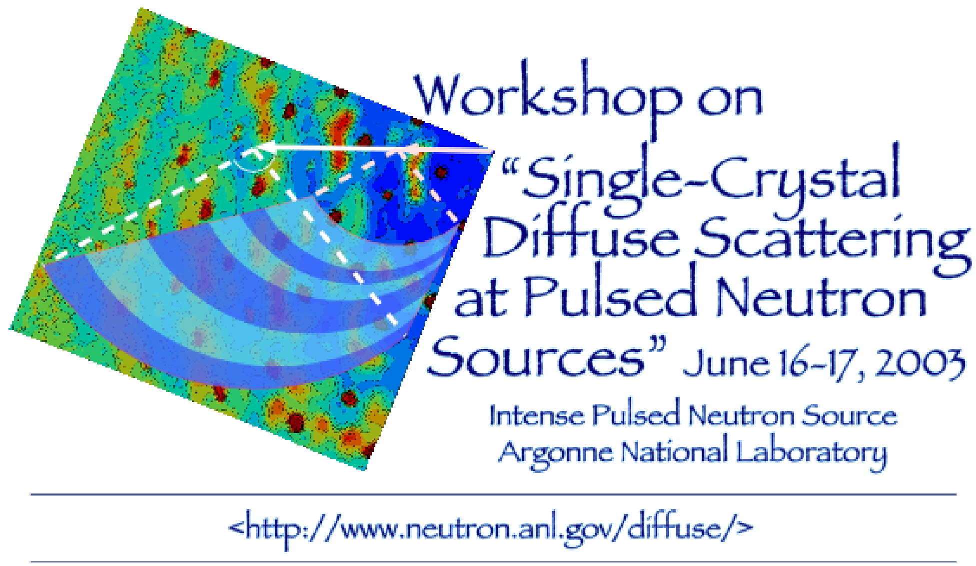


T. Proffen and T. R. Welberry J. Appl. Cryst. **31**, 318 (1998)

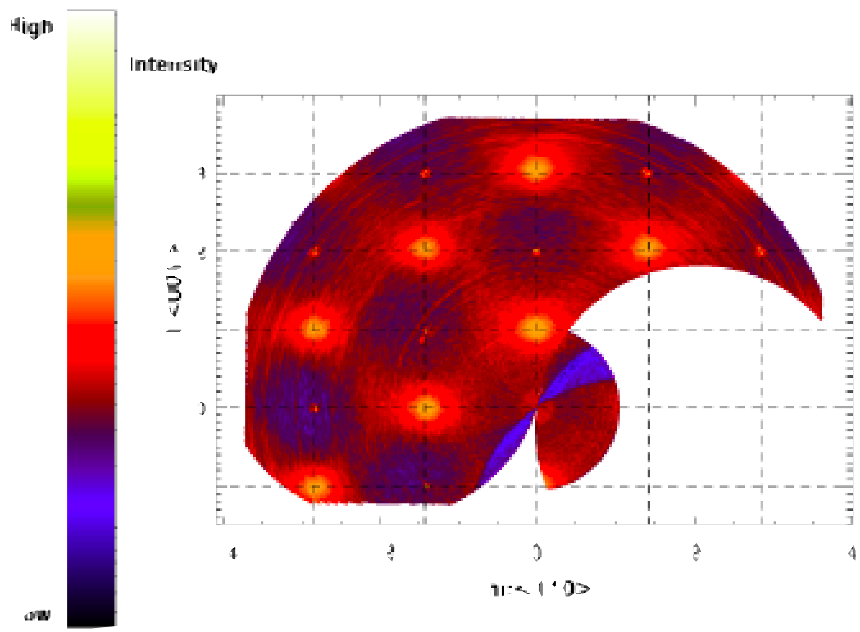
What is it good for?

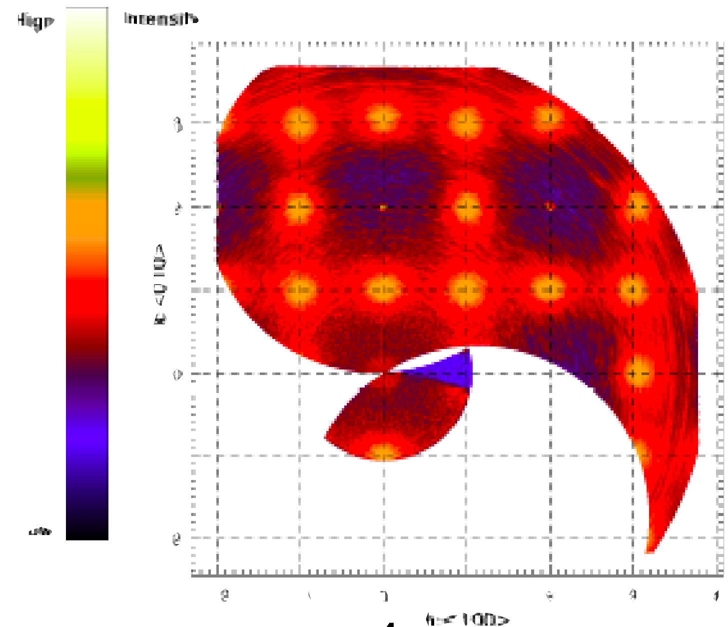
Science Impacted by Diffuse Scattering

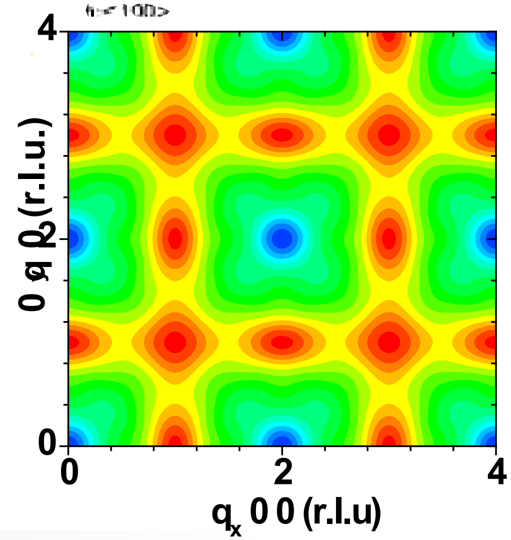
- Subjects identified at the *Workshop on Single Crystal Diffuse Scattering at Pulsed Neutron Sources*
  - Stripes in cuprate superconductors
  - Orbital correlations in transition metal oxides (including CMR)
  - Nanodomains in relaxor ferroelectrics
  - Defect correlations in fast-ion conductors
  - Geometrically frustrated systems
  - Critical fluctuations at quantum phase transitions
  - Orientational disorder in molecular crystals
  - Rigid unit modes in framework structures
  - Quasicrystals
  - Atomic and magnetic defects in metallic alloys
  - Molecular magnets
  - Defect correlations in doped semiconductors
  - Microporous and mesoporous compounds
  - Host-guest systems
  - Hydrogen-bearing materials
  - Soft matter - protein configurational disorder using polarization analysis of spin-incoherence
  - Low-dimensional systems
  - Intercalates
  - Structural phase transitions in geological materials



Diffuse Scattering from Metallic Alloys



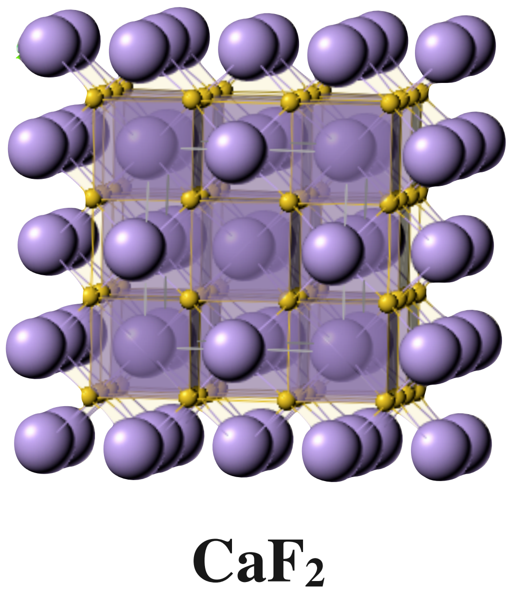


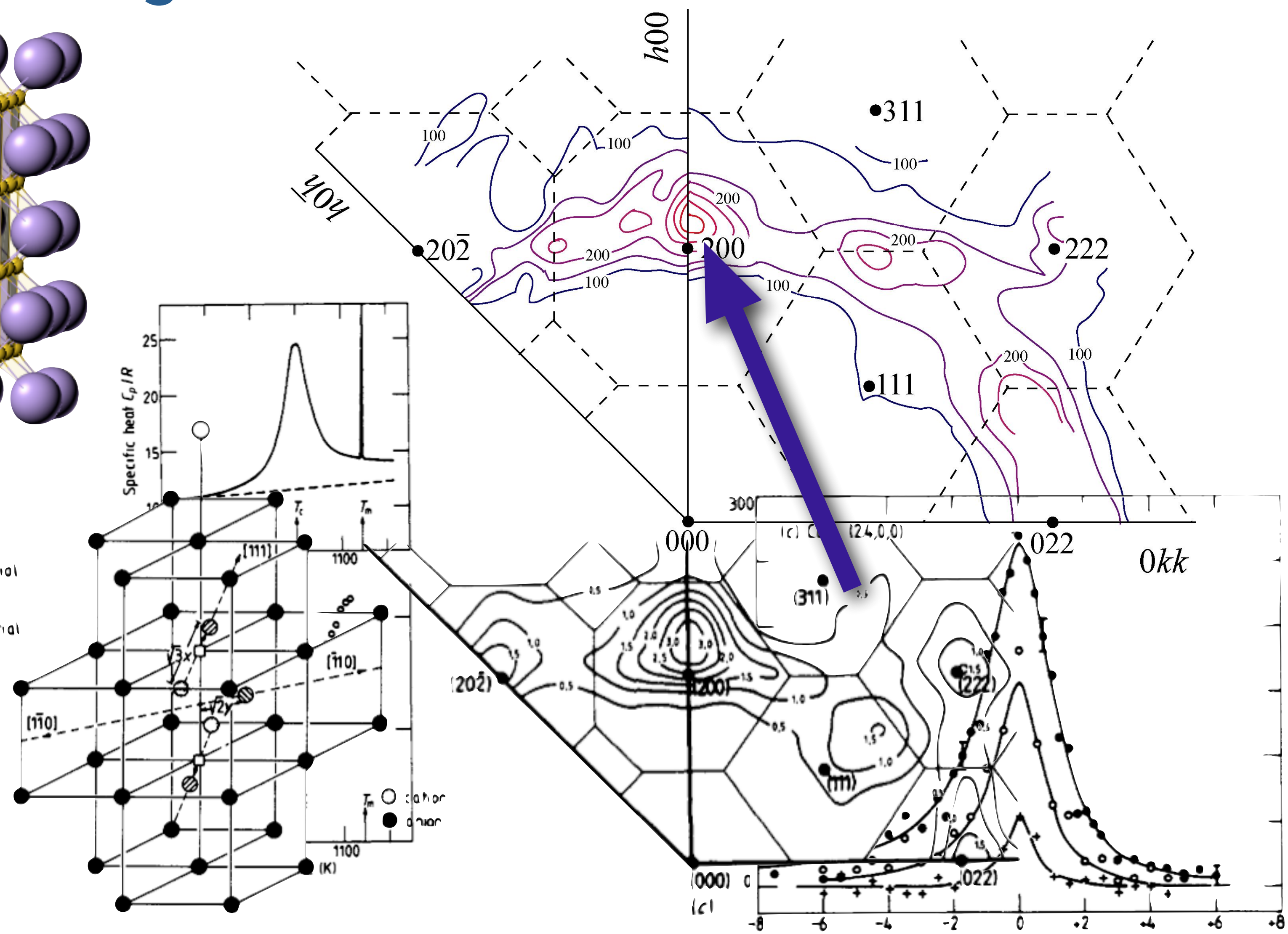


Short-range Order in Null Matrix $^{62}Ni_{0.52}Pt_{0.52}$

J. A. Rodriguez, S. C. Moss, J. L. Robertson, J. R. D. Copley, D. A. Neumann, and J. Major
Phys. Rev. B **74**, 104115

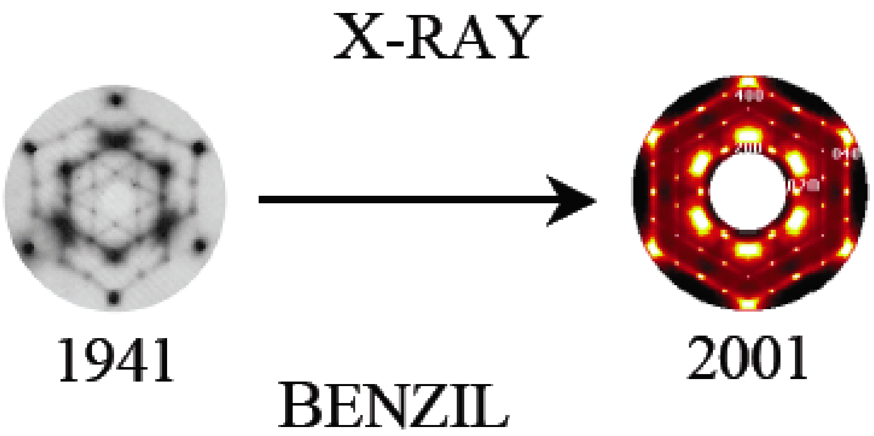
Diffuse Scattering from a Fast-Ion Conductor

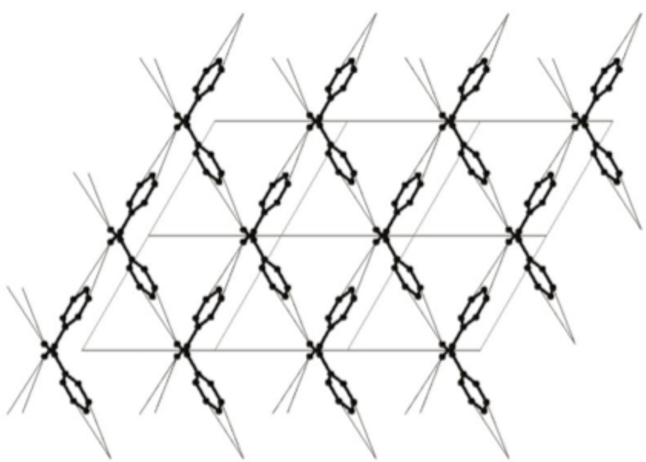


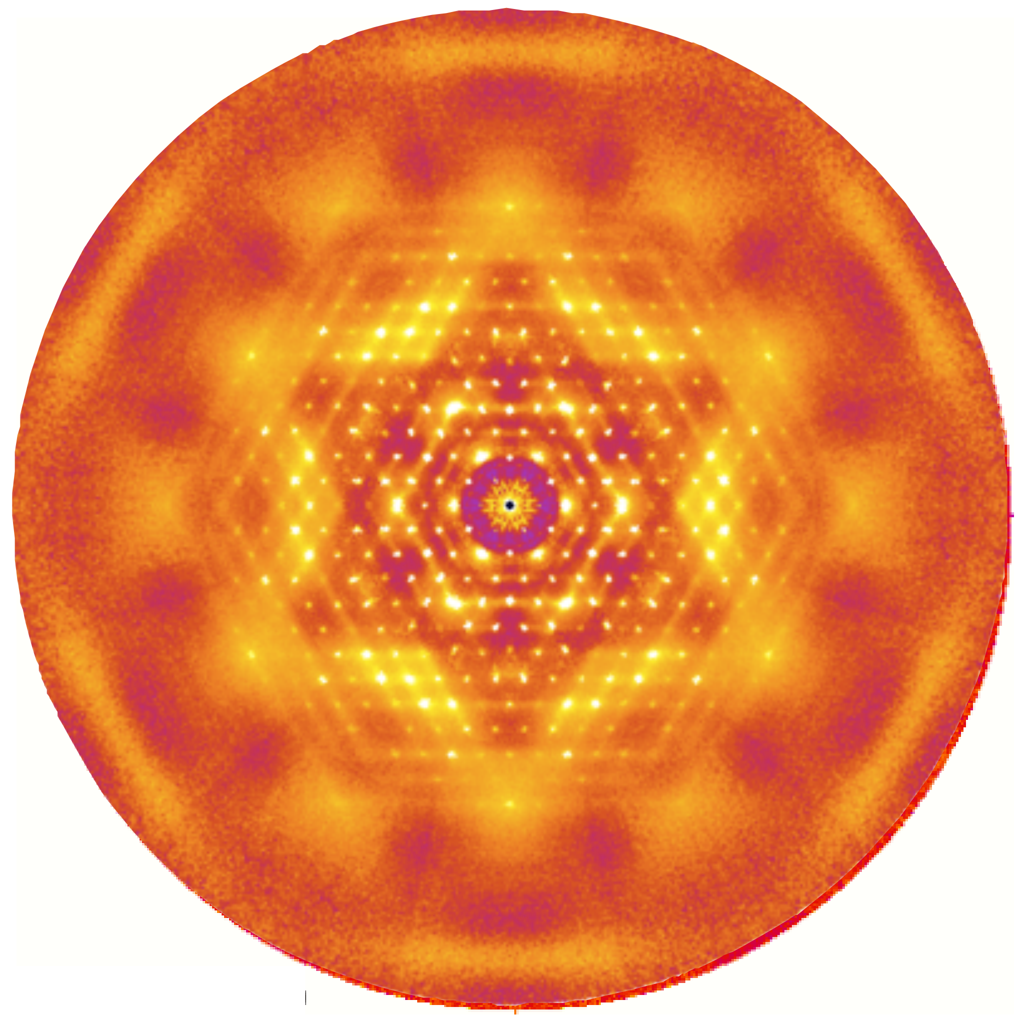


M. T. Hutchings *et al* J. Phys. C **17**, 3903 (1984)

Diffuse Scattering from Molecular Solids

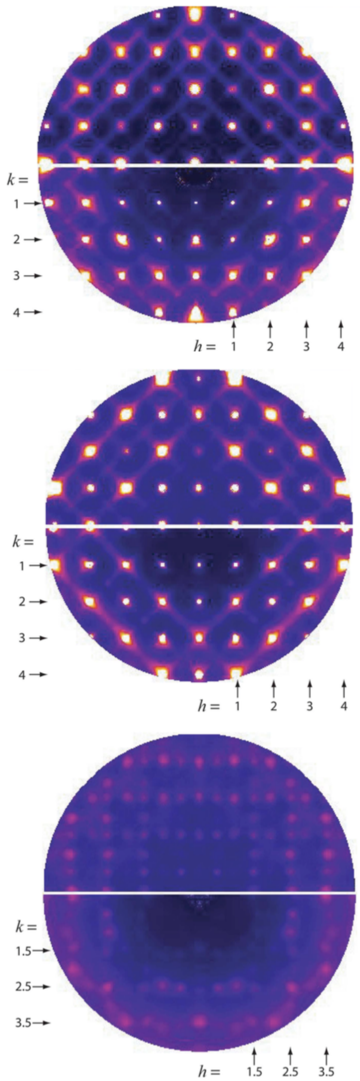


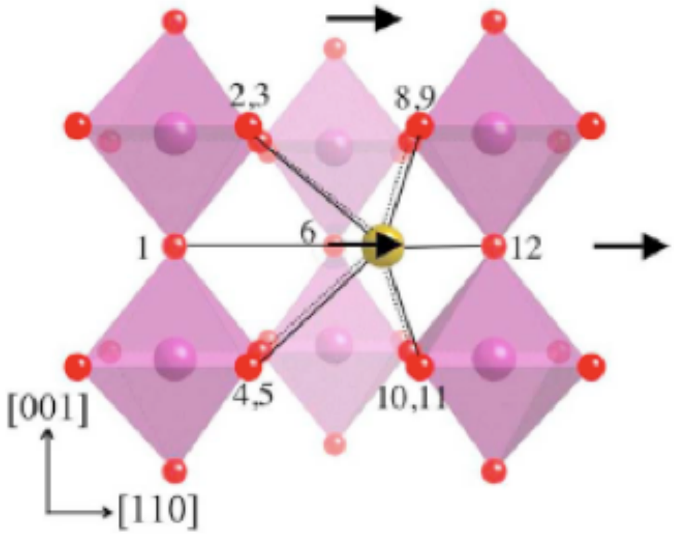




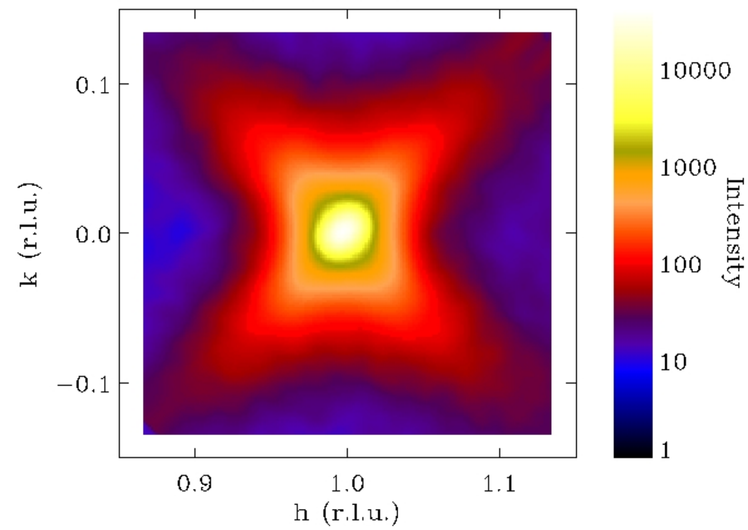
T. R. Welberry *et al* J. Appl. Cryst. **36**, 1400 (2003)

