

Use of raw data for diffraction space visualization: What are we missing in an integrated HKL file?

Jim Britten

McMaster University

Canada

Outline

Visualization of area detector scans

Supercells

Incommensurate scattering

Diffuse scattering

Twinning

Texture of thin films

Teaching Crystallography

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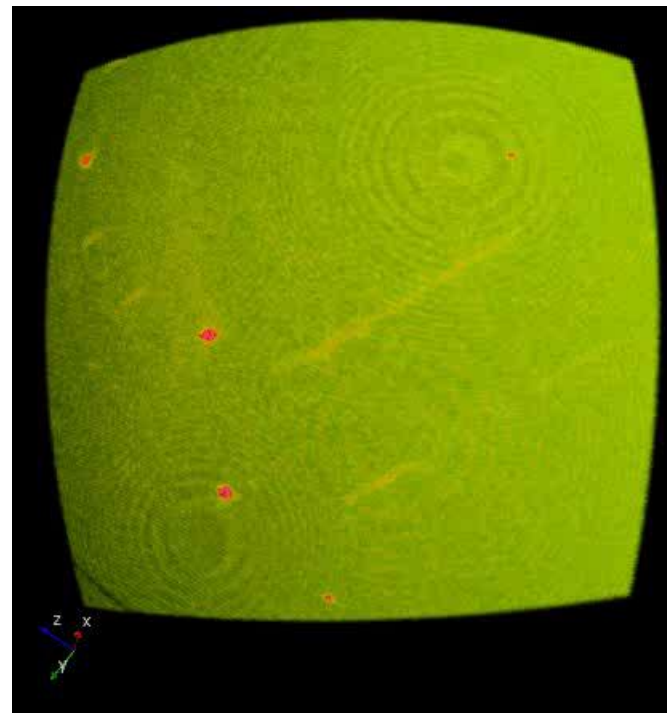
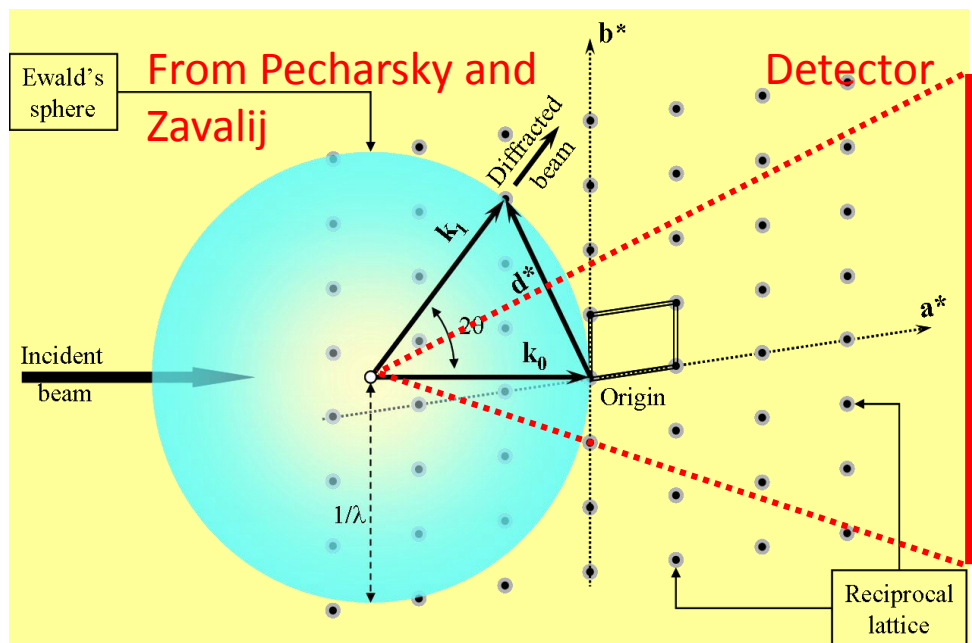
Twinning

Texture of thin films

Teaching Crystallography

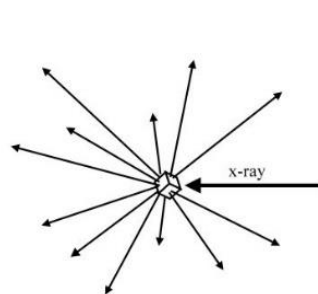
Other diffraction patterns worth saving

Rotate the sample in the beam and collect 2D frames.

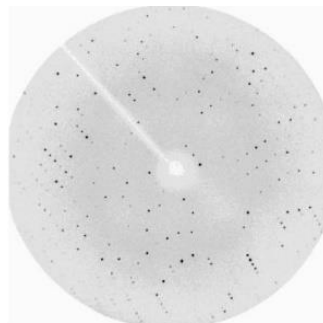


The 2D images can be mapped into reciprocal space – onto the surface of Ewald's Sphere

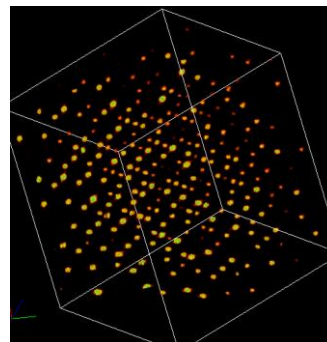
SCD - 2D image + scan \rightarrow 3D Int vs 2θ
XRD³ - 2D image + scan \rightarrow 3D Int vs 2θ



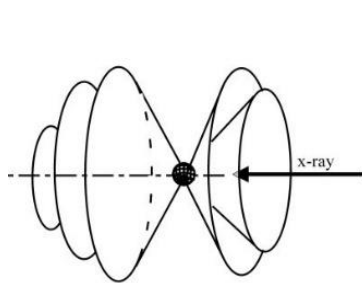
(a)



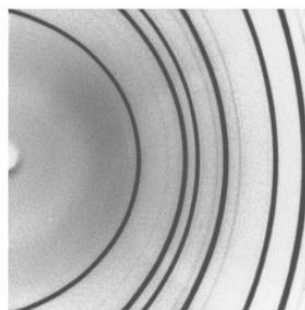
(b)