Diffuse Scattering from Relaxor Ferroelectrics

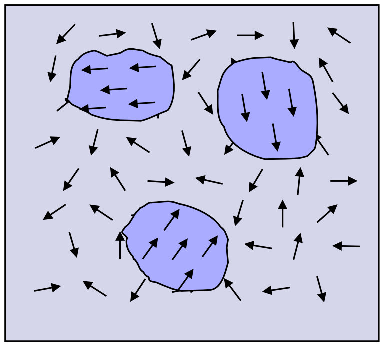


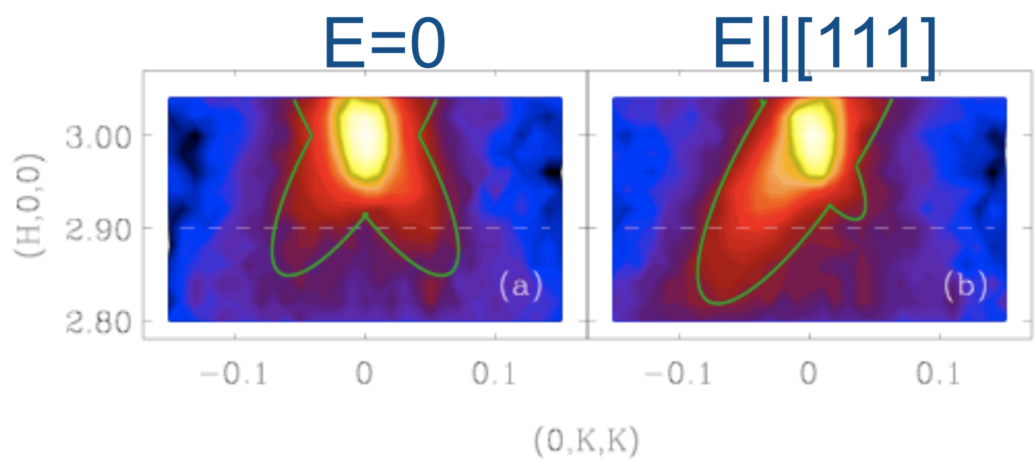


Lead Magnesium-Niobate



Lead Zinc-Niobate

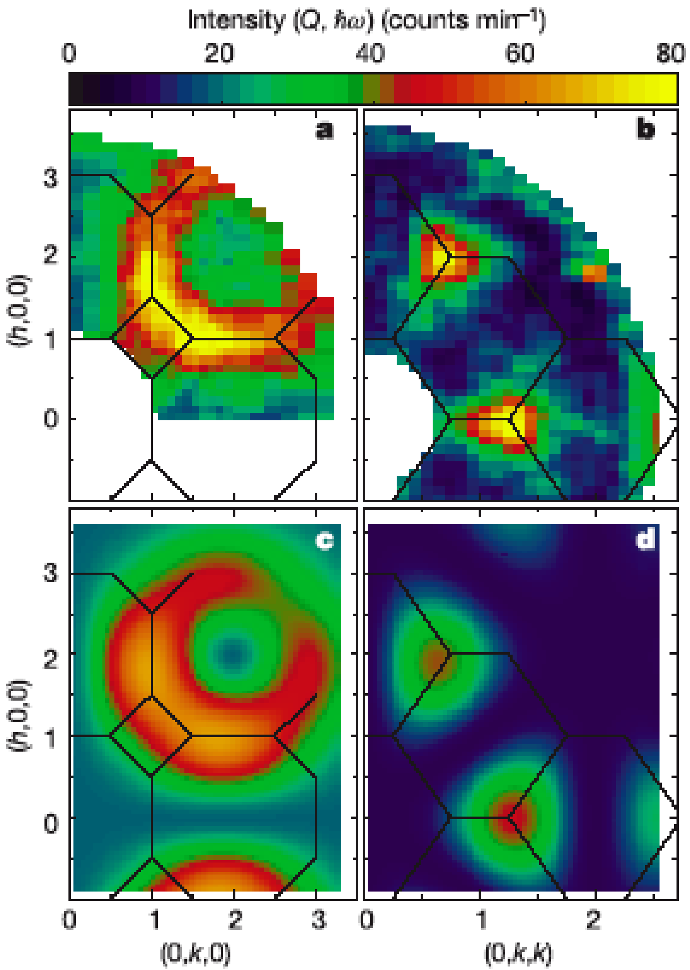


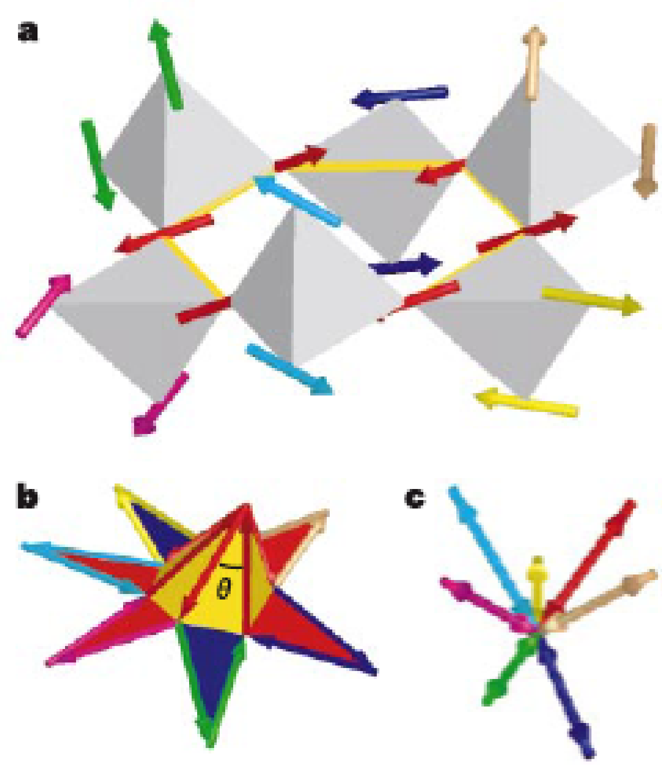


T. R. Welberry *et al* J. Appl. Cryst. **38**, 639 (2005)

G. Xu, P. M. Gehring, G. Shirane, Phys. Rev. B **72**, 214106 (2005).

Magnetic Diffuse Scattering from Geometric Frustration





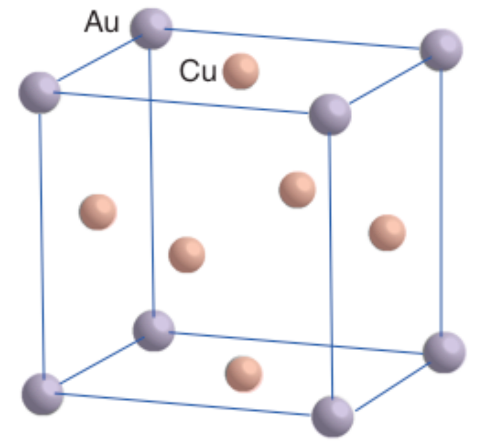
$ZnCr_2O_4$

S.-H. Lee *et al* Nature **418**, 856 (2002)

How do I model it?

A Few Equations

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* (2004)



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

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

- **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**

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

- **Warren Size Effect**

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

- **Borie and Sparks Correlations**

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

Three-Dimensional Pair Distribution Functions

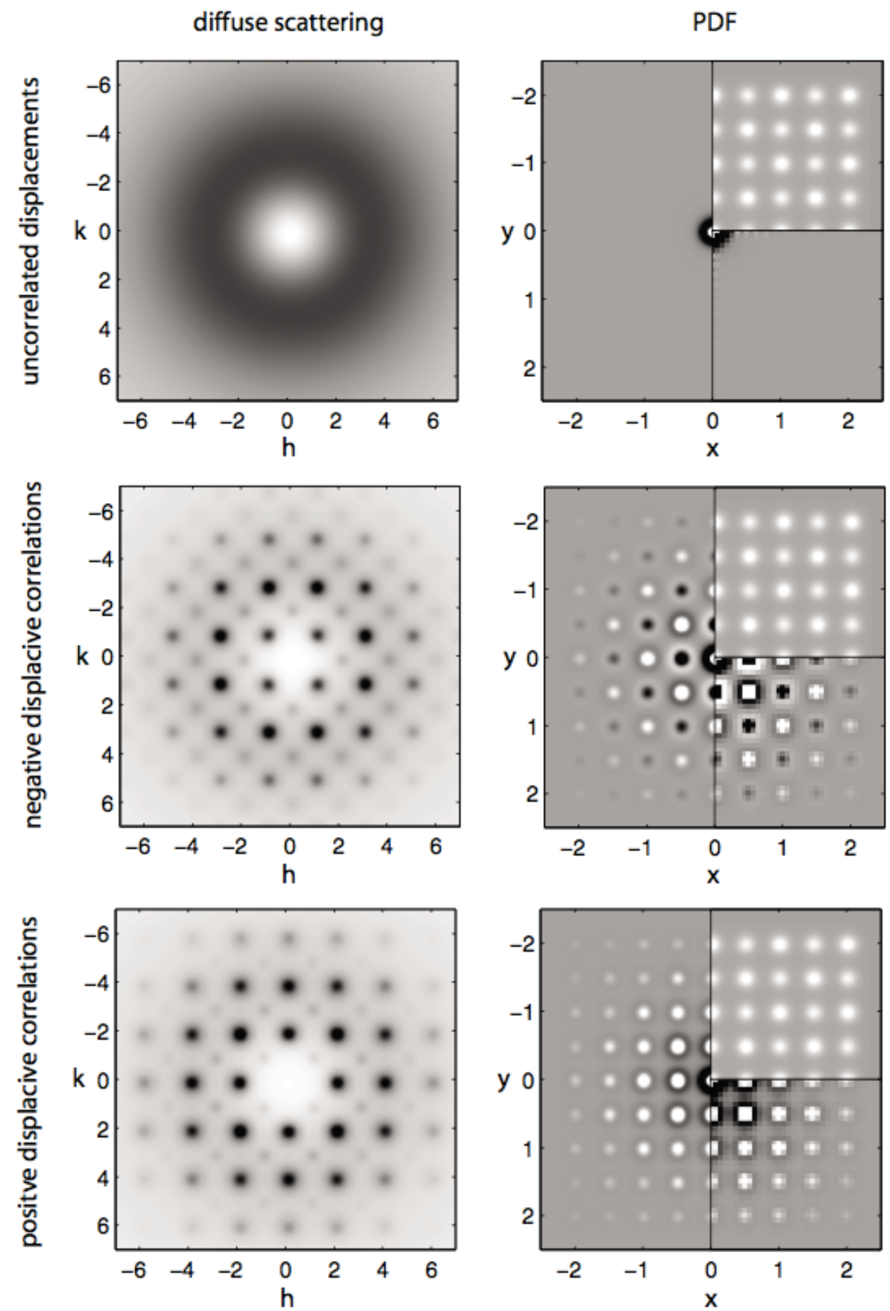
- The ability to measure three-dimensional S(**Q**) over a wide range of reciprocal space provides the 3D analog of PDF measurements.
  - Total PDFs if Bragg peaks and diffuse scattering can be measured simultaneously
  - Δ-PDFs if the Bragg peaks are eliminated
    - using the punch and fill method
- This would allow a model-independent view of the measurements in real space.

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

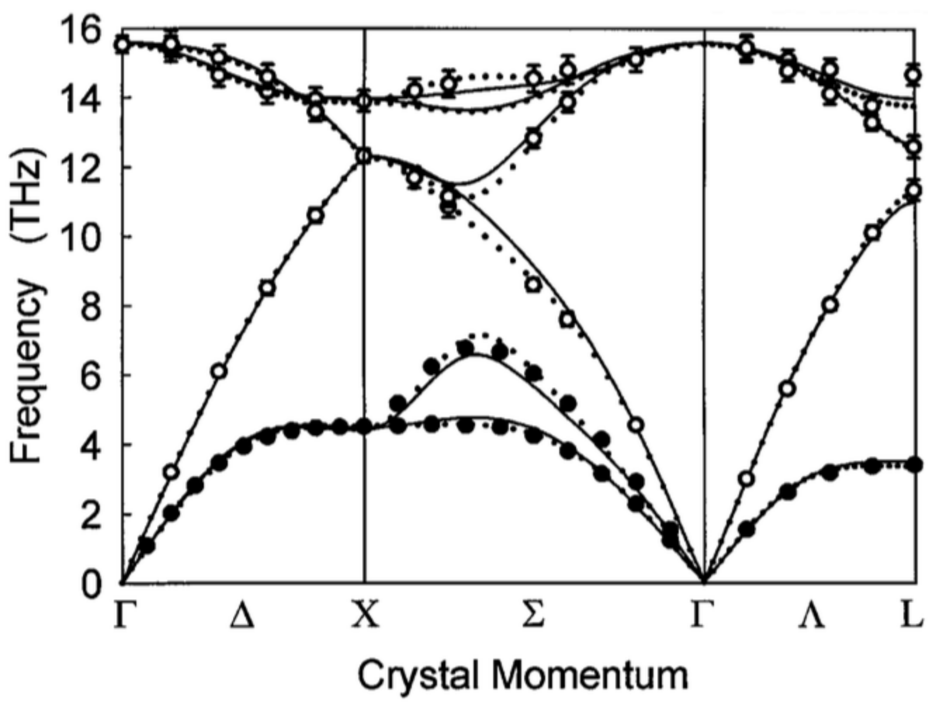
Thomas Weber* and Arkadiy Simonov

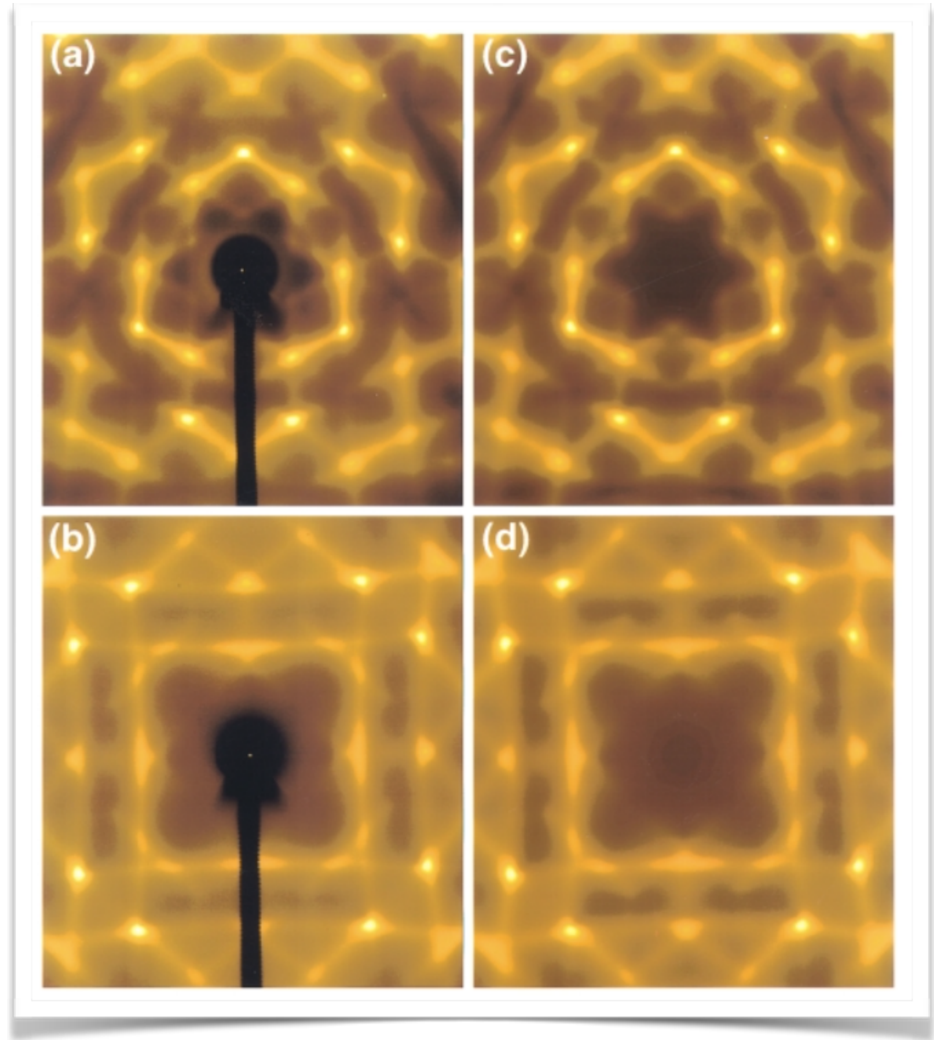
Laboratory of Crystallography, ETH Zurich Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland



Thermal Diffuse Scattering

- 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**





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

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

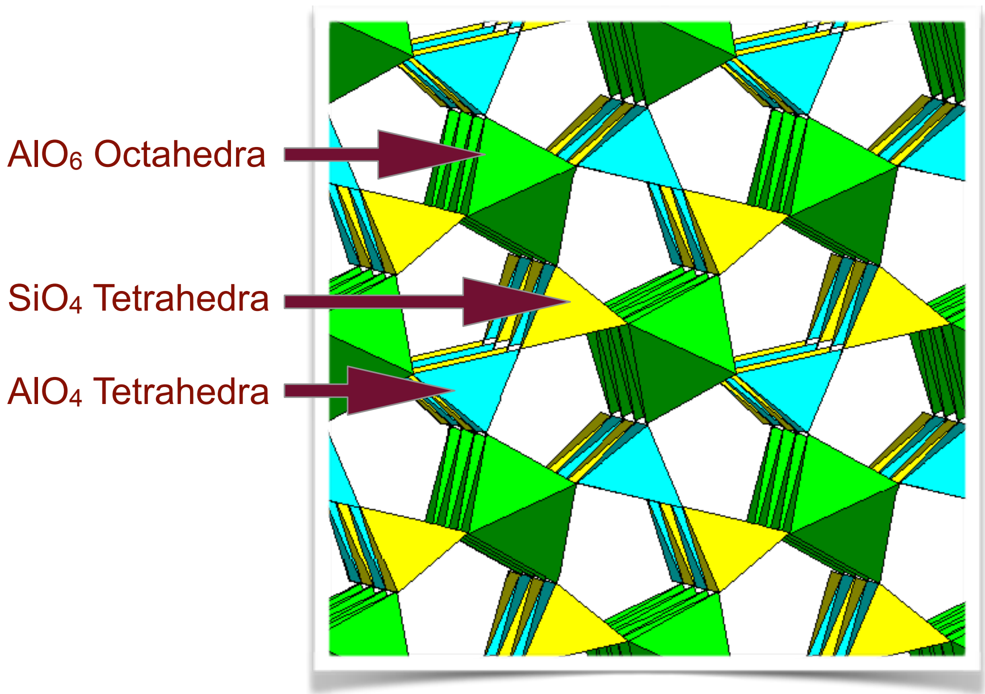
Some Rules of Thumb (*thanks to* Hans Beat Bürgi)

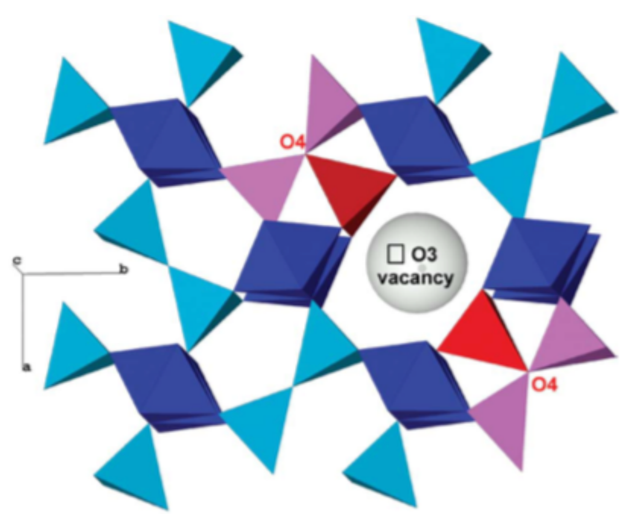
Reciprocal space		Direct space
Only sharp Bragg reflections	→	3D-periodic structure • no defects
Sharp diffuse rods	→	2D-periodic structure • perpendicular to the streaks • disordered in streak directions
Sharp diffuse planes	→	1D-periodic structure • perpendicular to the planes • disordered within the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