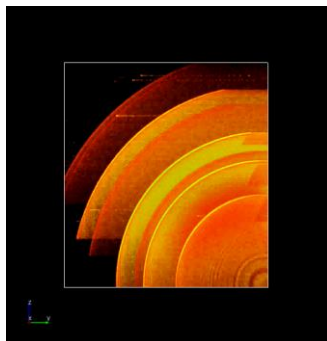
**Single
Crystal**



(c)



(d)

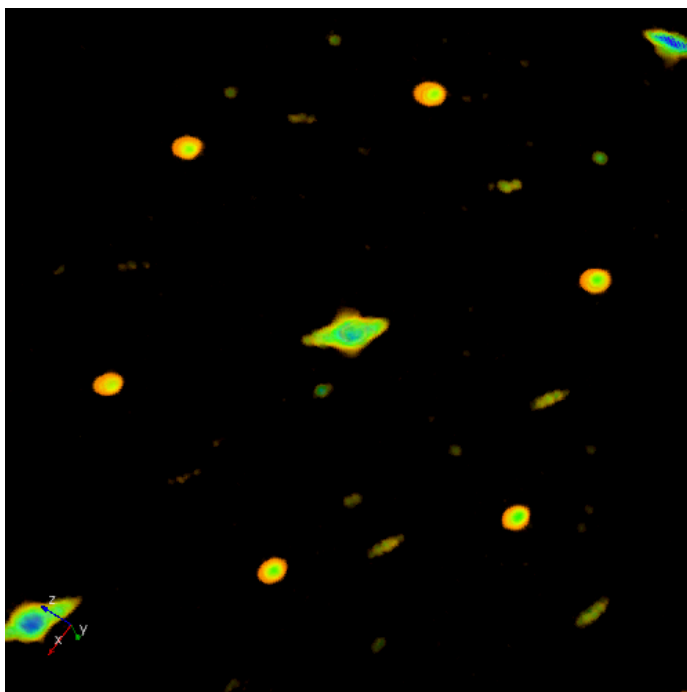


**Powder or
polycrystalline
solid**

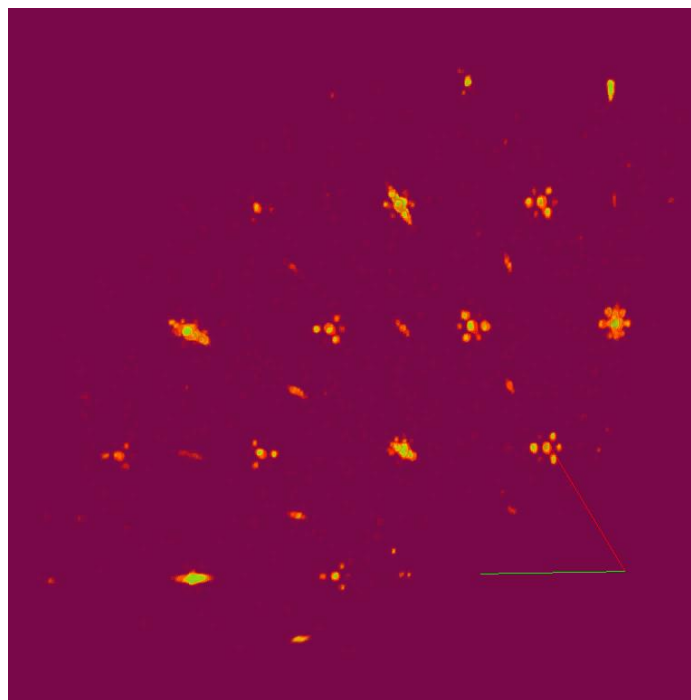
From Bob He's book: Two-Dimensional X-Ray Diffraction

Single Crystal With Long *and* Short Range Ordering (LuFe_2O_4)

Y.J. Kim, Toronto



80C



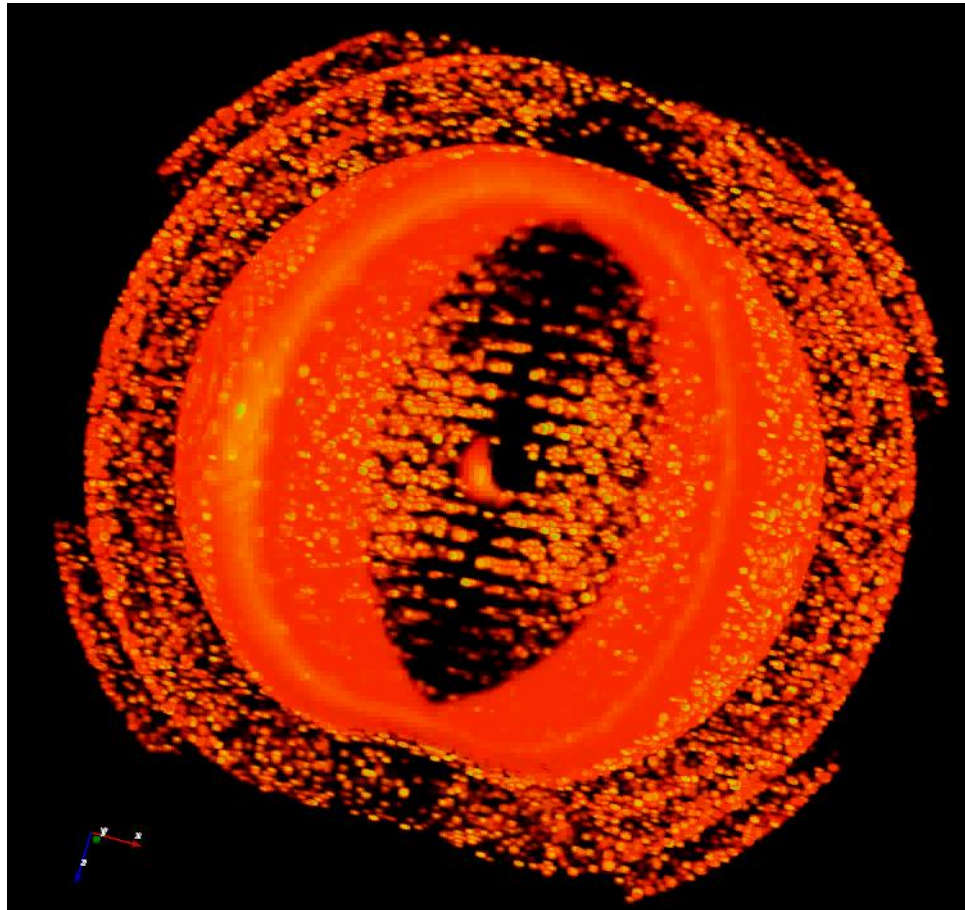
173C

When should small molecule crystallographers
publish raw diffraction data? IUCr21