Case Study 1: Mullite

Mullite - A Case Study

- 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



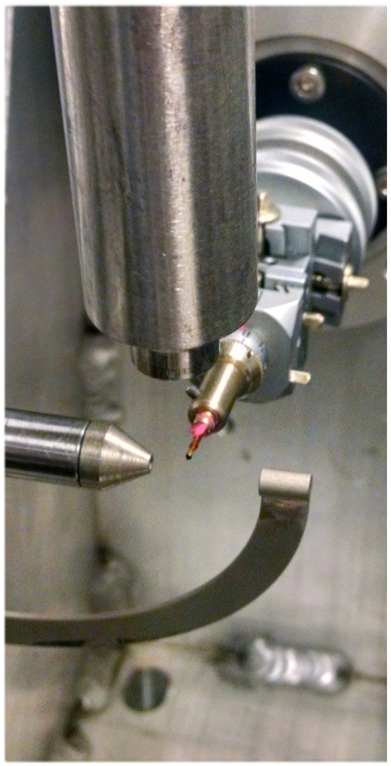


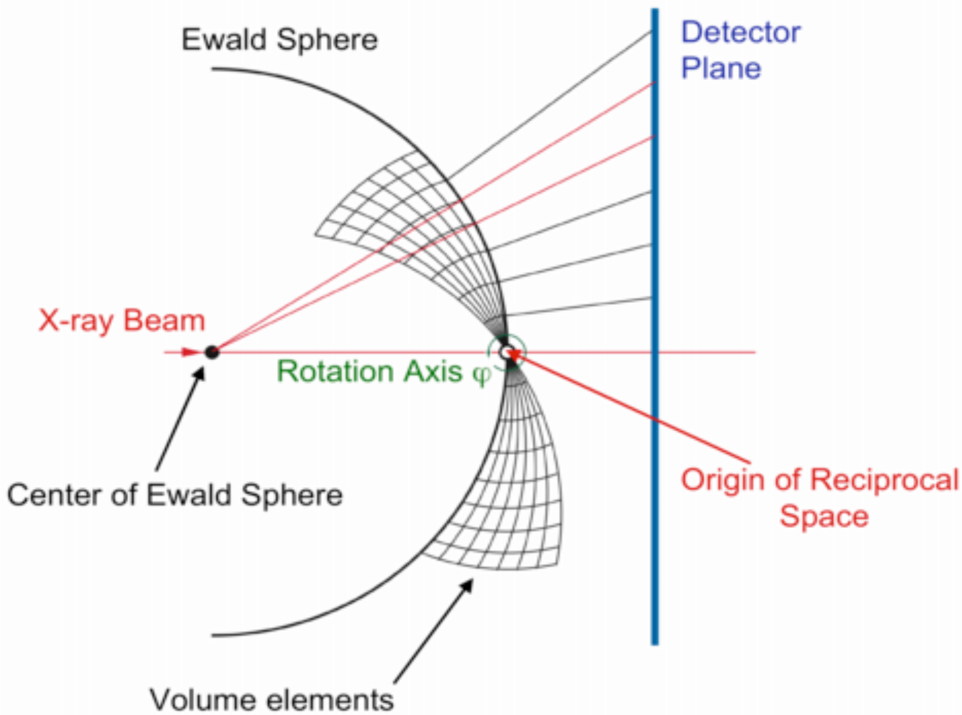
Sillimanite: Al_2SiO_5

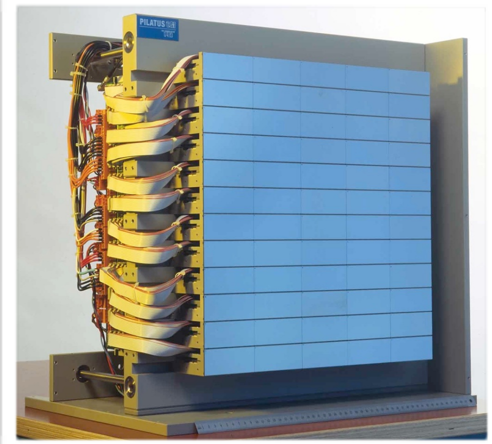
Mullite: $Al_2(Al_{2+2x}Si_{2-2x})O_{10+x}$

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

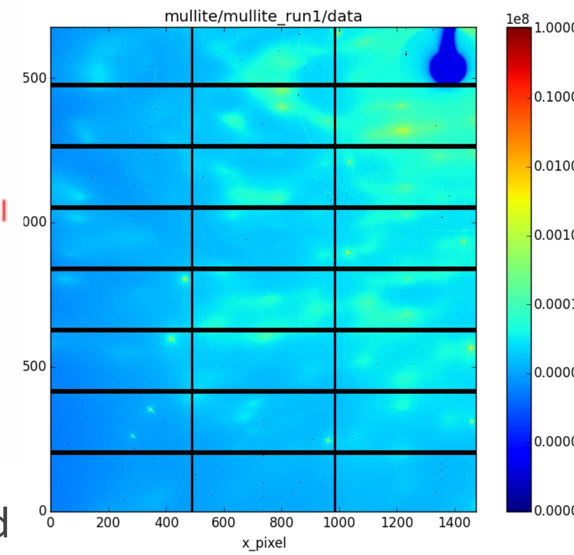
Measuring X-ray Diffuse Scattering with Continuous Rotation Method





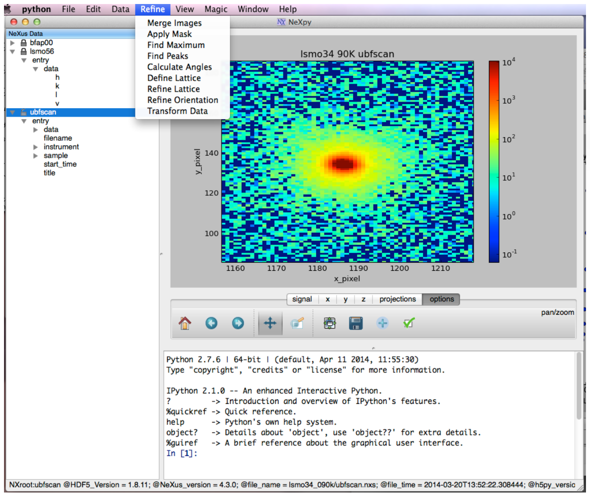


Pilatus 2M Detector

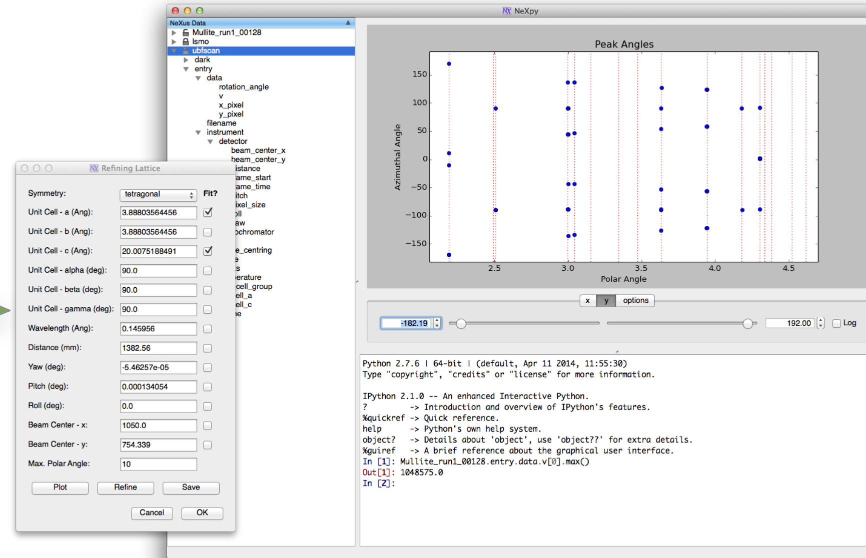


- The sample is continuously rotated in shutterless mode at 1° per second
- A fast area detector (*e.g.*, a Pilatus 2M) acquires images at 10 frames per second
  - *i.e.*, 3600 x 8MB frames ~ 30GB every 6 minutes
- The detector needs low background, high dynamic range, and energy discrimination
  - Ideally, this is performed with high-energy x-rays, *e.g.*, 80 to 100 keV

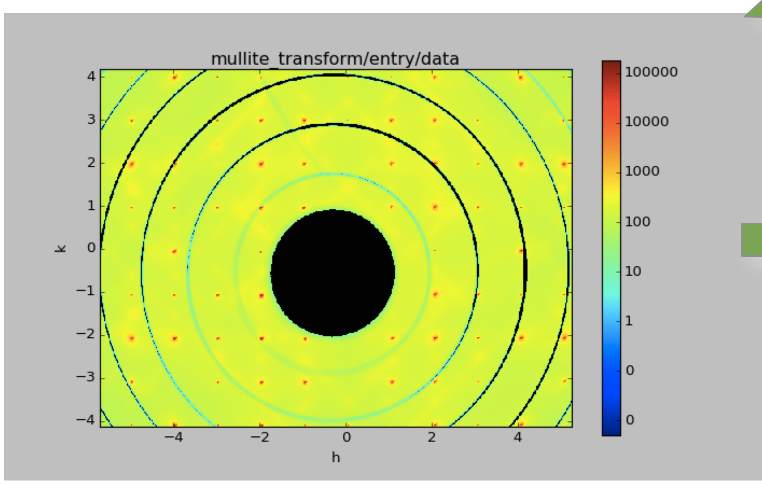
Data Reduction Workflows



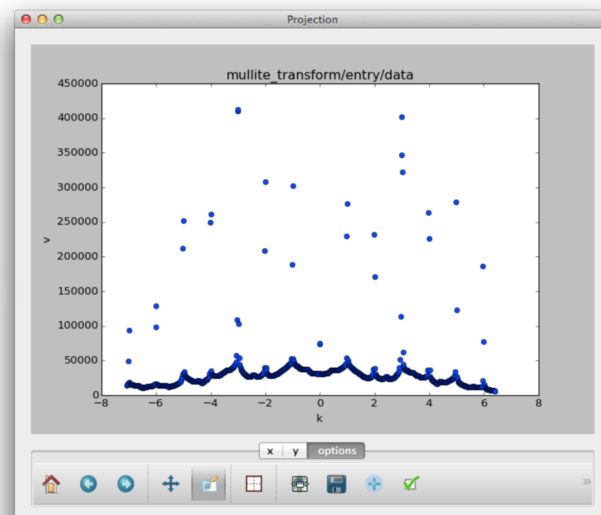
Peak Search



Refinement and Orientation



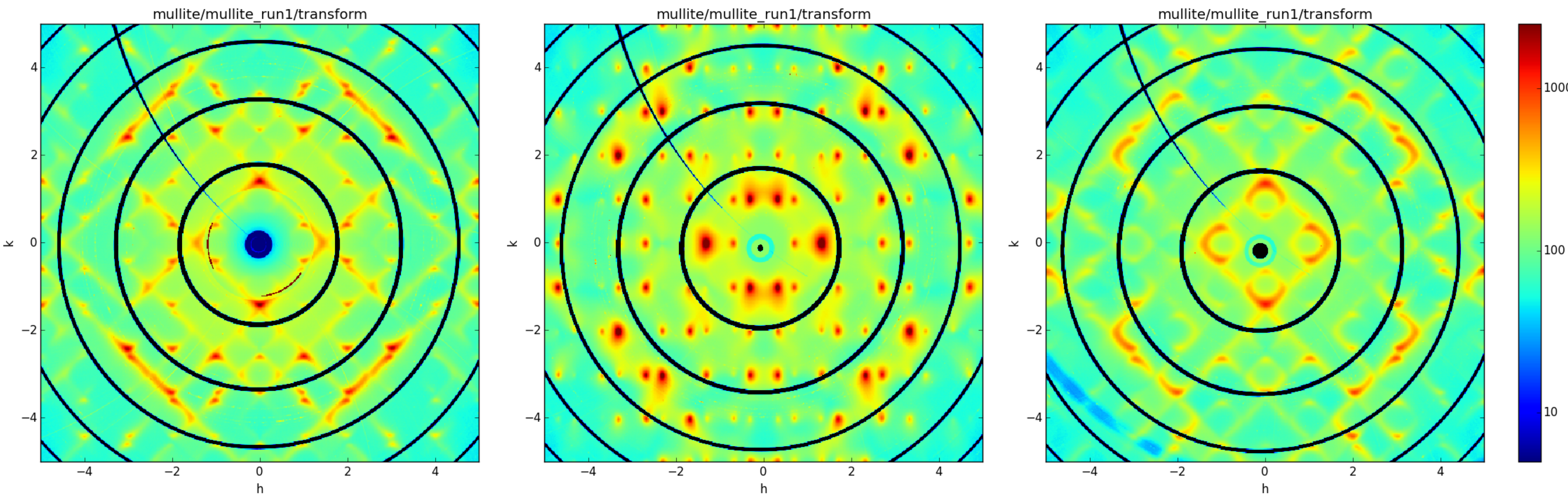
Coordinate Transformation



Data Projections

3D Diffuse Scattering in Mullite

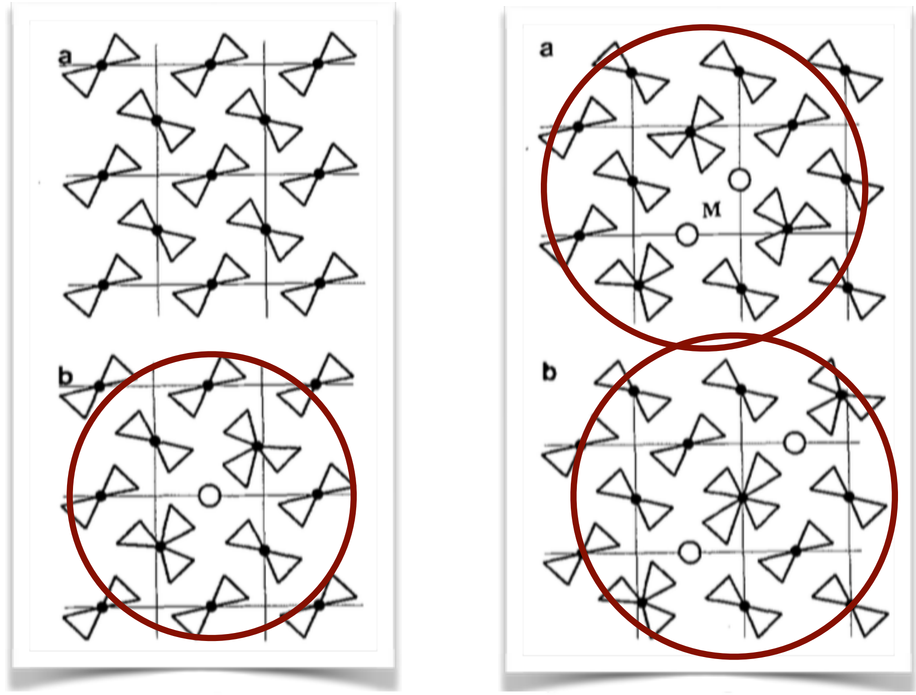
- There is strong diffuse scattering throughout reciprocal space
- The shape of the diffuse scattering is strongly dependent on the value of Ql
- There are incipient superlattice peaks at **Q** = 0.5 *c** + 0.31 *a**



Ql=0.16 | Ql=0.5 | Ql=0.75

Monte Carlo Analysis

- 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

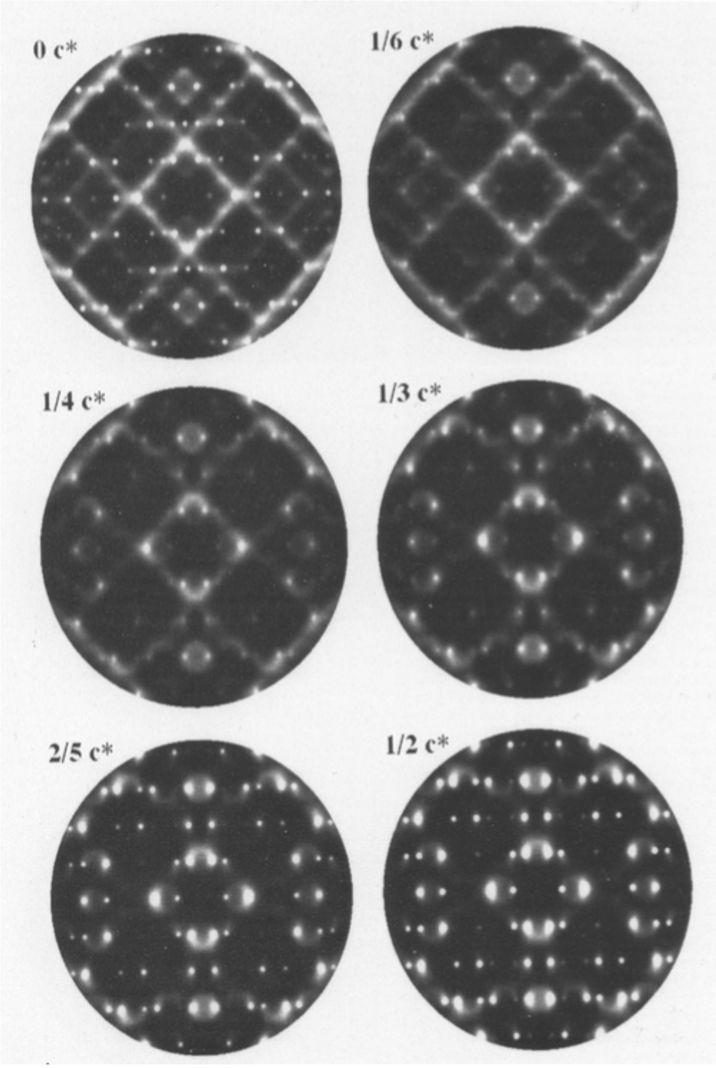
$$P_i = \frac{e^{-V_i}}{1+e^{-V_i}},$$

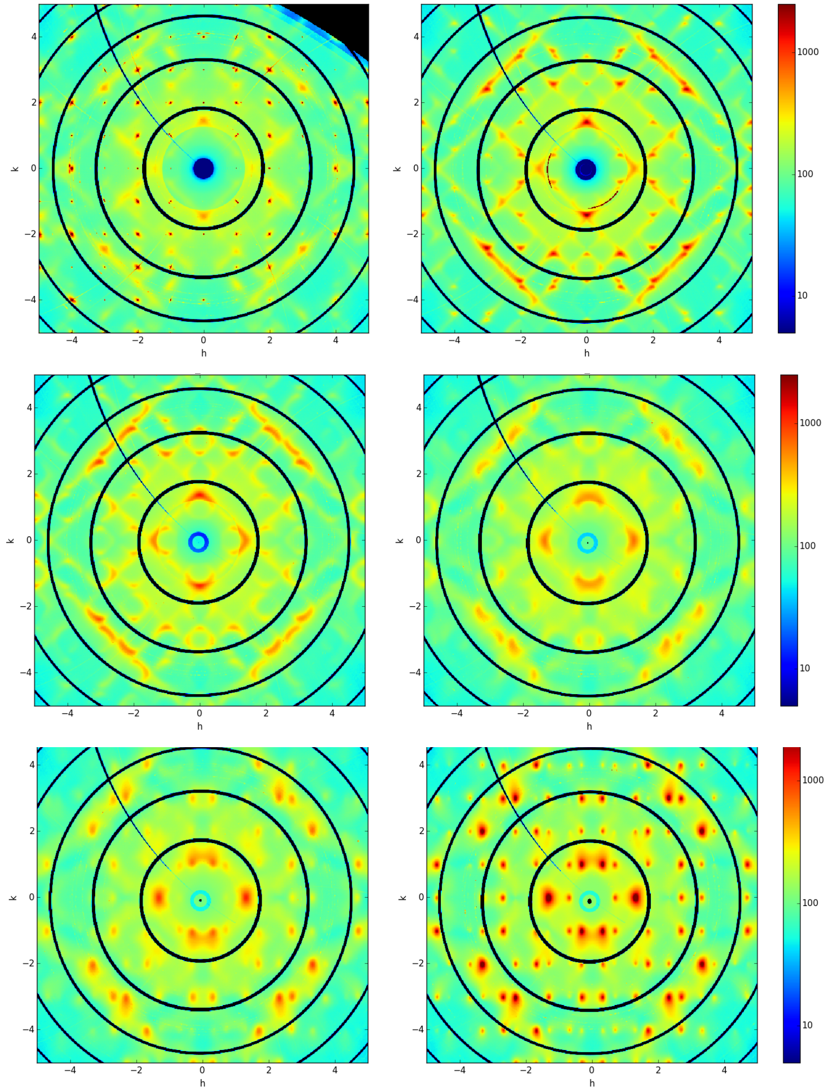
where,

$$V_i = \frac{\sum_j E_{ij}}{kT} + \frac{(N_v - N_v^o)^2}{N_v^o}\,\mathrm{sgn}\,(N_v - N_v^o).$$