Protein Single Crystal

Alba Guarne
Tamiza Nanji

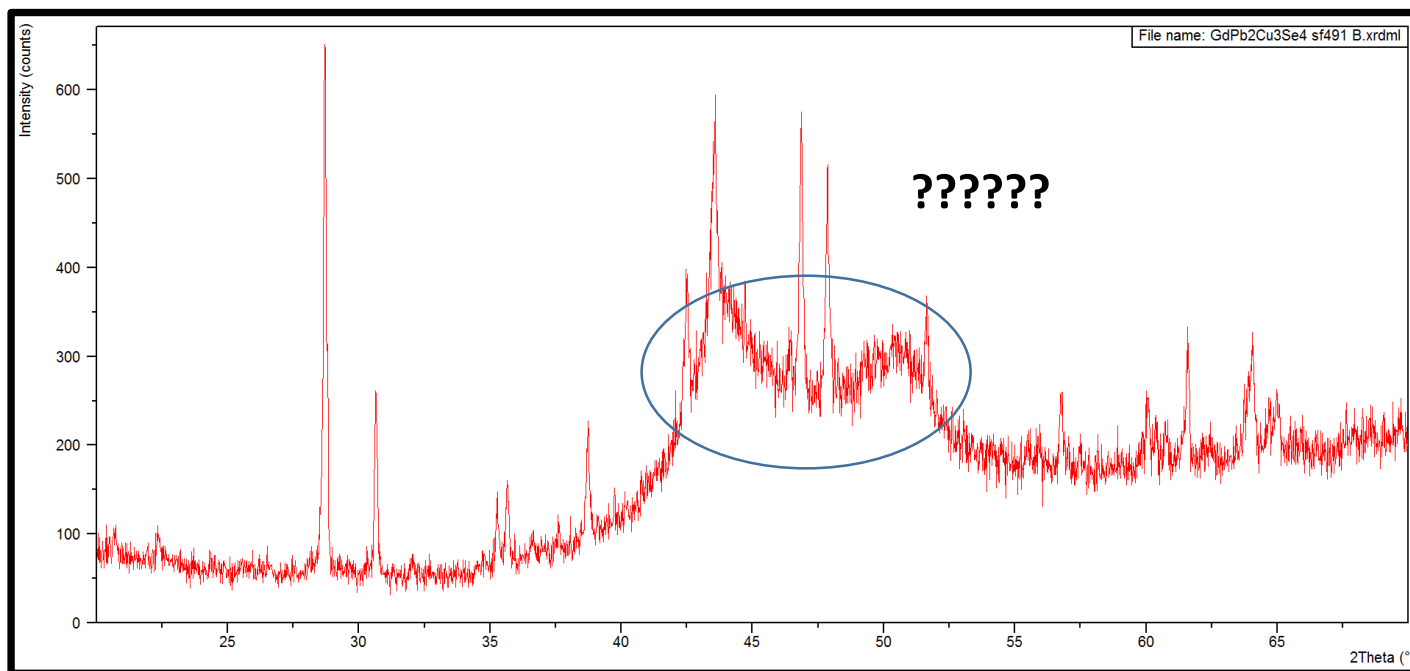
Rigaku
R-Axis4++
Image Plate



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GdPb₂Cu₃Se₄ 1200°C for 4 hrs (Plates)

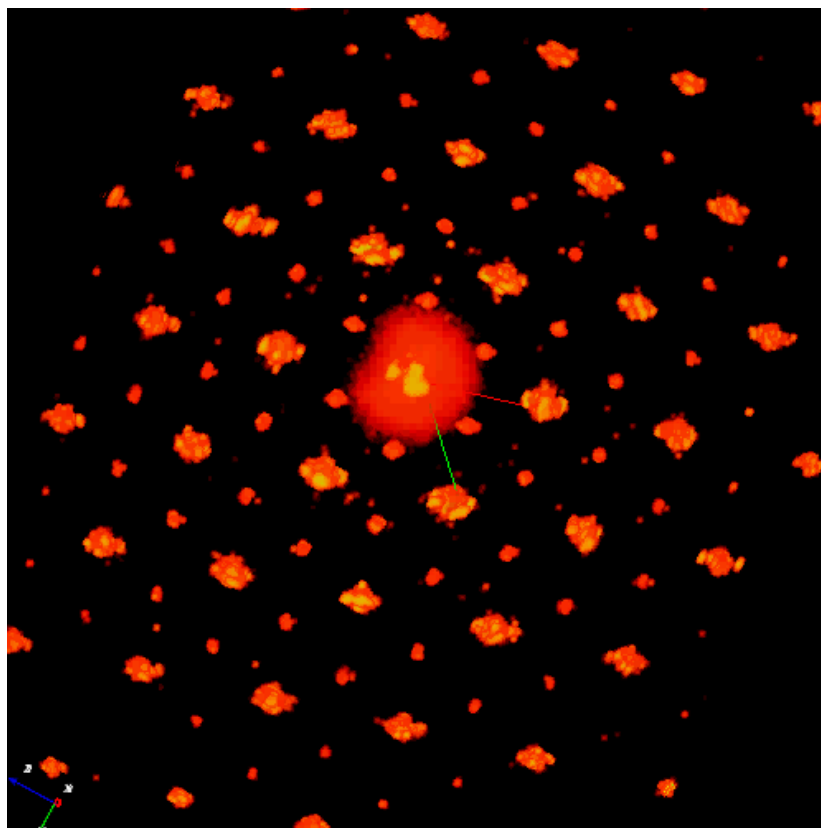
XRD pattern from Panalytical X'Pert Pro Diffractometer, Cu K α ₁



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$\text{GdPb}_2\text{Cu}_3\text{Se}_4$

Pawel Grochulski. Look at a single grain of the powder on a protein beamline.



Canadian Macromolecular Crystallography
Facility, 08B1-1 (CMCF-BM) Beamline

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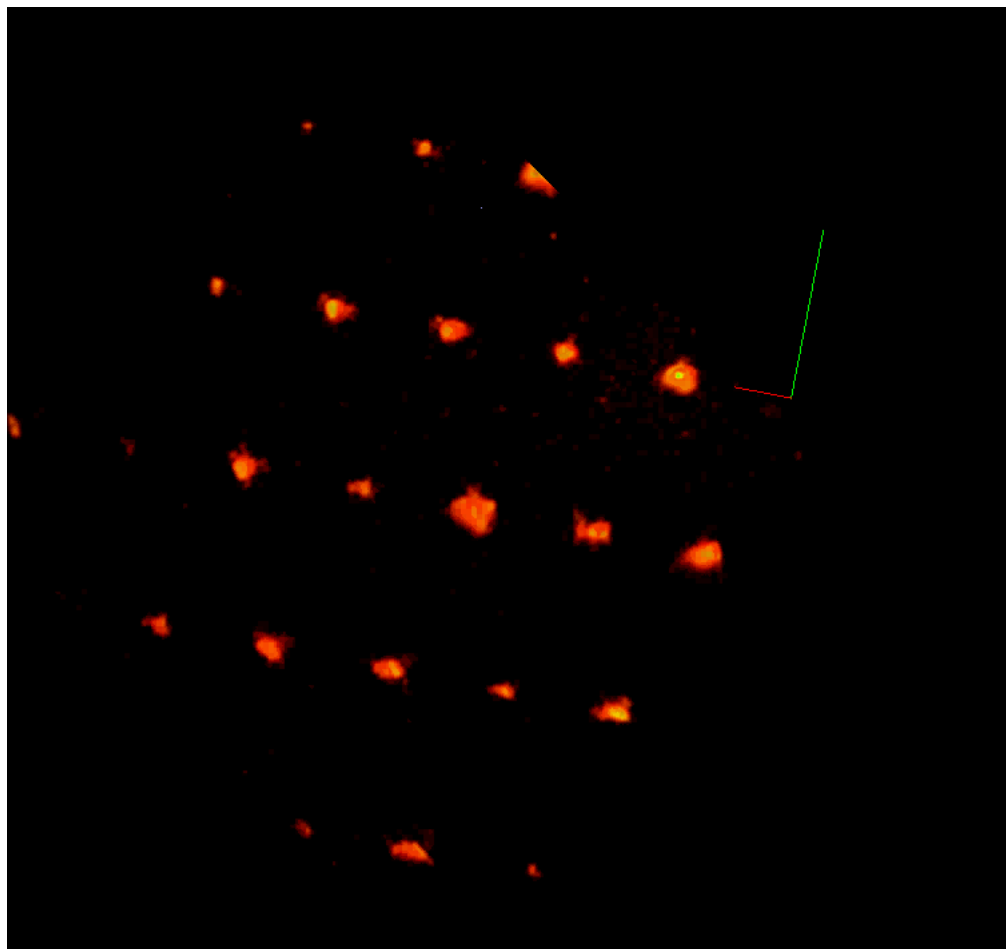
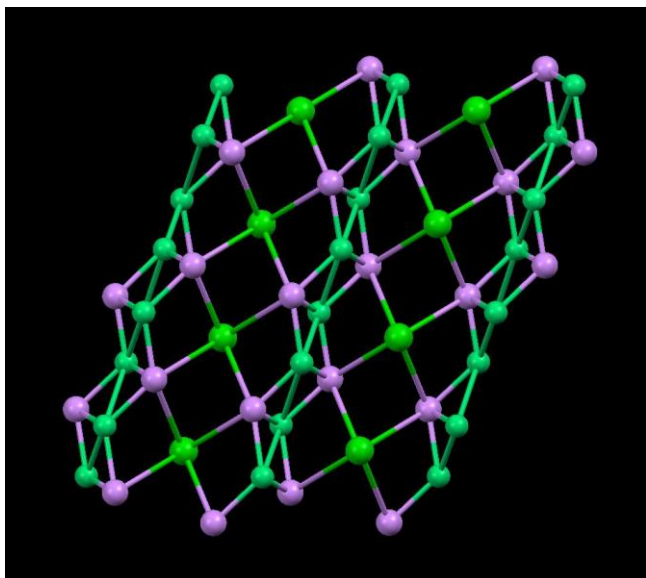
Teaching Crystallography

Other diffraction patterns worth saving

Supercell

Athena Safa-Sefat
Yurij Mozharivskij

Ba-As-Ni



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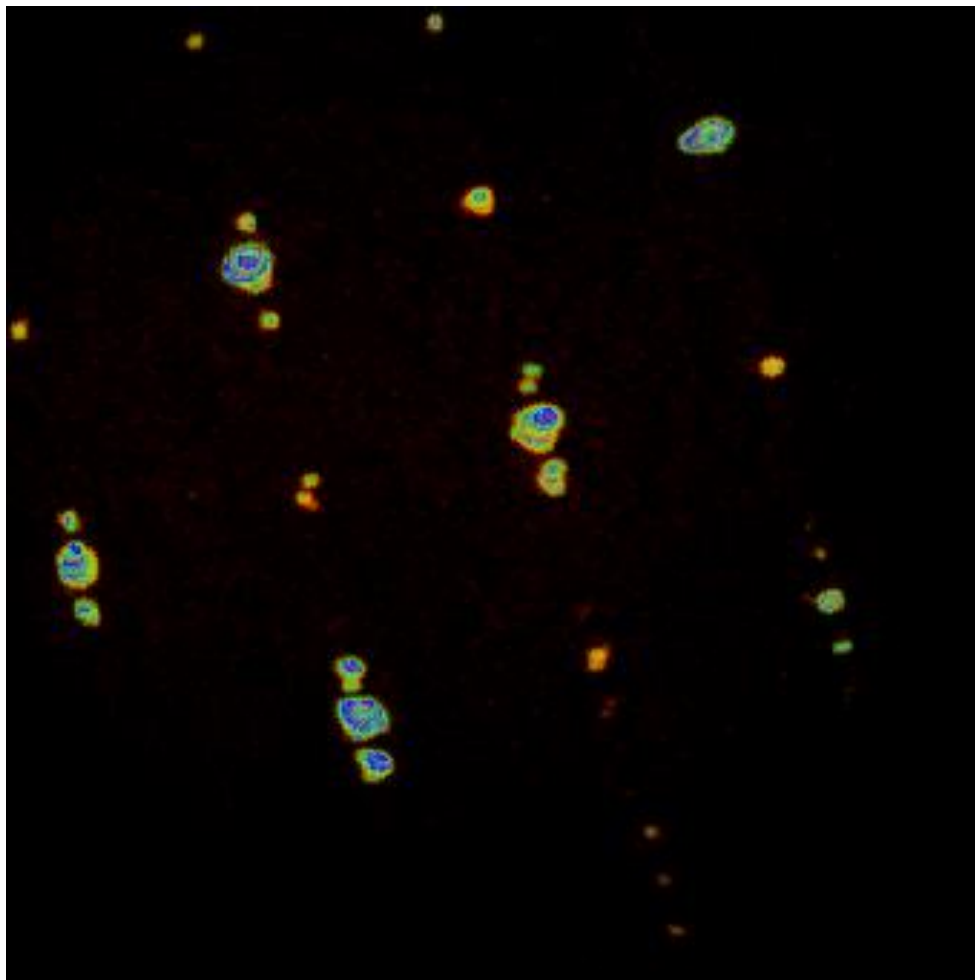
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Aperiodic Incommensurate Crystal