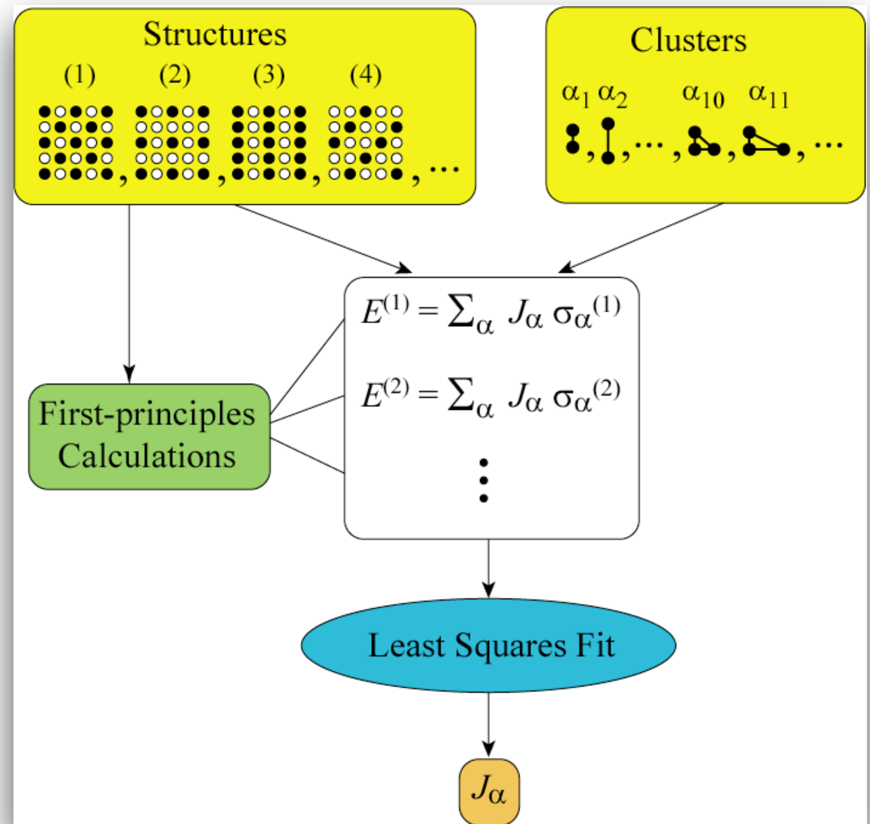
B. D. Butler, T. R. Welberry, & R. L. Withers, Phys Chem Minerals **20**, 323 (1993)

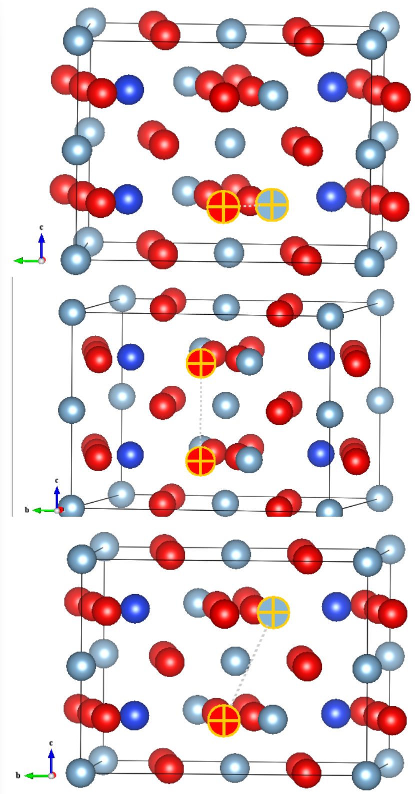
Monte Carlo Analysis Results

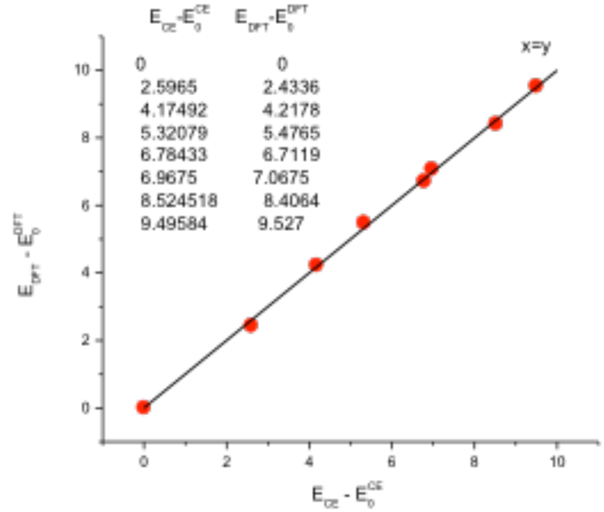




Vacancy Short-Range Order in Mullite
A First-Principles Approach

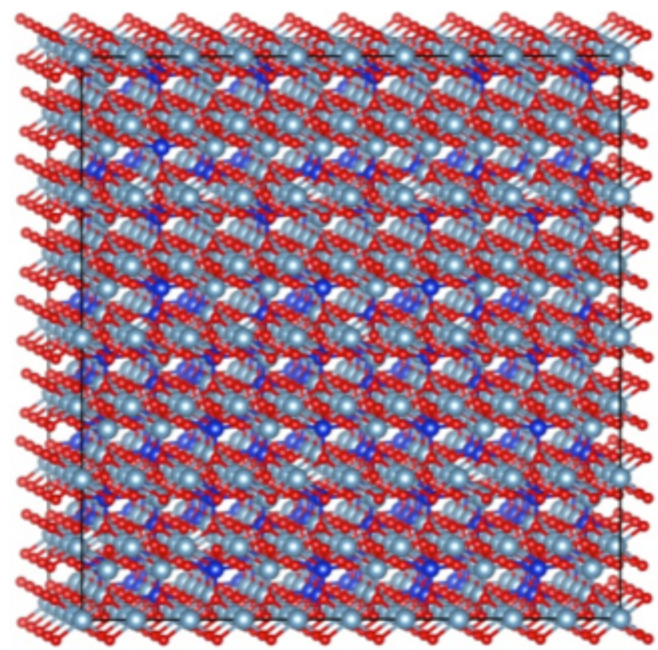






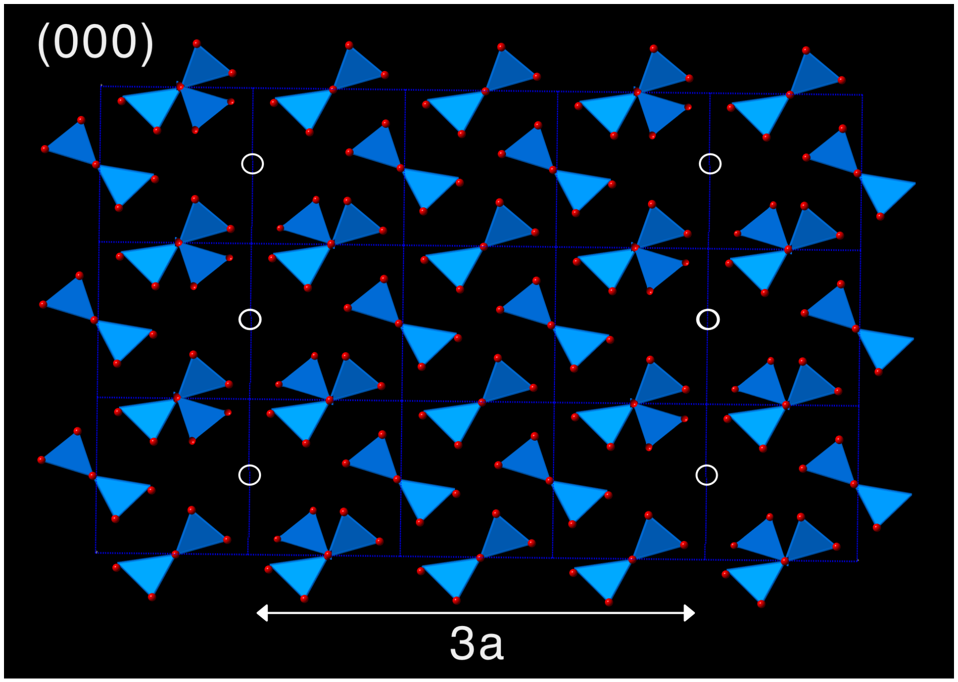
$$E(\sigma) = J_0 + \sum_i \sigma_i J_i + \sum_{i,j} J_{ij}\sigma_i\sigma_j + \sum_{ijk} J_{ijk}\sigma_i\sigma_j\sigma_k + \ldots$$

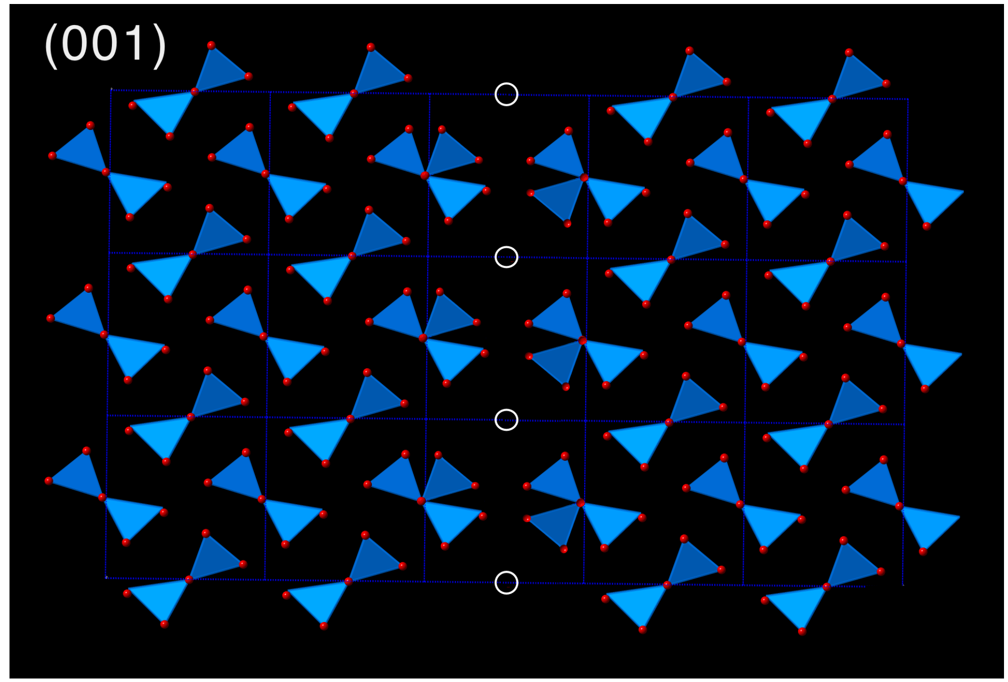
Peter Zapol & Anh Ngo



Lowest Energy 3:2 Mullite Structure from Kinetic Monte Carlo Calculation

Nearly-Commensurate Vacancy Stripes in Mullite





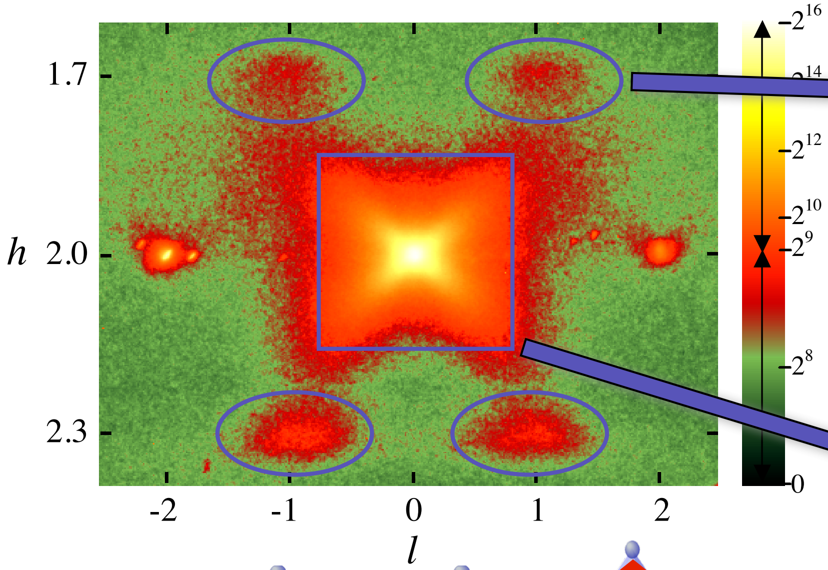
c = 0

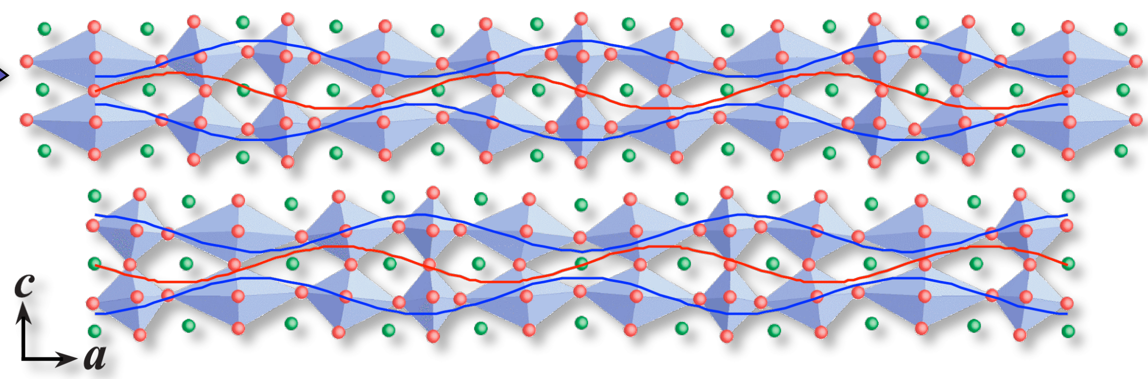
c = 1.0

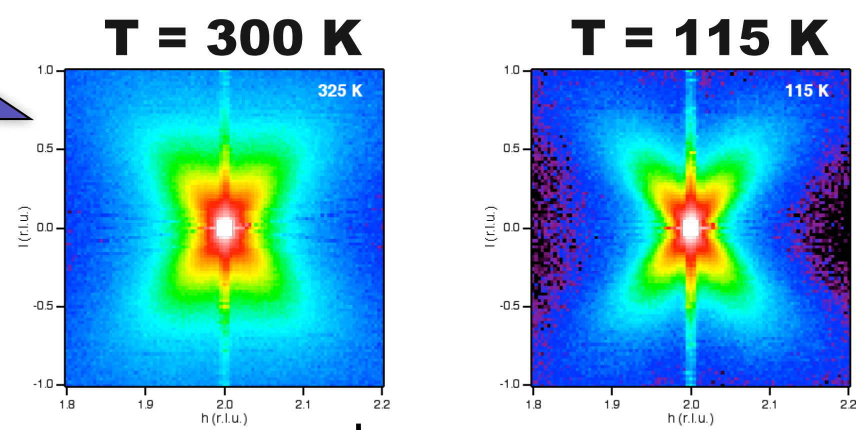
$$\mathbf{q} = \pm\frac{1}{2}\mathbf{c}^* \pm \frac{1}{3}\mathbf{a}^*$$

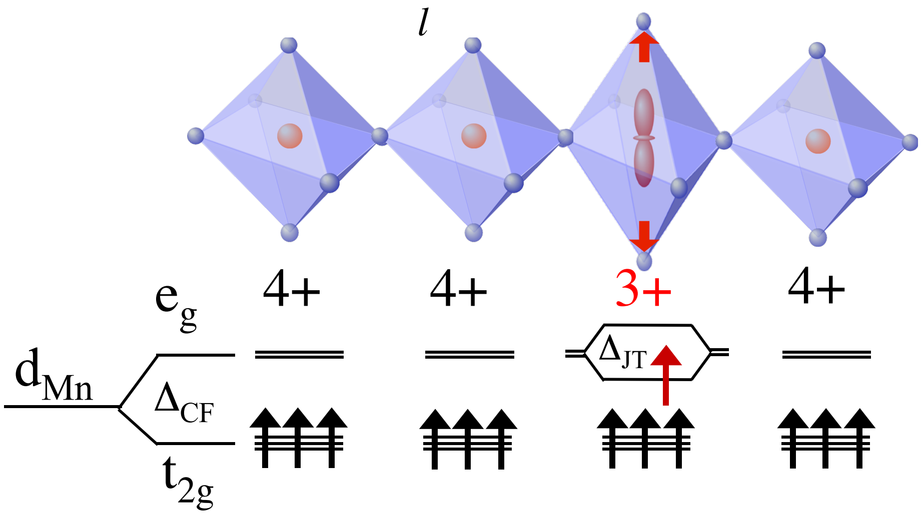
Case Study 1: Bilayer Manganites

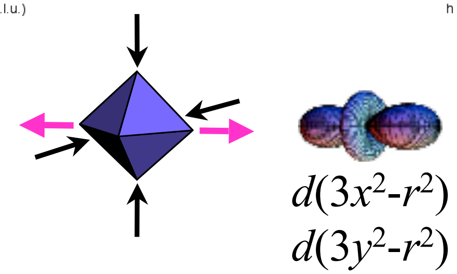
Diffuse Scattering from Jahn-Teller Polarons











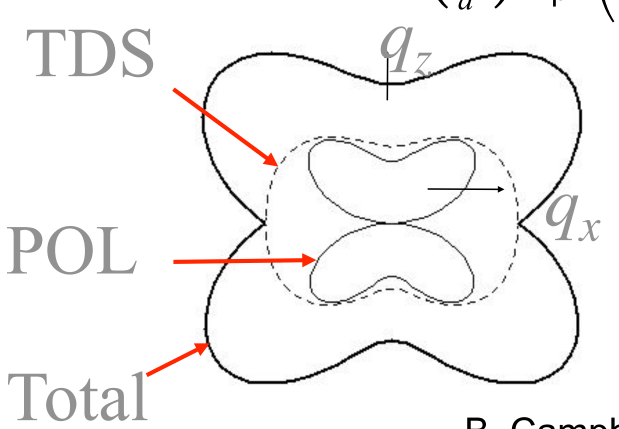
Huang Scattering

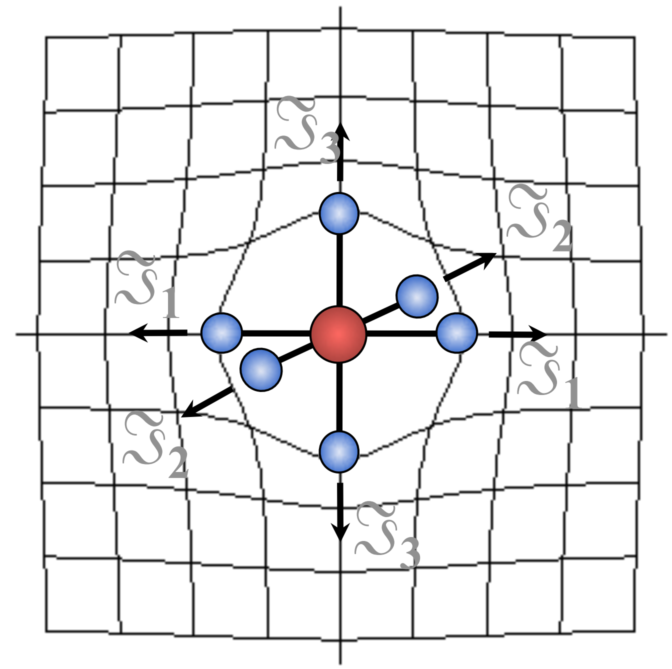
$$I(\mathbf{Q}) = \sum_{m,n} e^{i\mathbf{Q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} f_m f_n e^{-W_m} e^{-W_n} \left\langle (\mathbf{Q}\cdot\mathbf{u}_m)(\mathbf{Q}\cdot\mathbf{u}_n) \right\rangle$$

$$I_{POL}(\mathbf{Q}) = N\left|F_{\mathbf{G}}\right|^2 \sum_{\alpha,\beta,\gamma,\delta} Q_\beta Q_\delta \left(\sum_{j,j'} \frac{\varepsilon_{\alpha,\mathbf{q},j}\,\varepsilon^*_{\beta,\mathbf{q},j}\,\varepsilon^*_{\gamma,\mathbf{q},j'}\,\varepsilon_{\delta,\mathbf{q},j'}}{\omega^2_{\mathbf{q},j}\,\omega^2_{\mathbf{q},j'}} \right) \sum_{m,n} \Im_{m,\alpha} \Im_{n,\gamma}\, e^{i\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)}$$

$$I_{TDS}(\mathbf{Q}) = N\left|F_{\mathbf{G}}\right|^2 \left(\frac{kT}{2M}\right) \sum_{\beta,\delta} Q_\beta Q_\delta \left(\sum_{j} \frac{\varepsilon^*_{\beta,\mathbf{q},j}\,\varepsilon_{\delta,\mathbf{q},j}}{\omega^2_{\mathbf{q},j}} \right)$$