Bruce Gaulin – Bi Cu Oxide Superconductor

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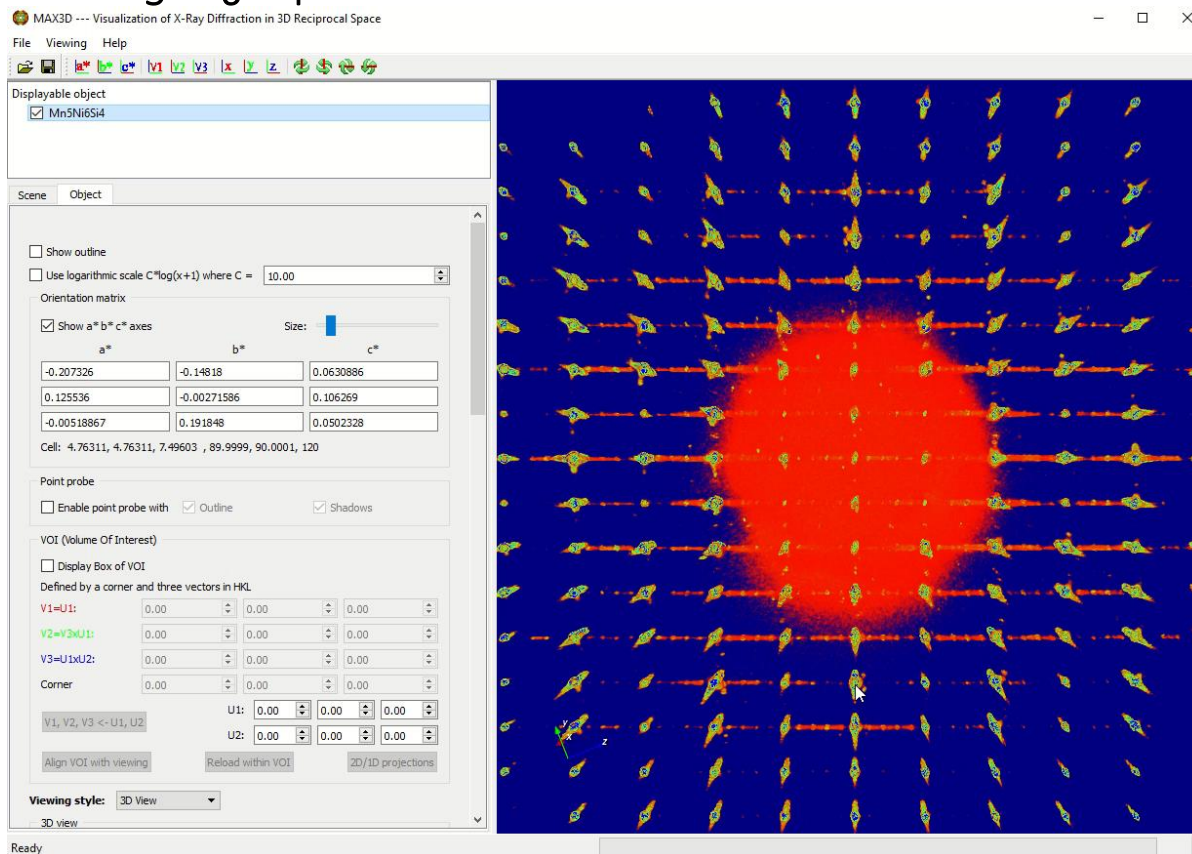
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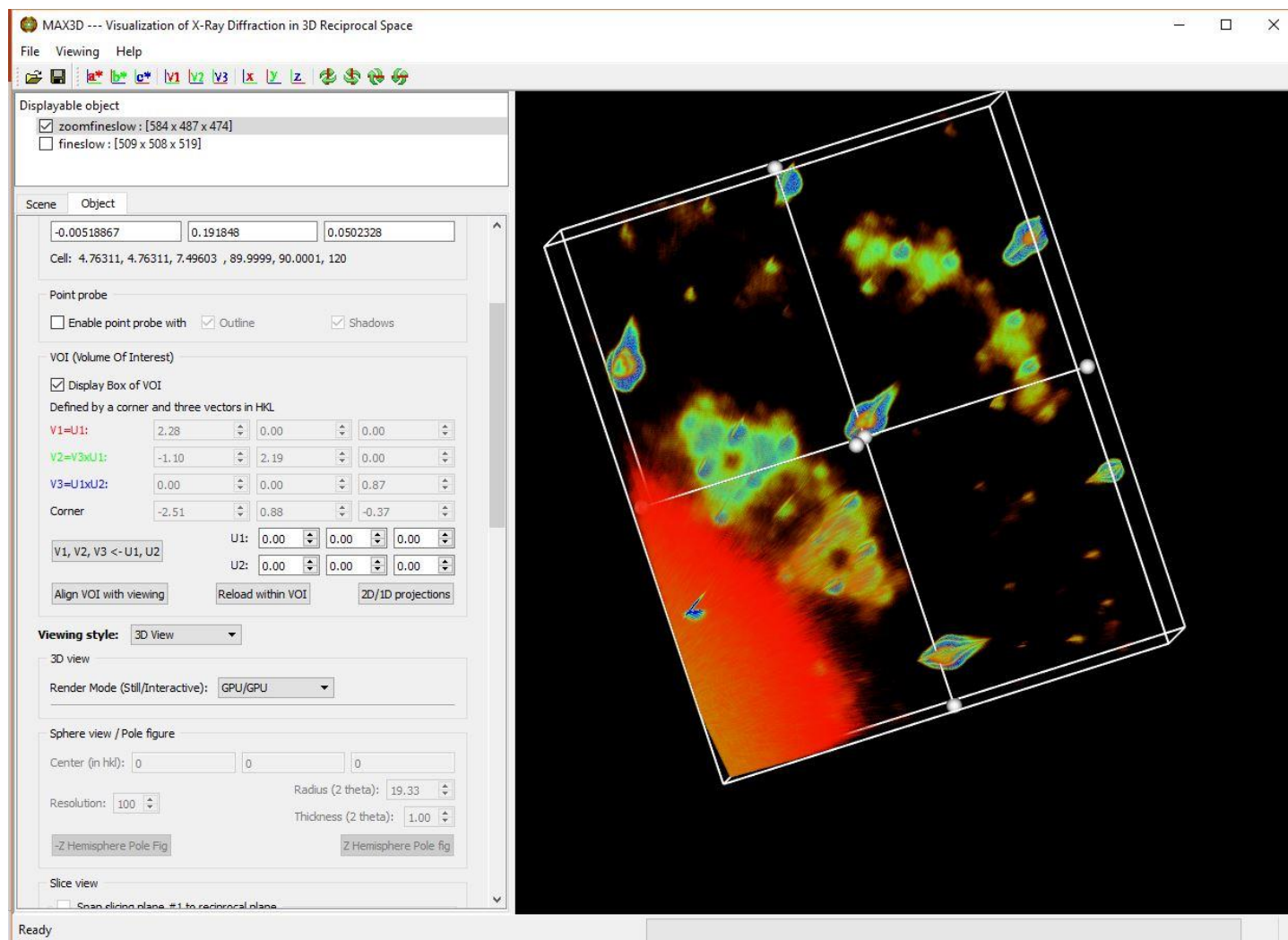
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$\text{Mn}_5\text{Ni}_6\text{Si}_4$; Marek Niewczas, Sheikh Ahmed

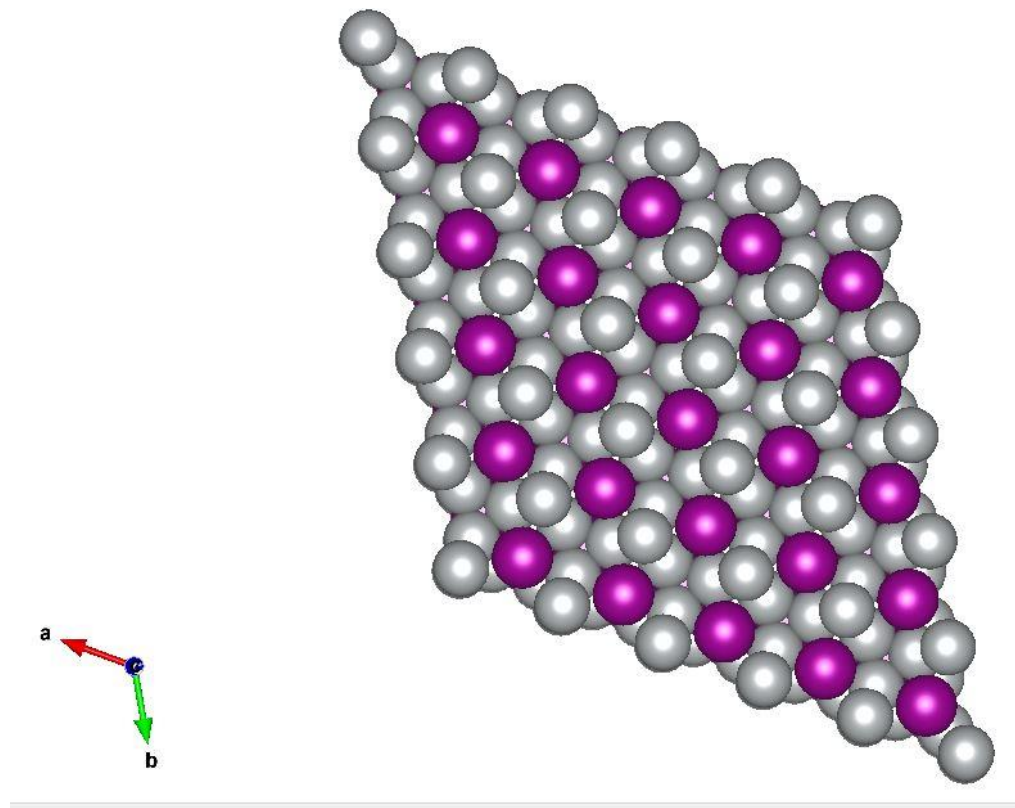


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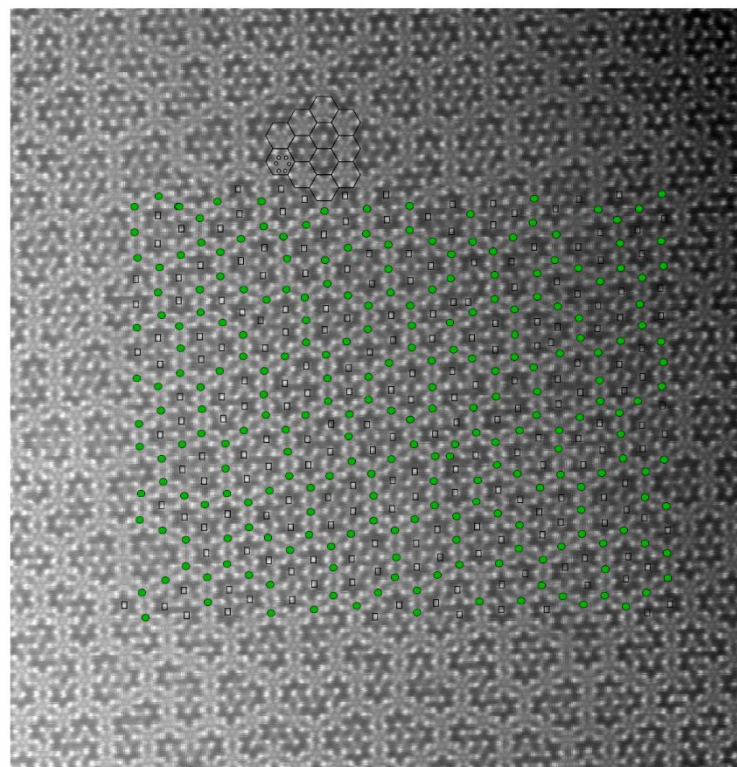