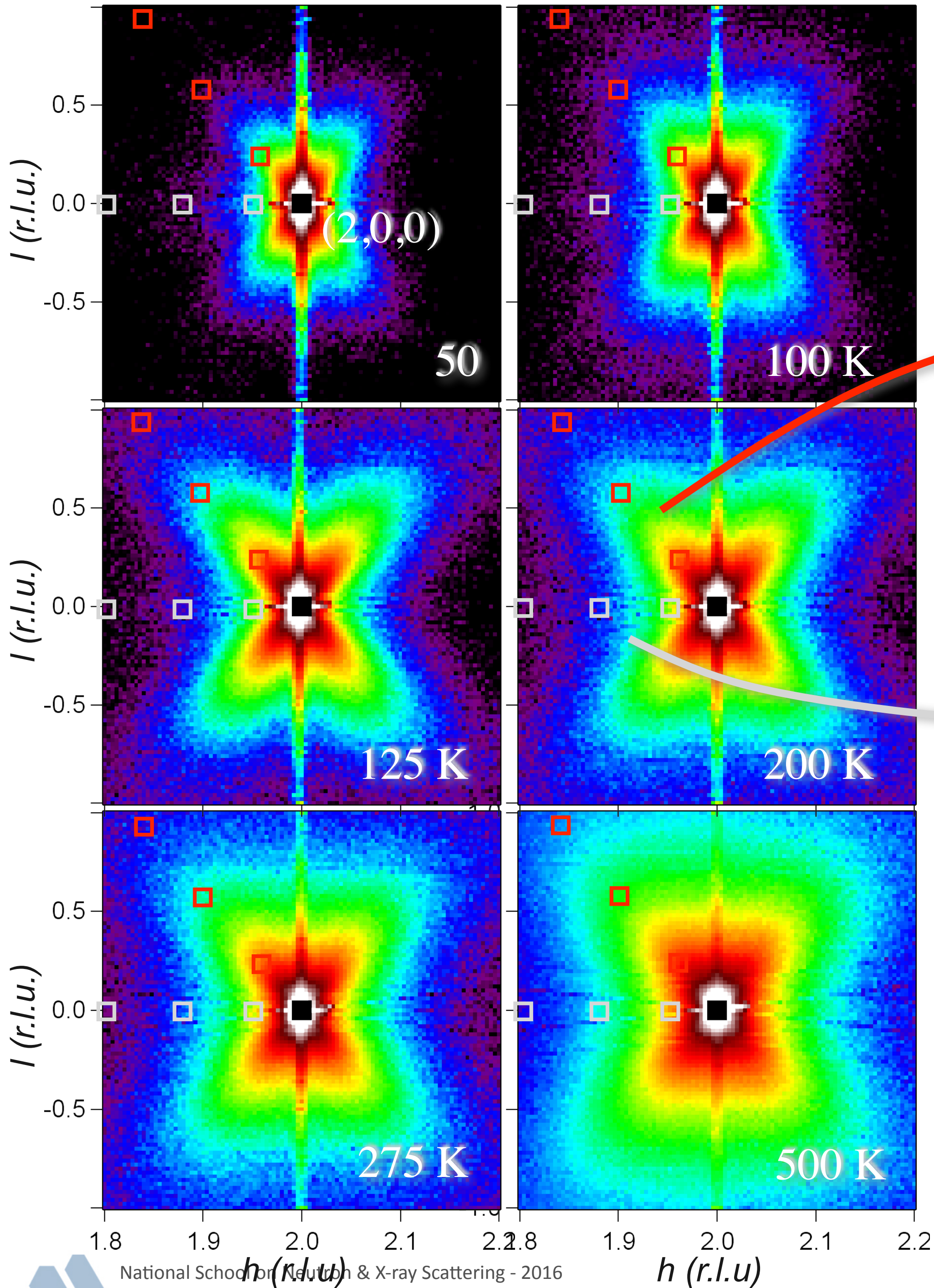
$$u_{m,\delta} = \int \frac{d^3 q}{\left(\frac{2\pi}{a}\right)^3} \sum_{\beta} \left(\sum_{j} \frac{\varepsilon^*_{\beta,\mathbf{q},j}\,\varepsilon_{\delta,\mathbf{q},j}}{\omega^2_{\mathbf{q},j}} \right) \sum_{n} \Im_{n,\beta}\, e^{i\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)}$$

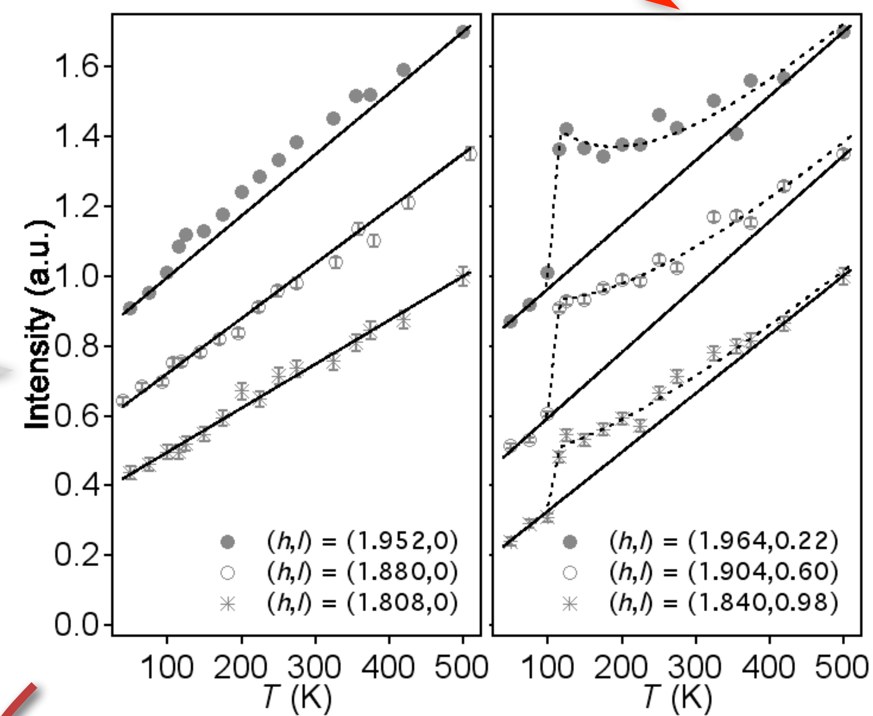




B. Campbell *et al* Phys. Rev. B. **67**, 020409 (2003)

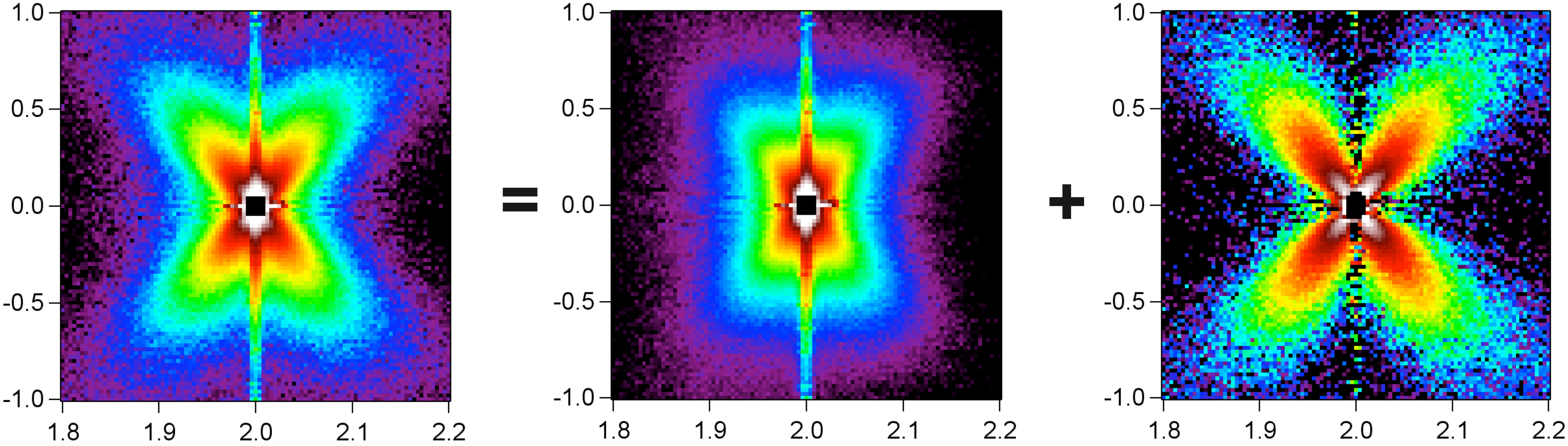
single crystal synchrotron x-ray scattering
11-ID-D, APS@Argonne





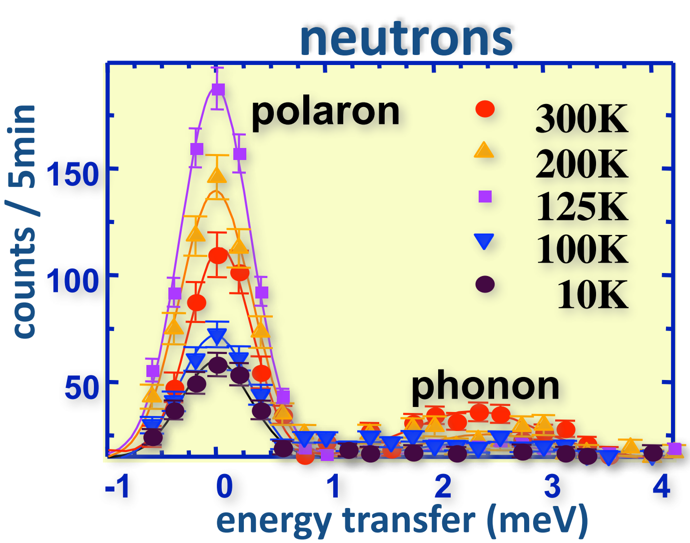
this allows us to subtract background from thermal diffuse scattering!

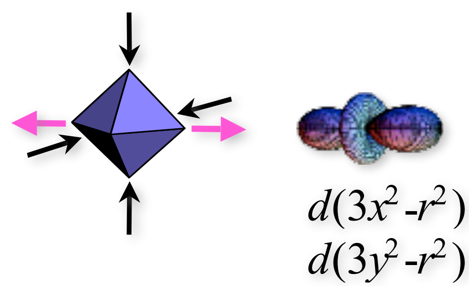
TDS + Huang scattering



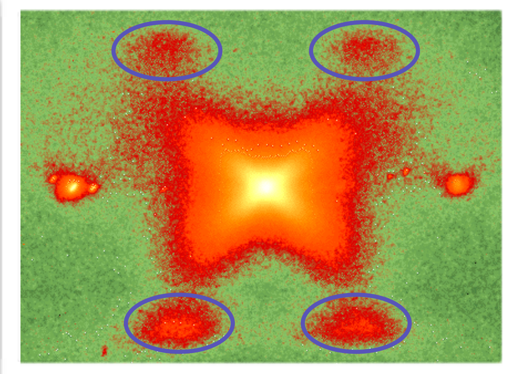
TDS

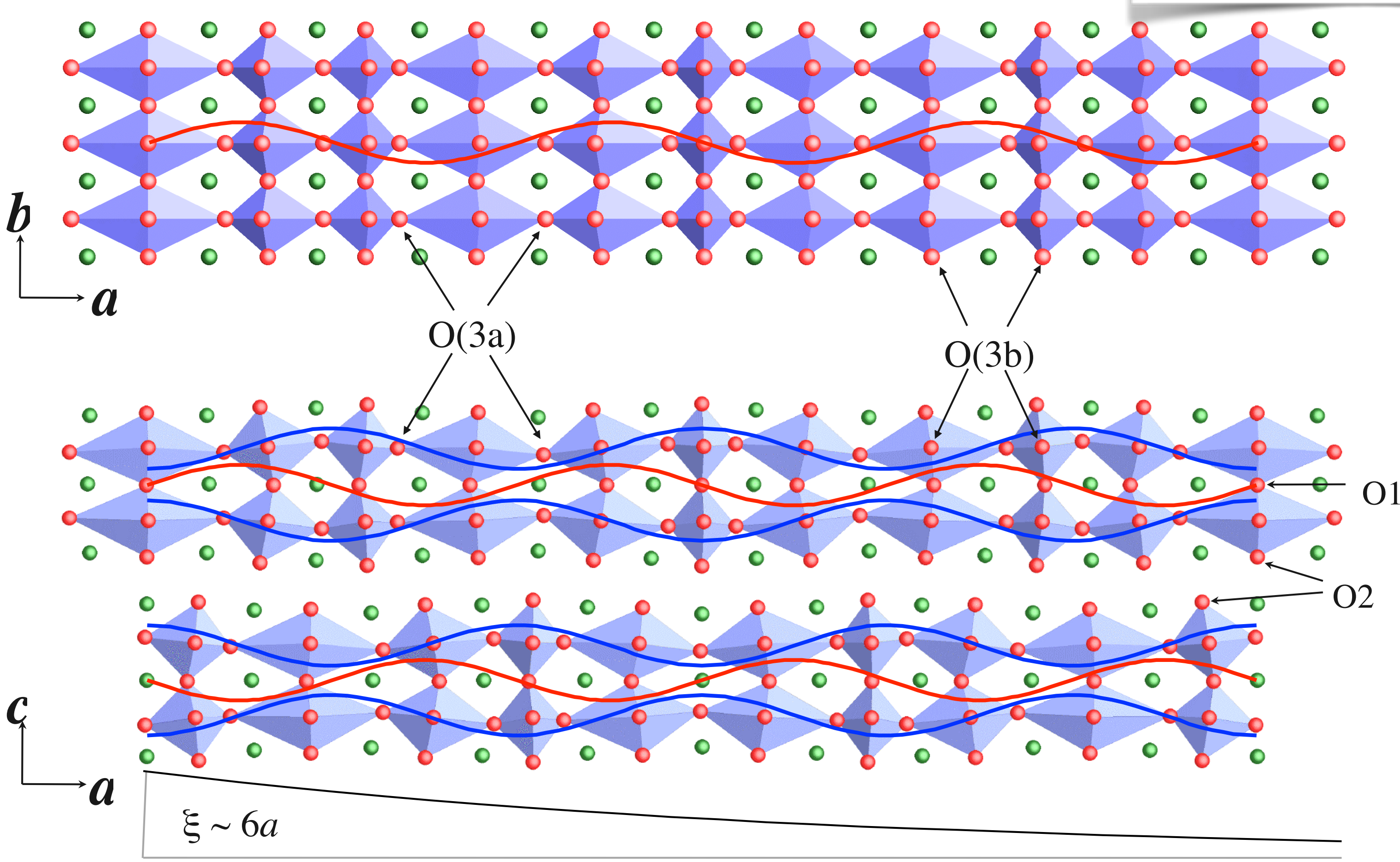
polaron

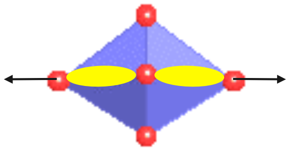




Cooperative Jahn-Teller Distortions



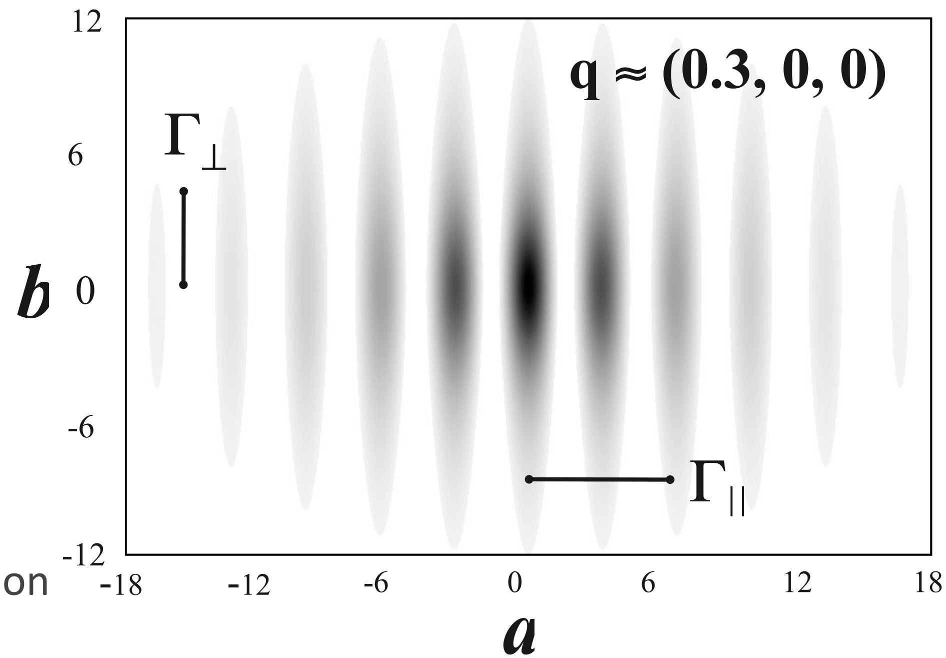


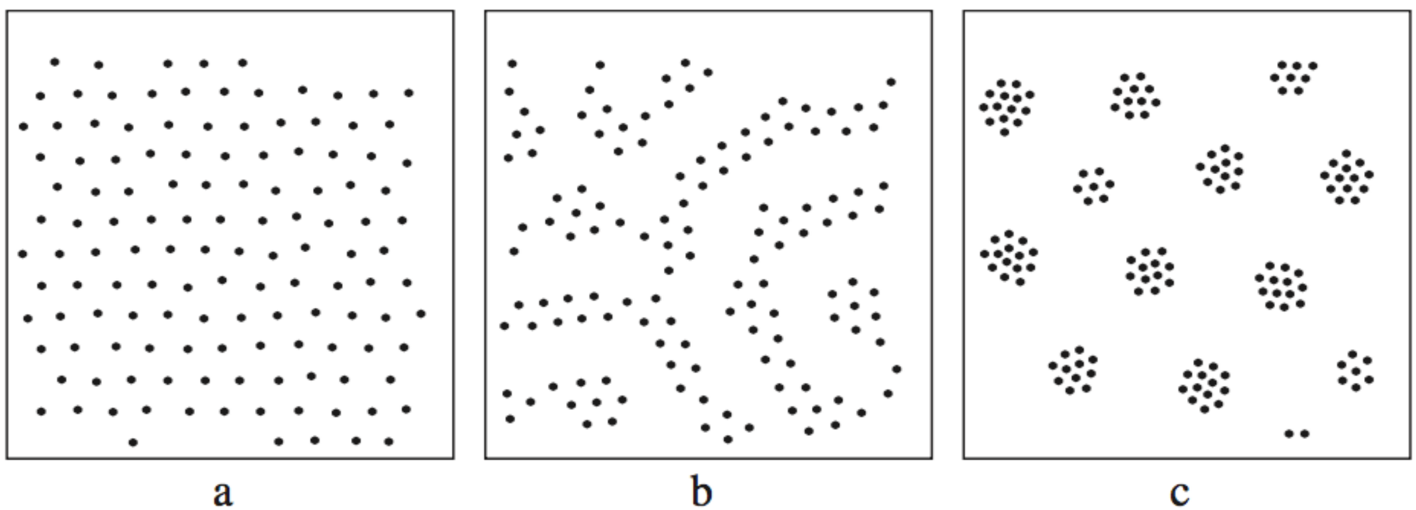


B. J. Campbell, R. Osborn, D. N. Argyriou, L. Vasiliu-Doloc, J. F. Mitchell, S. K. Sinha, U. Ruett, C. D. Ling, Z. Islam, and J. W. Lynn, Physical Review B **65**, 014427 (2001)

Origins of Stripe Formation

- Stripe formation is a very common motif of disordered systems
- It is the response of a system with interactions that compete on different length scales
  - *e.g.*, long-range repulsion *vs* short-range attraction