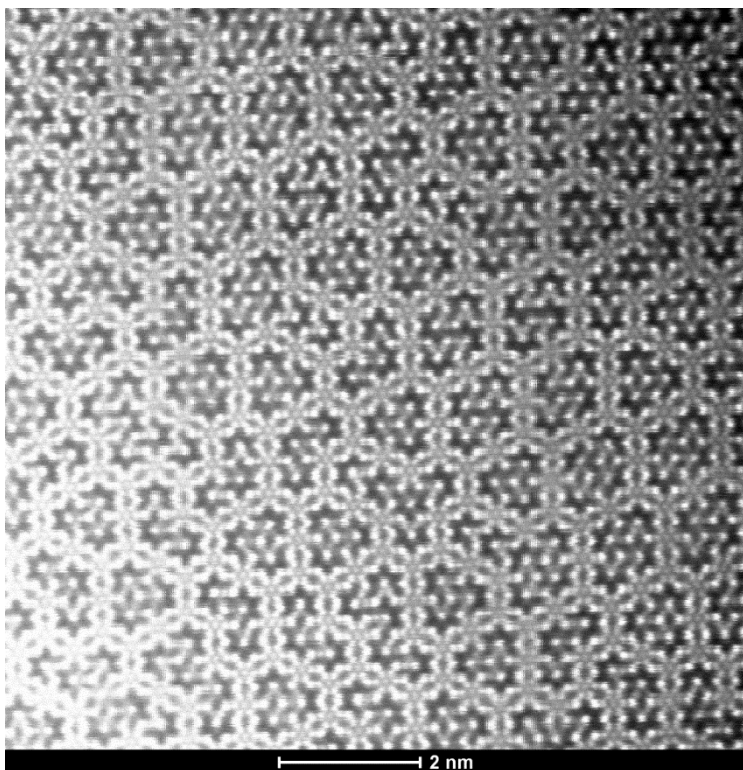


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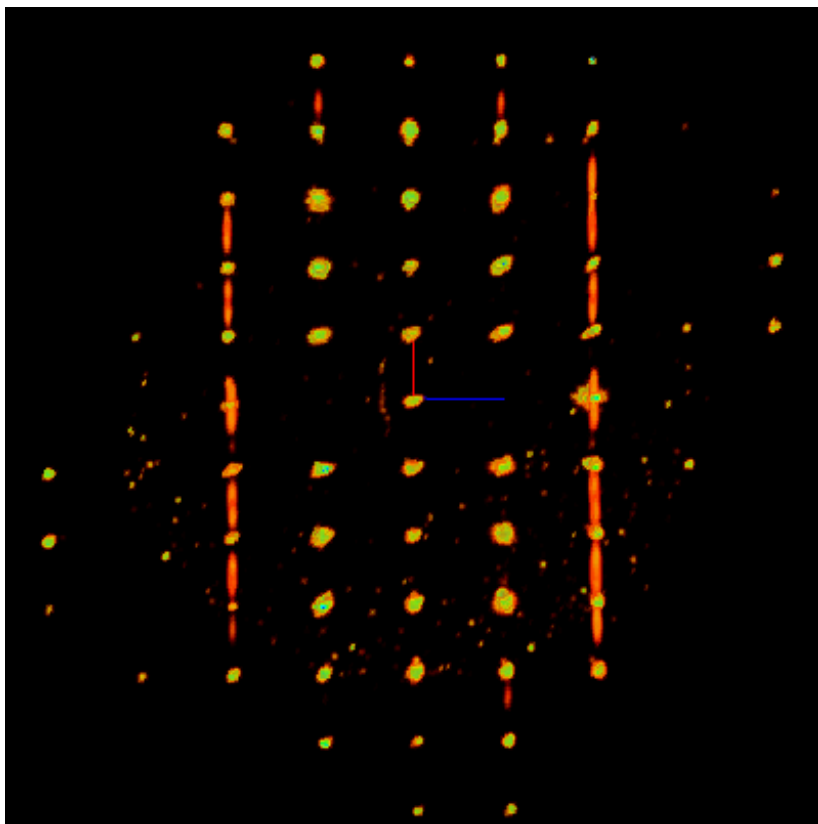