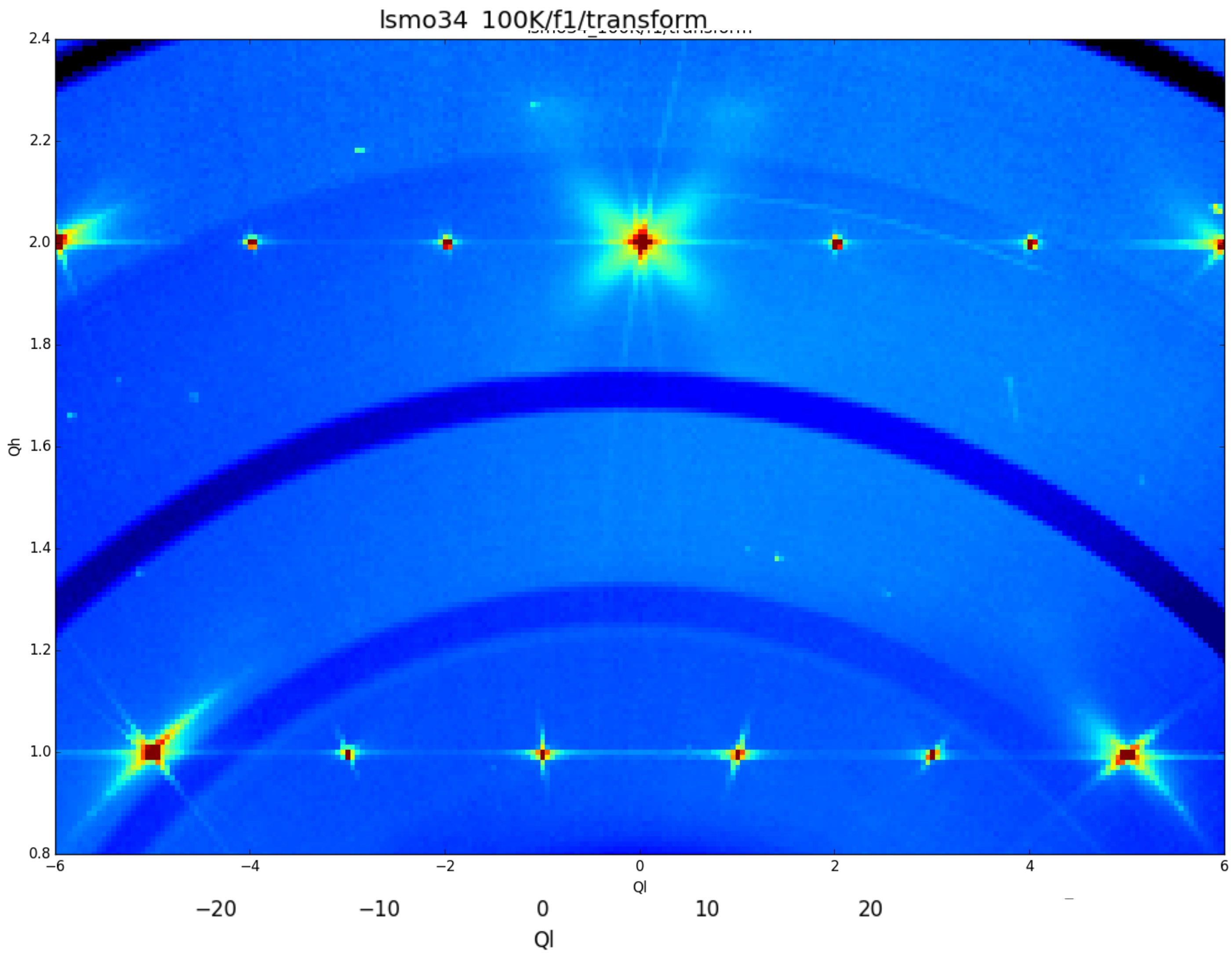




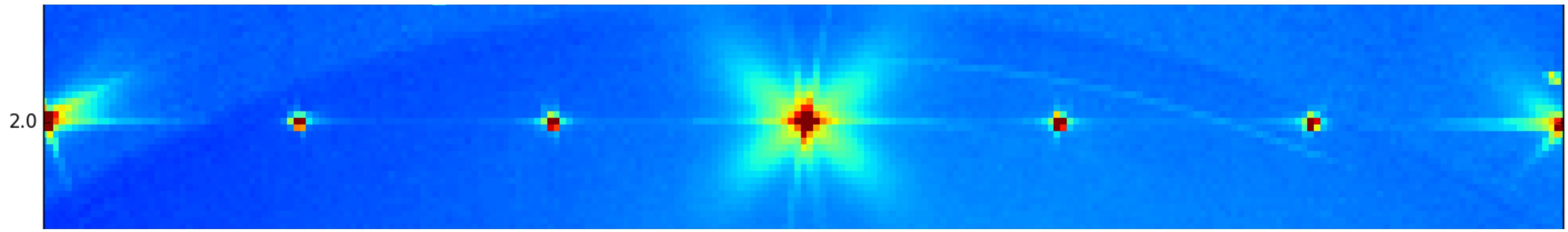
Wigner Lattice | Stripes | Phase Separation

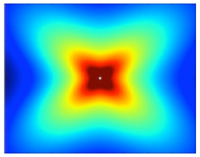
C. Reichhardt, C. J. Olsen, I. Martin & A. Bishop, EPL **61**, 221–227 (2003).

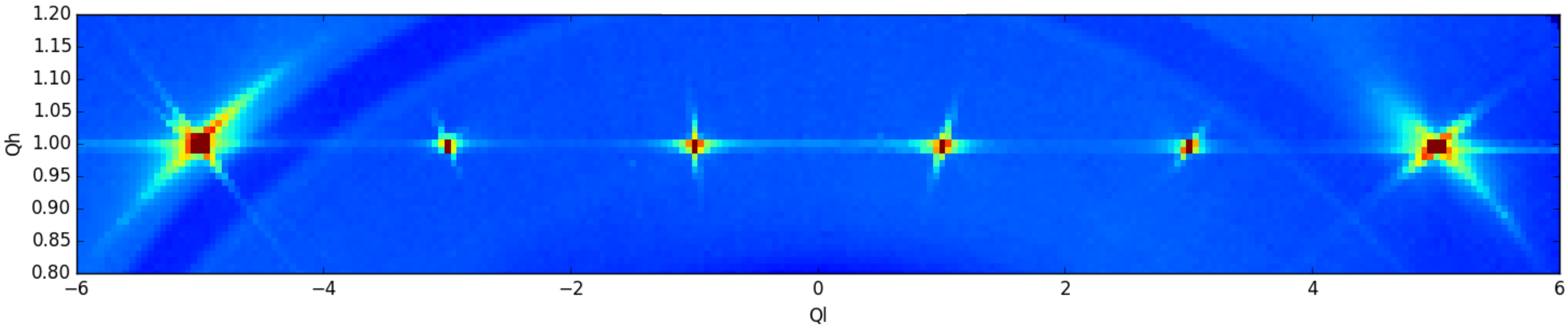
Bilayer Manganites Revisited



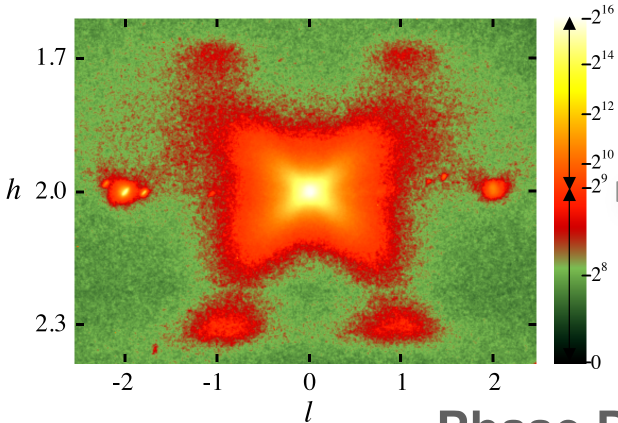
Huang Scattering as a Function of (Qh, Qk, Ql)

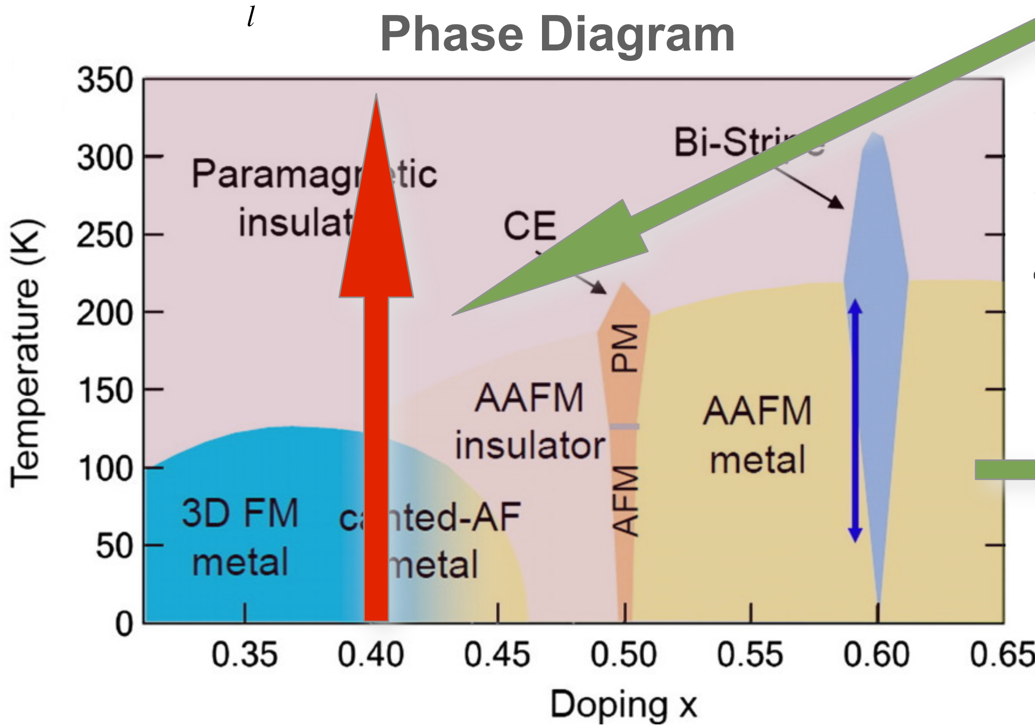


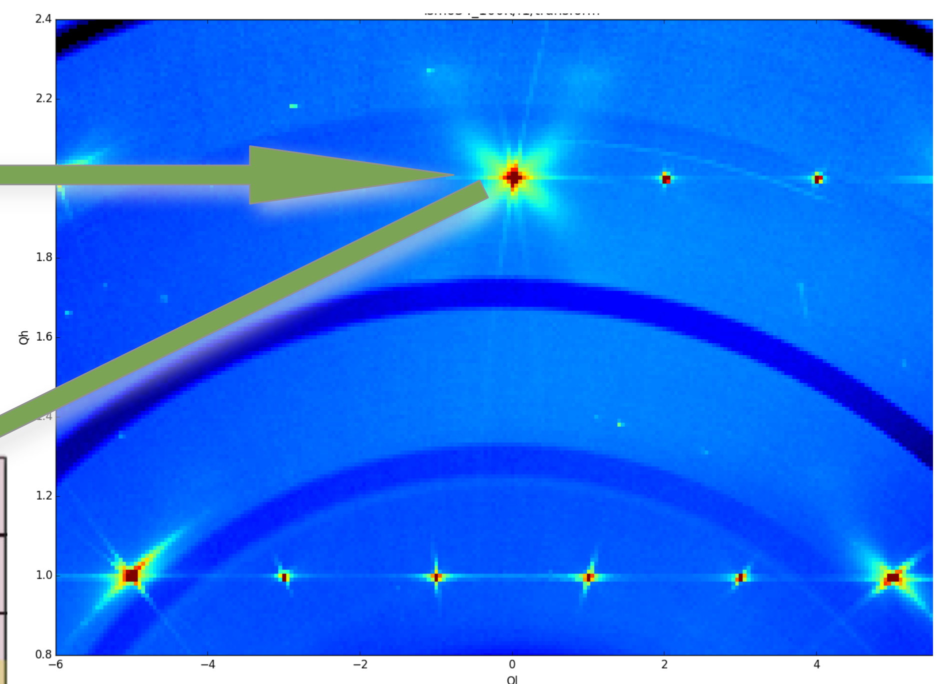




Expanding the Concept of a Data Set





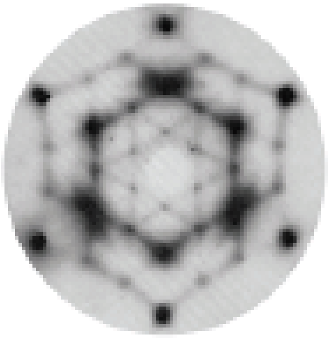


Correlated Data Analysis/ Machine Learning

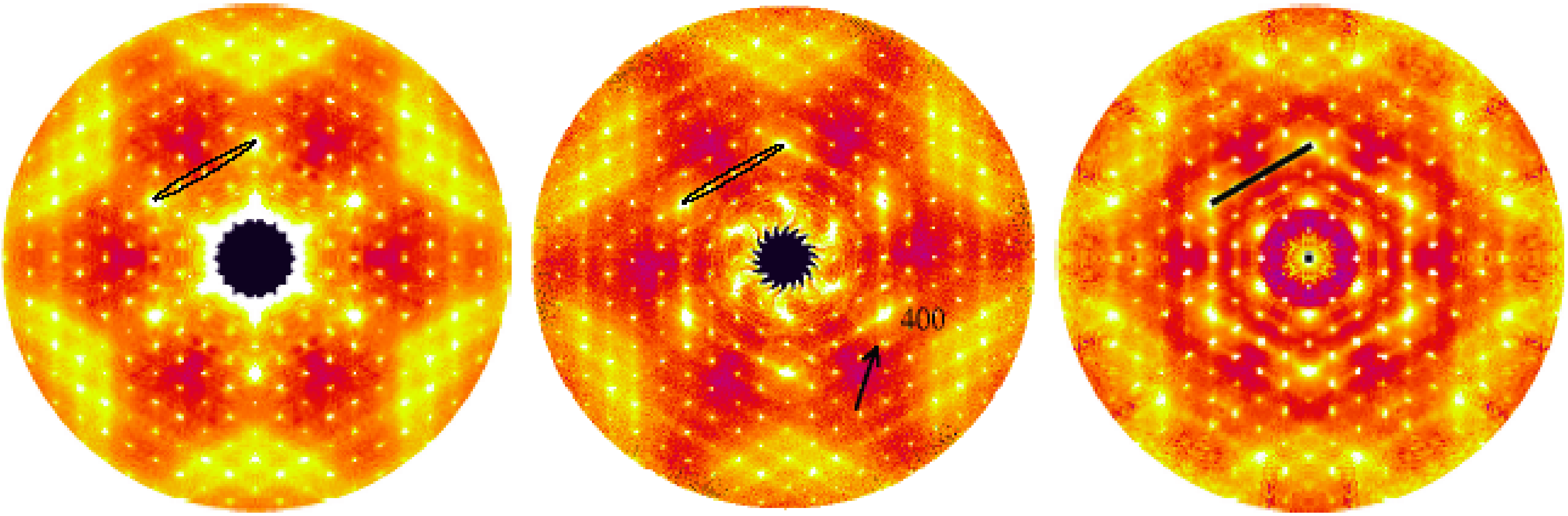
Total Data: S(Q, T, *x*)

How do I look at static disorder?

Importance of Elastic Discrimination



BENZIL



Detector 1
2θ~142.5°

Detector 2
2θ~90.0°

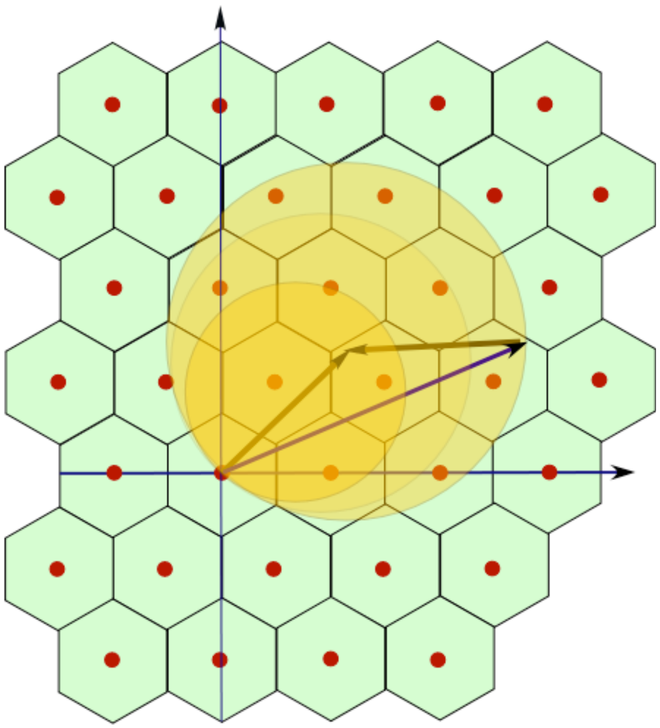
Detector 3
2θ~37.5°

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

Measuring Large Volumes of Reciprocal Space

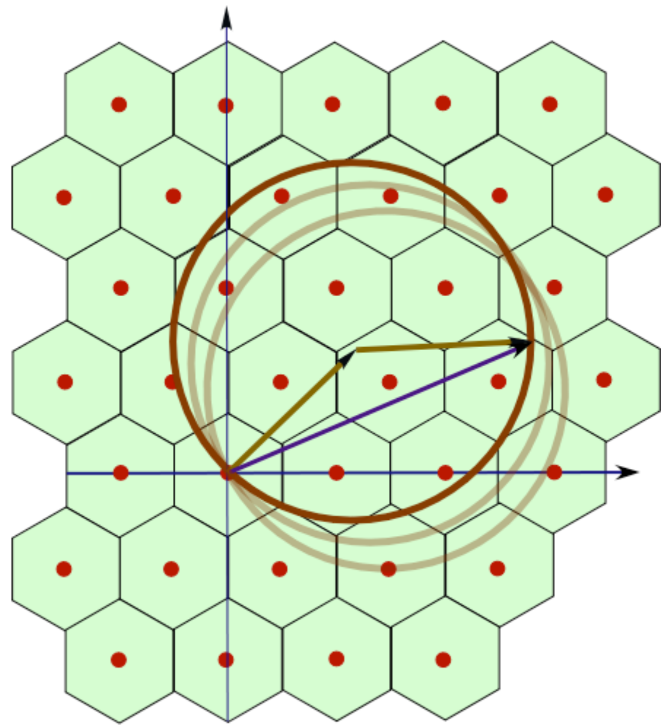
Conventional Time-of-Flight Neutron Methods

White Beam:
efficient



NO energy discrimination

Fixed k_i :
energy resolved



NOT efficient

Cross Correlation Chopper

TOF Laue Diffractometer

- highly efficient data collection
- wide dynamic range in Q

Statistical Chopper

- elastic energy discrimination
- optimum use of white beam

Sample with :

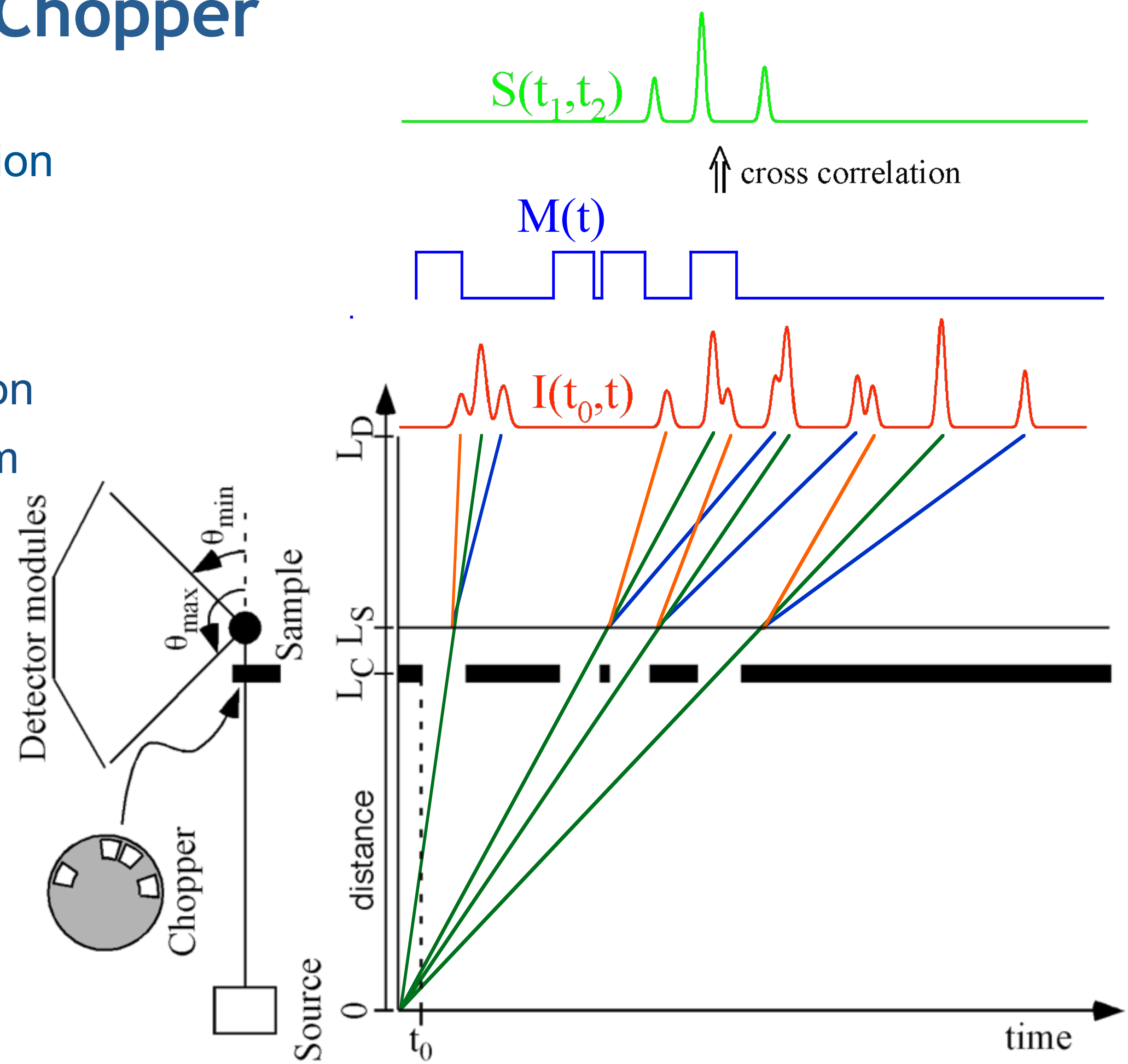
elastic scattering

$$\hbar\omega = 0$$

inelastic excitations

$$\hbar\omega = +E_0$$

$$\hbar\omega = -E_0$$



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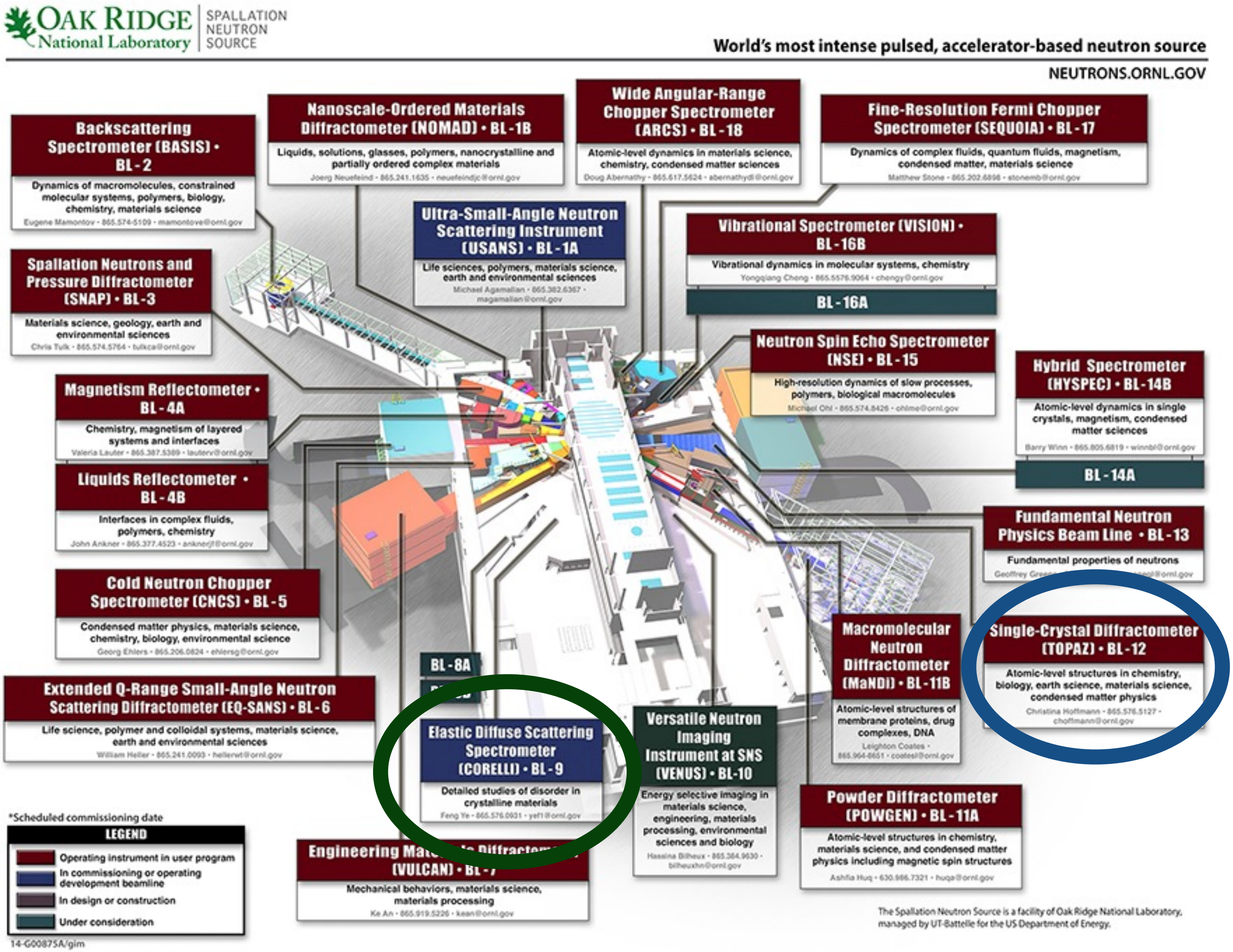

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In design or construction
Under consideration
14-G00875A/gim
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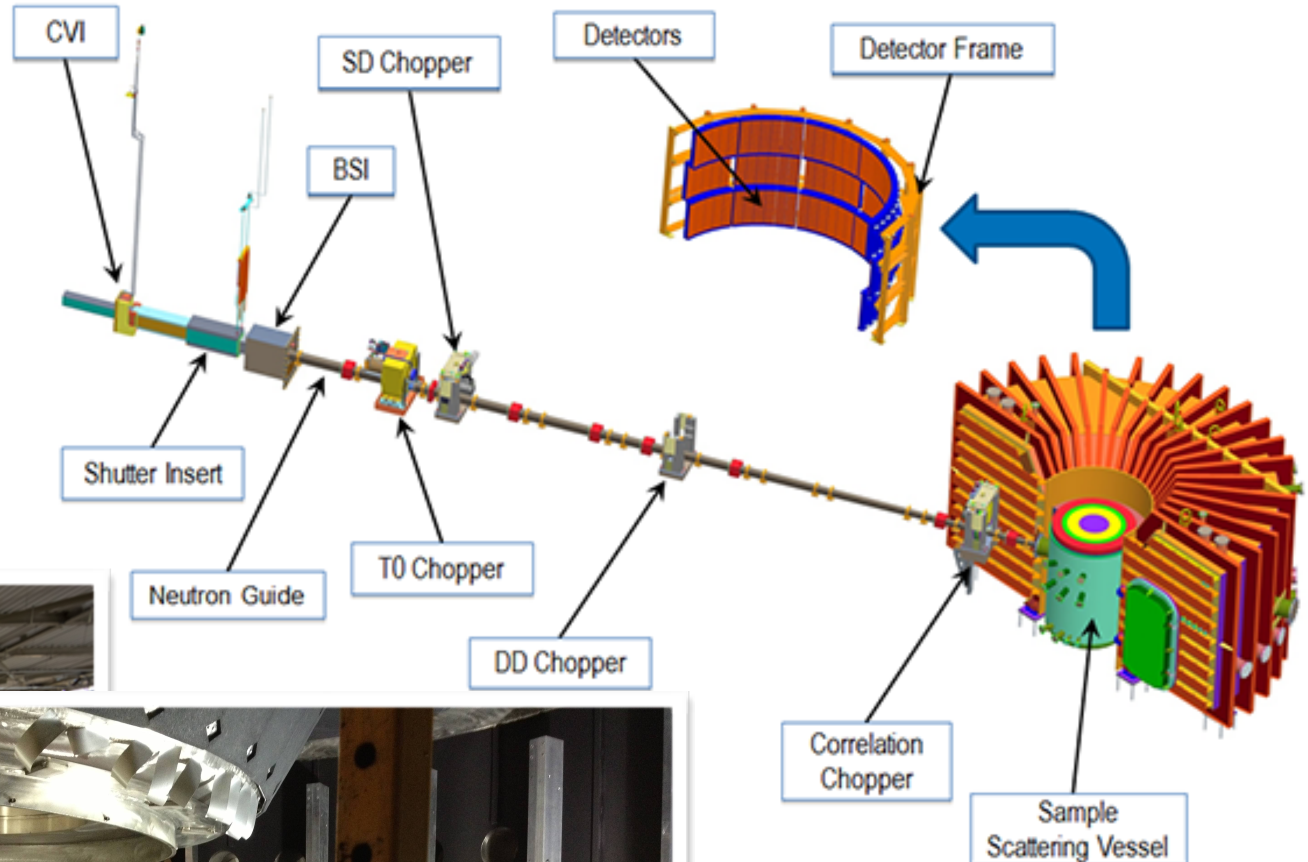
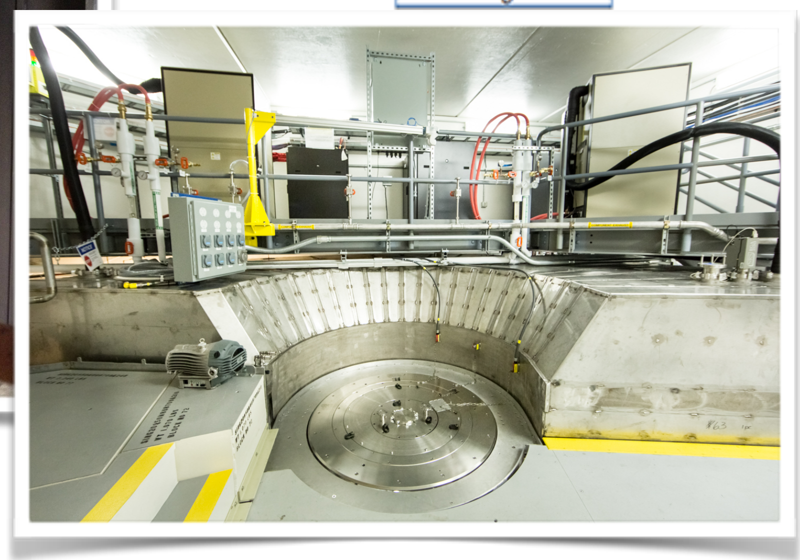
Arcangelo Corelli (1653-1713)

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.

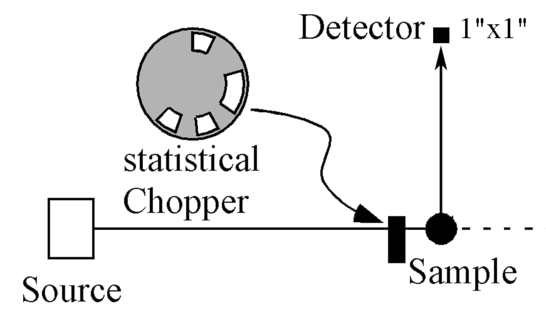
Corelli

Instrument Scientists
Feng Ye
Yaohua Liu

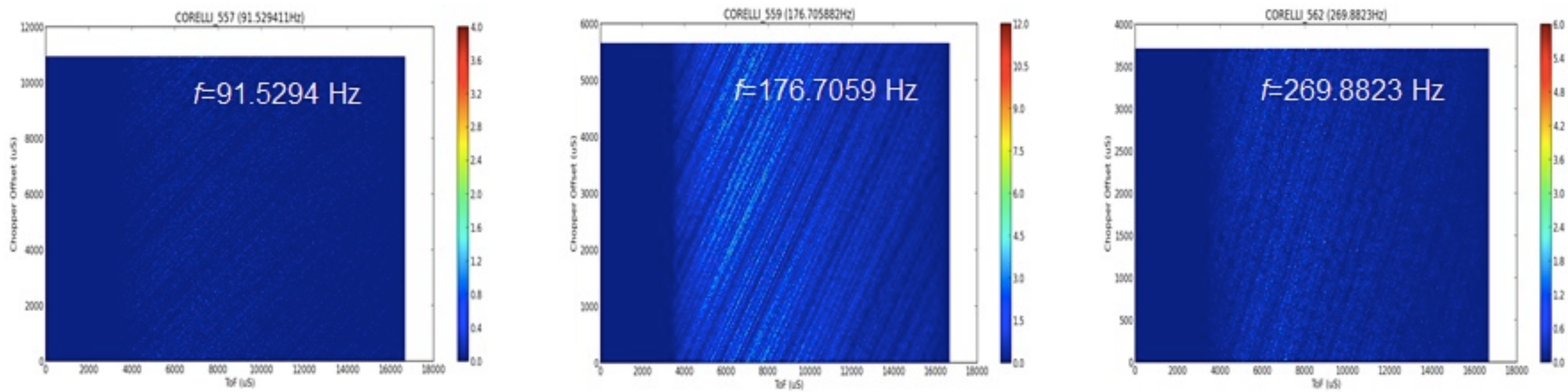




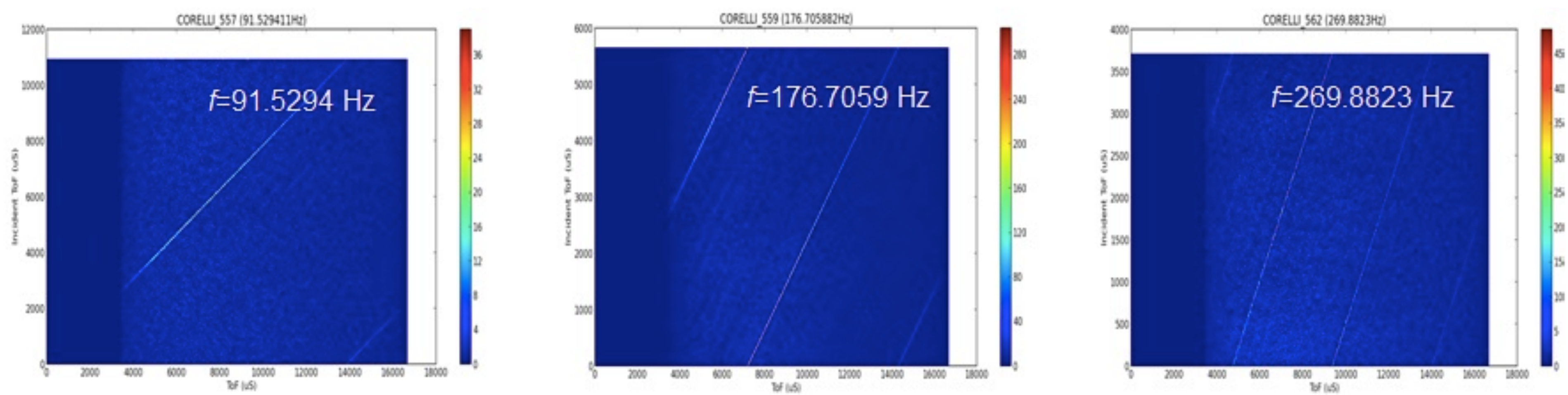
Cross Correlation in Action



Before cross-correlation

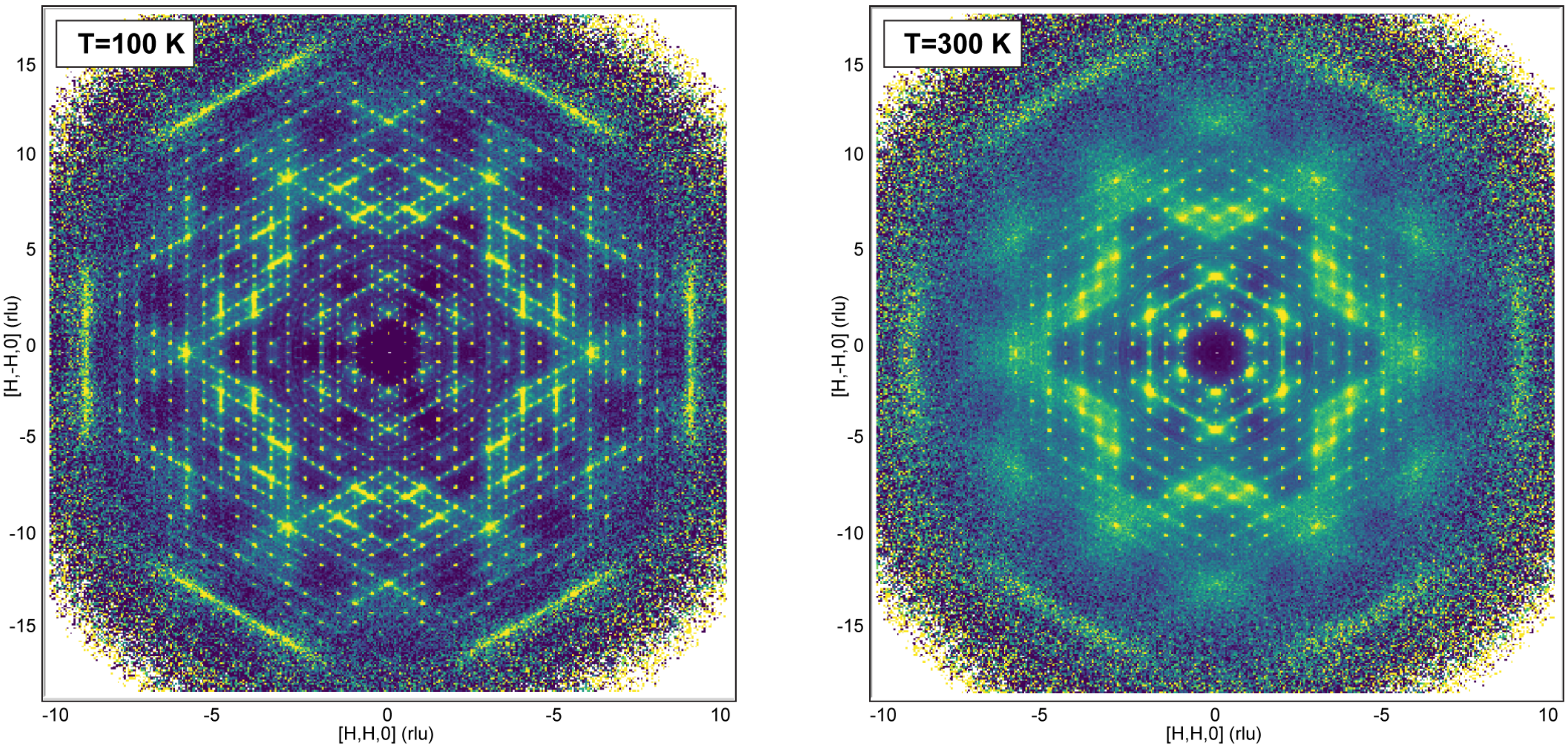


After cross-correlation



First Results

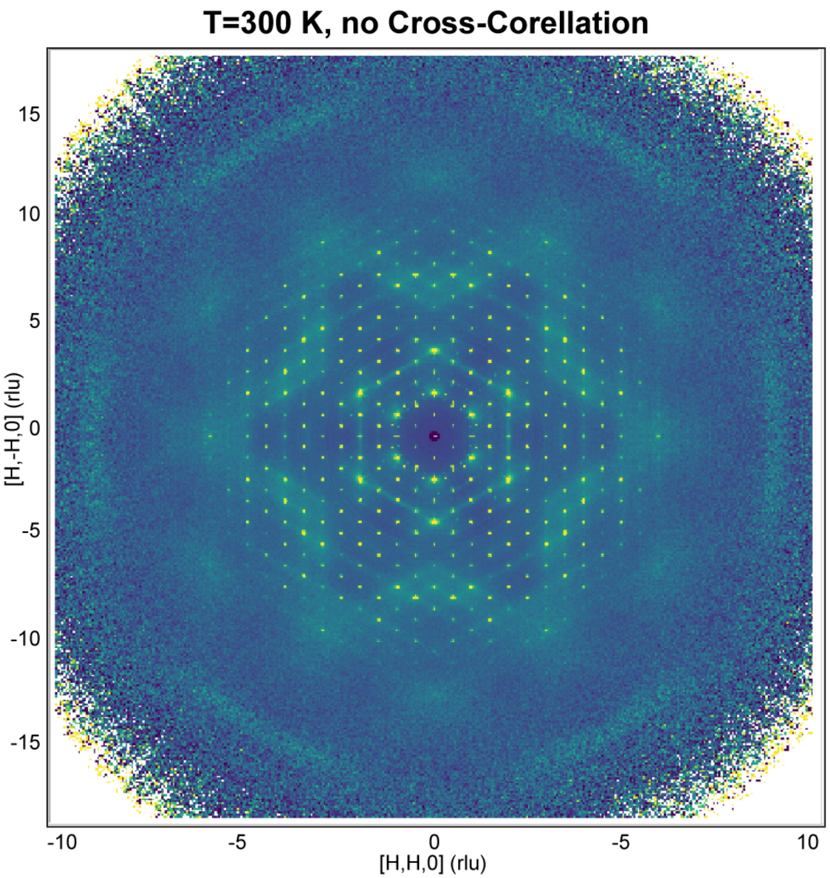
Benzil $C_{14}H_{10}O_2$

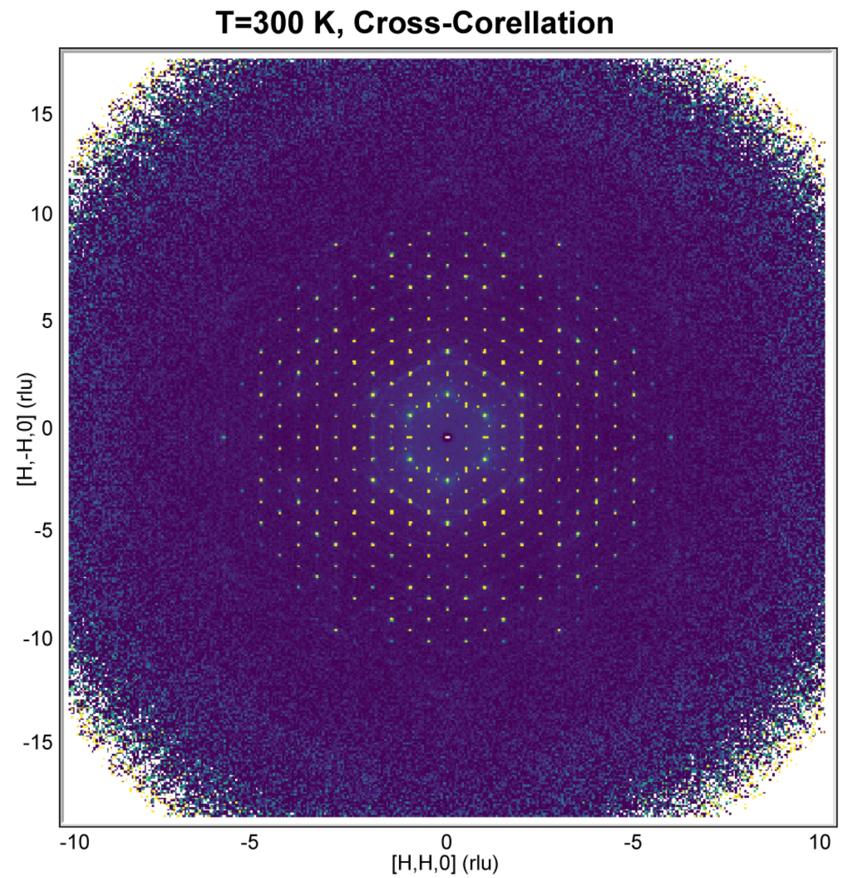


Acknowledgement: Richard Welberry (PI) and Christina Hoffmann

Does Cross Correlation Work?

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

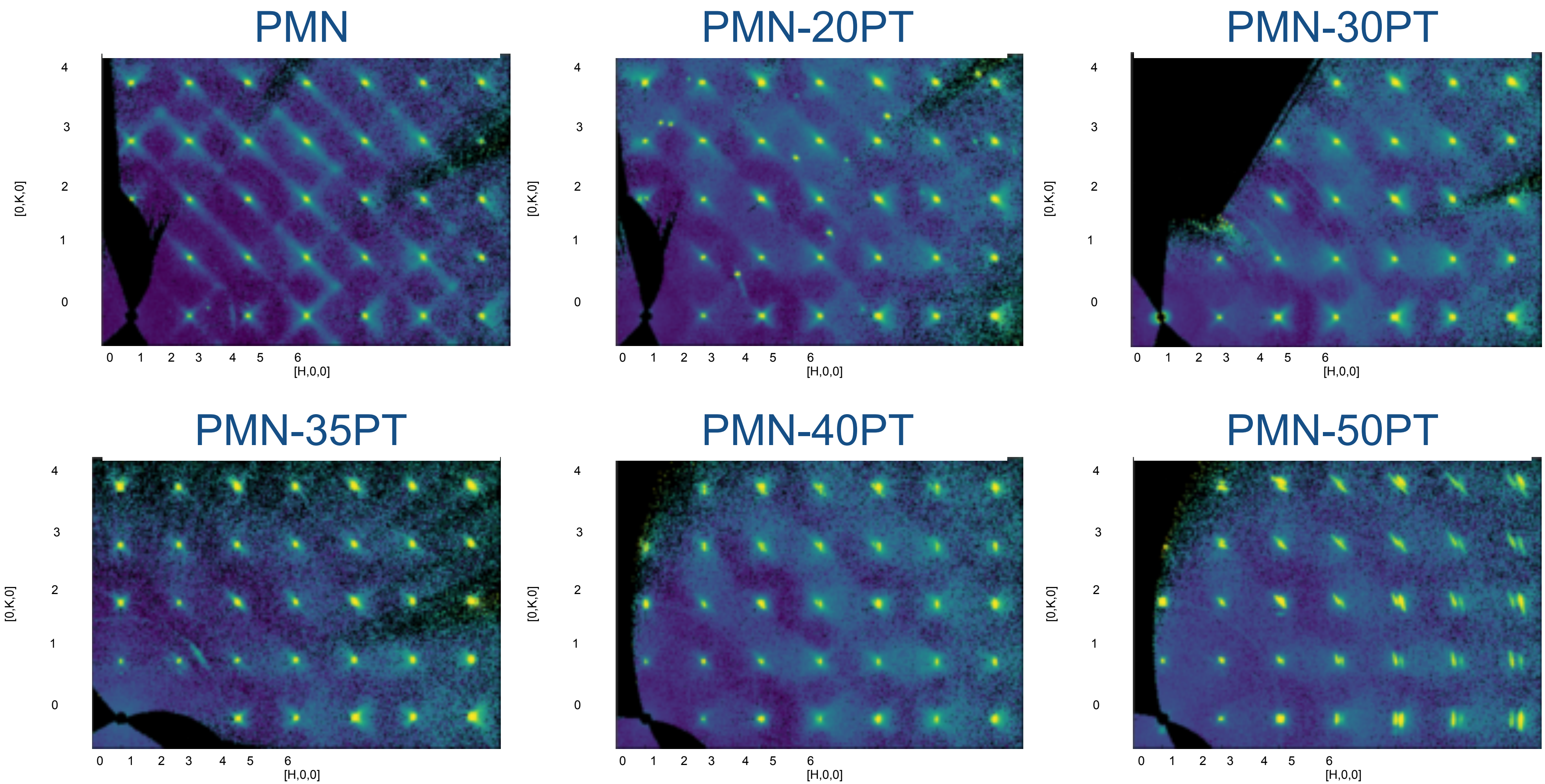




Acknowledgement: Richard Welberry (PI) and Christina Hoffmann

First Results

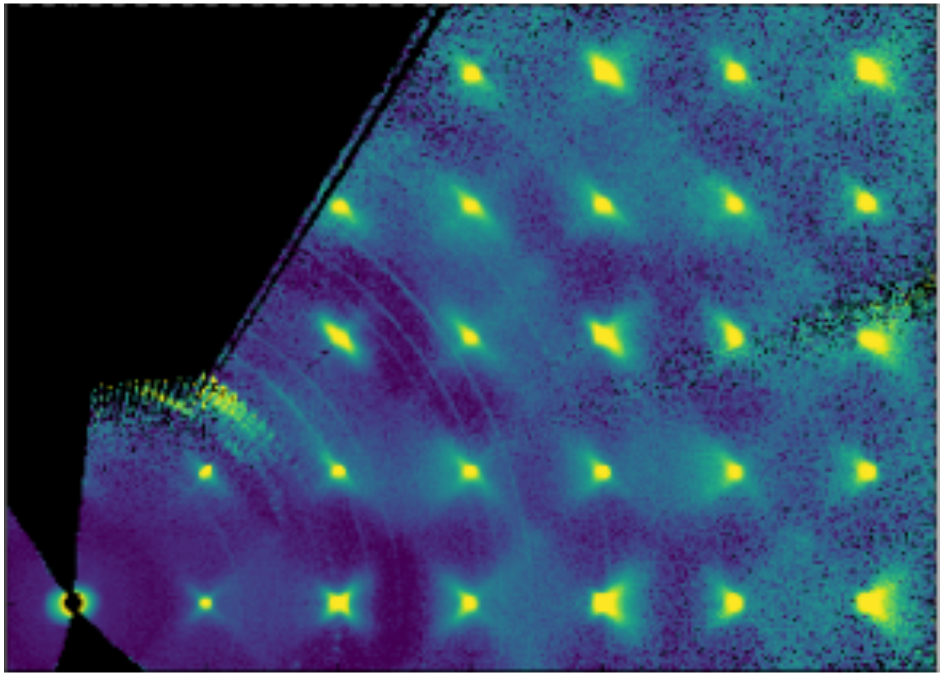
Relaxor Ferroelectrics - $Pb(Mg_{1/3}Nb_{2/3})O_3$-30%$PbTiO_3$



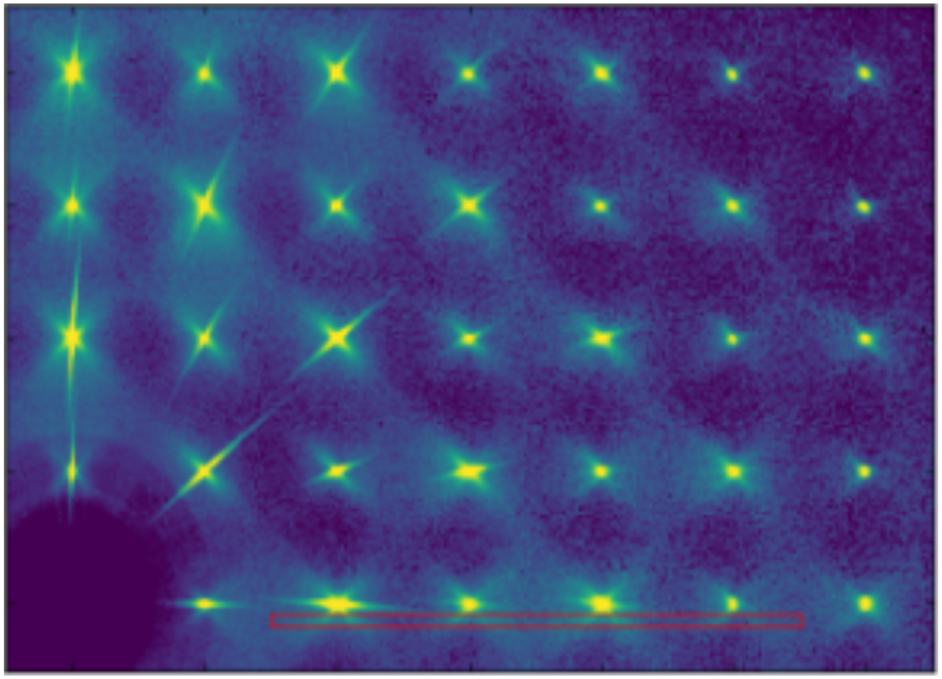
Acknowledgement: Matt Krogstad, Daniel Phelan, Stephan Rosenkranz

Complementarity of Neutrons and X-rays

$Pb(Mg_{1/3}Nb_{2/3})O_3$-30%$PbTiO_3$



Corelli Neutrons

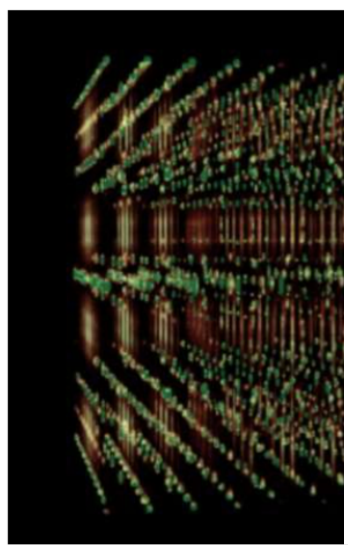


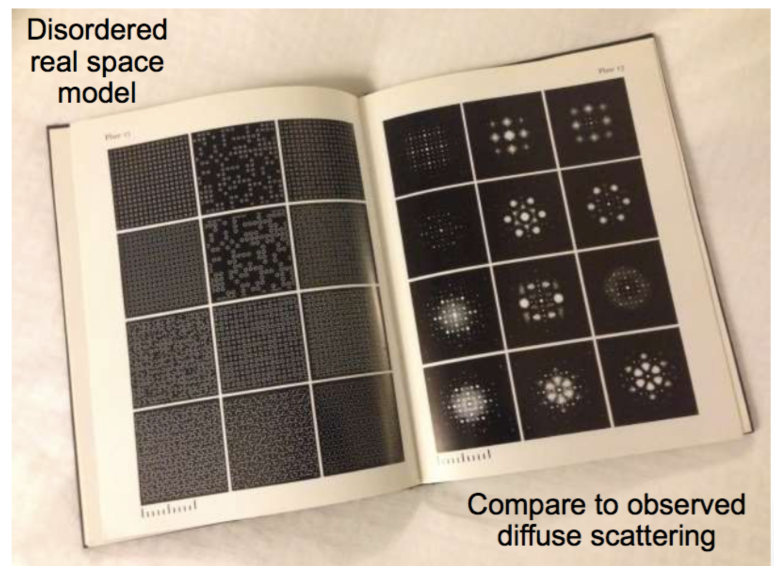
CHESS 55keV X-rays

Acknowledgement: Matt Krogstad, Daniel Phelan, Stephan Rosenkranz

The Future

- High-Energy X-rays
  - Absorption lengths similar to neutrons
  - Most existing detectors have low efficiency but alternatives exist, *e.g.* CdTe
- Micro-diffuse scattering
  - Benefiting from increased brightness of, *e.g.,* APS Upgrade
- Increasing use of *ab initio* computational modeling
  - Allowing more complex systems to be investigated
  - Less dependence on intuition in modeling
- Enhanced analysis tools
  - Machine learning
  - Correlated data analysis
  - Easier co-refinement of neutrons and x-rays





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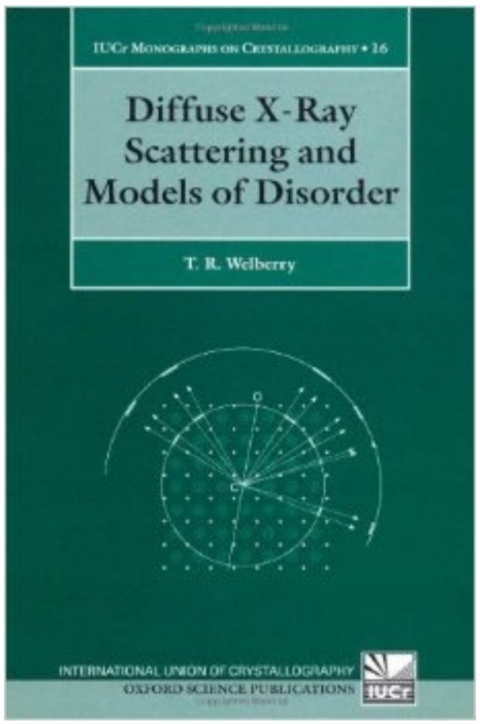
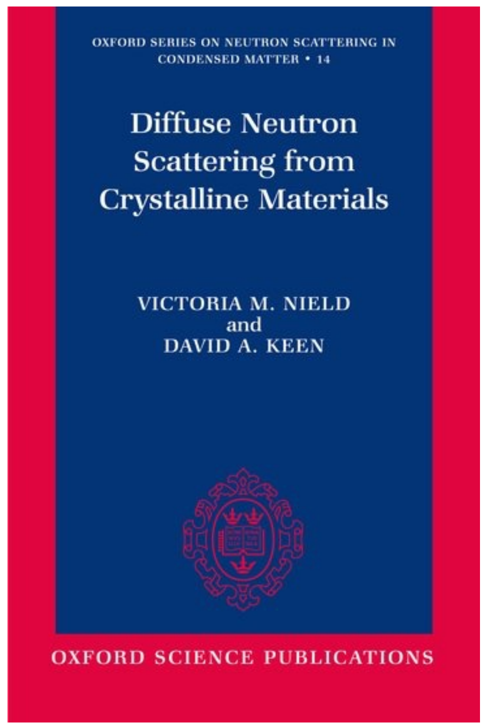
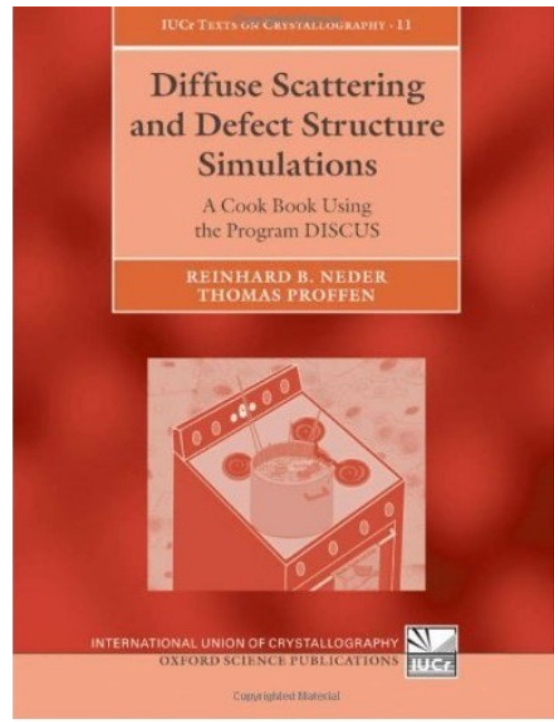


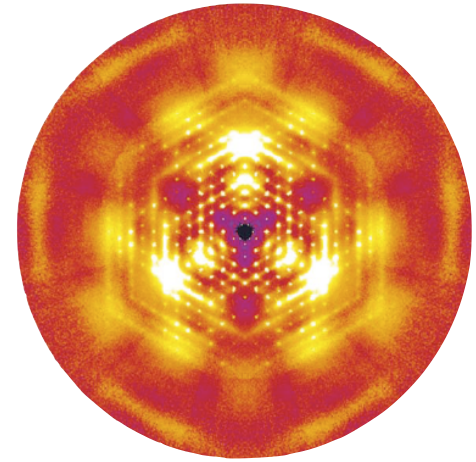


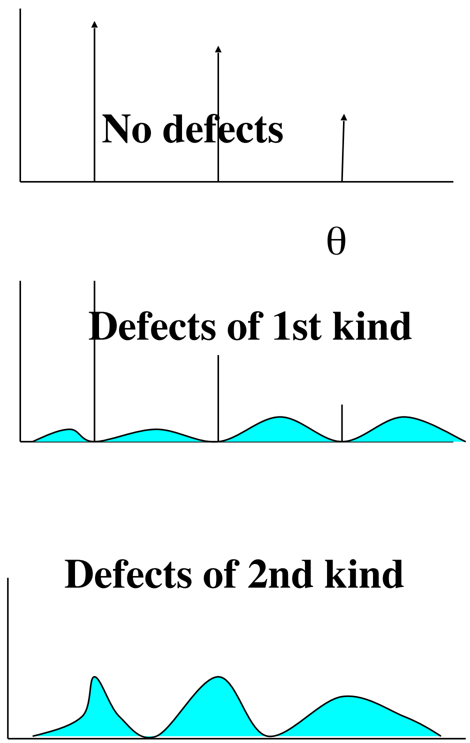


Diffuse Scattering Song

- Come eager young scholars - so tender and new
  I'll teach you diffraction - what I says mostly true
  Between the Bragg Peaks lies a world where you see
  Fluctuations and defects- they stand out plane-ly
- *Chorus*
  For its dark as a dungeon between the Bragg peaks
  But here in the darkness - each defect speaks
  It gathers- from throughout- reciprocal space
  And re-distributes all over the place.
- Between the Bragg peaks - one thing that we see
  Is TDS on our CCD
  Intensity totals are conserved- you can't win
  It steals from the Bragg peaks that stay very thin
- Substitutional alloys can cause quite a stir
  The shorter the length scale the greater the blur
  With care you can find out the bond length between
  Each atom pair type-the measurements clean
- Dislocations and other- type 2 defects
  Destroy the Bragg peaks -they turn them to wrecks
  But near the Bragg peaks- you still can see
  Intense diffraction continuously
- Many -are- the defects you find
  Between the Bragg peaks where others are blind
  So go tell your friends and impress your boss
  You've new understanding -with one hours loss

Gene Ice





Krivoglaz Classifications