HRTEM



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Diffuse Scattering

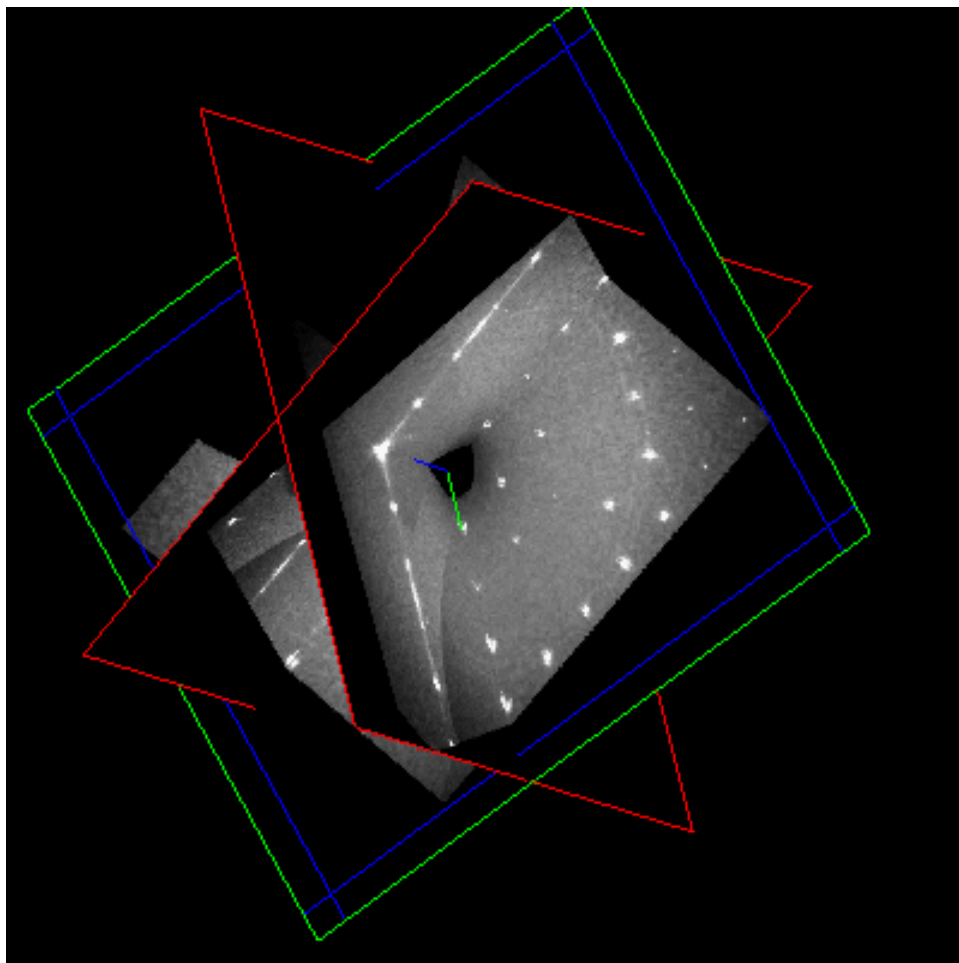


Columns of hexanaphthylbenzene are ordered along the stacking axis. The columns have a partial rotational disorder relative to one another. The refined structure shows a multiple orientations for the naphthyls. The configuration of the molecule in the ordered stack cannot be determined.

Hexanaphthylbenzene. Laura Harrington, Mike McGlinchey

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Diffuse Scattering

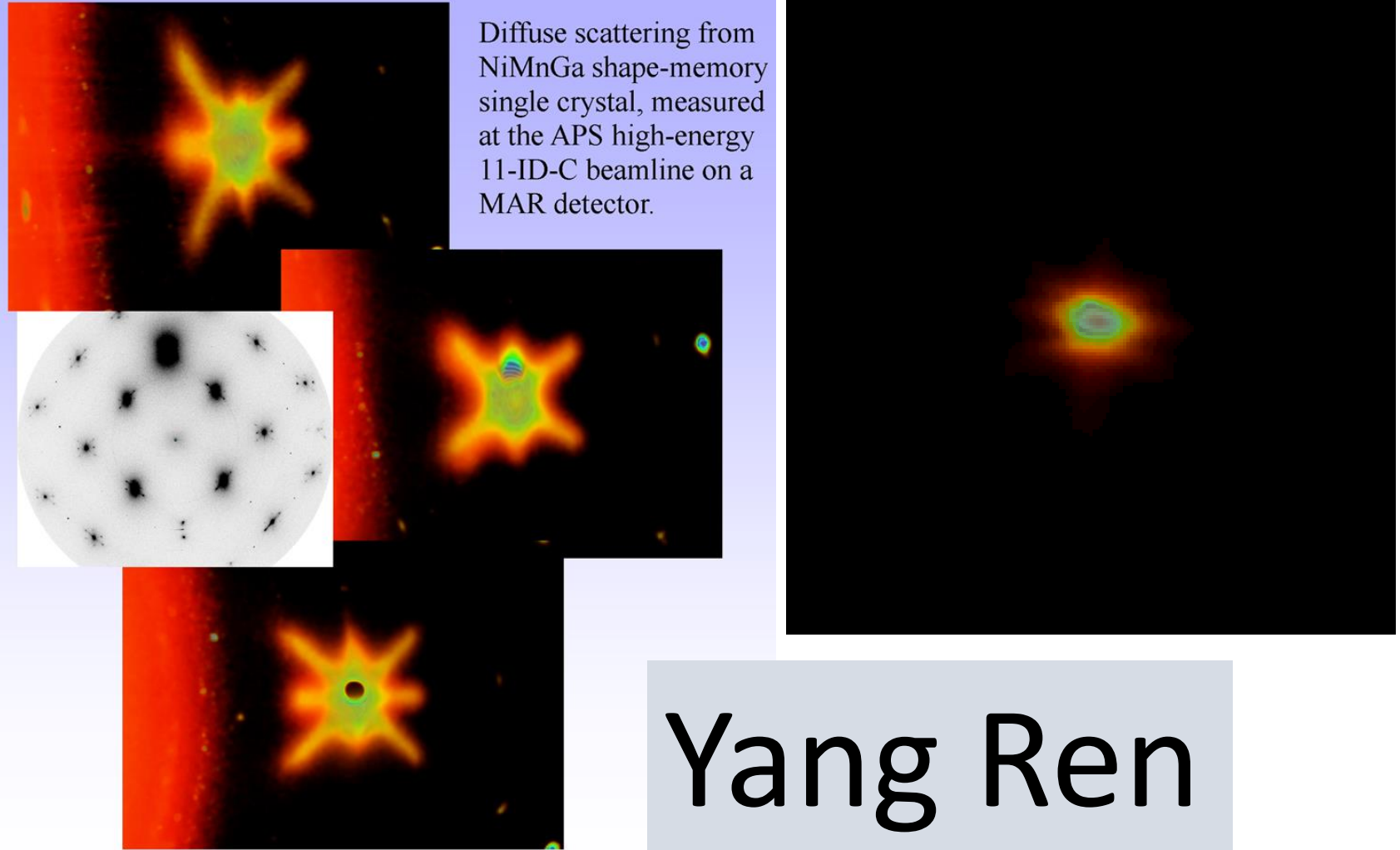


Hexanaphthylbenzene. Laura Harrington, Mike McGlinchey

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Diffuse Scattering

Diffuse scattering from NiMnGa shape-memory single crystal, measured at the APS high-energy 11-ID-C beamline on a MAR detector.



Yang Ren

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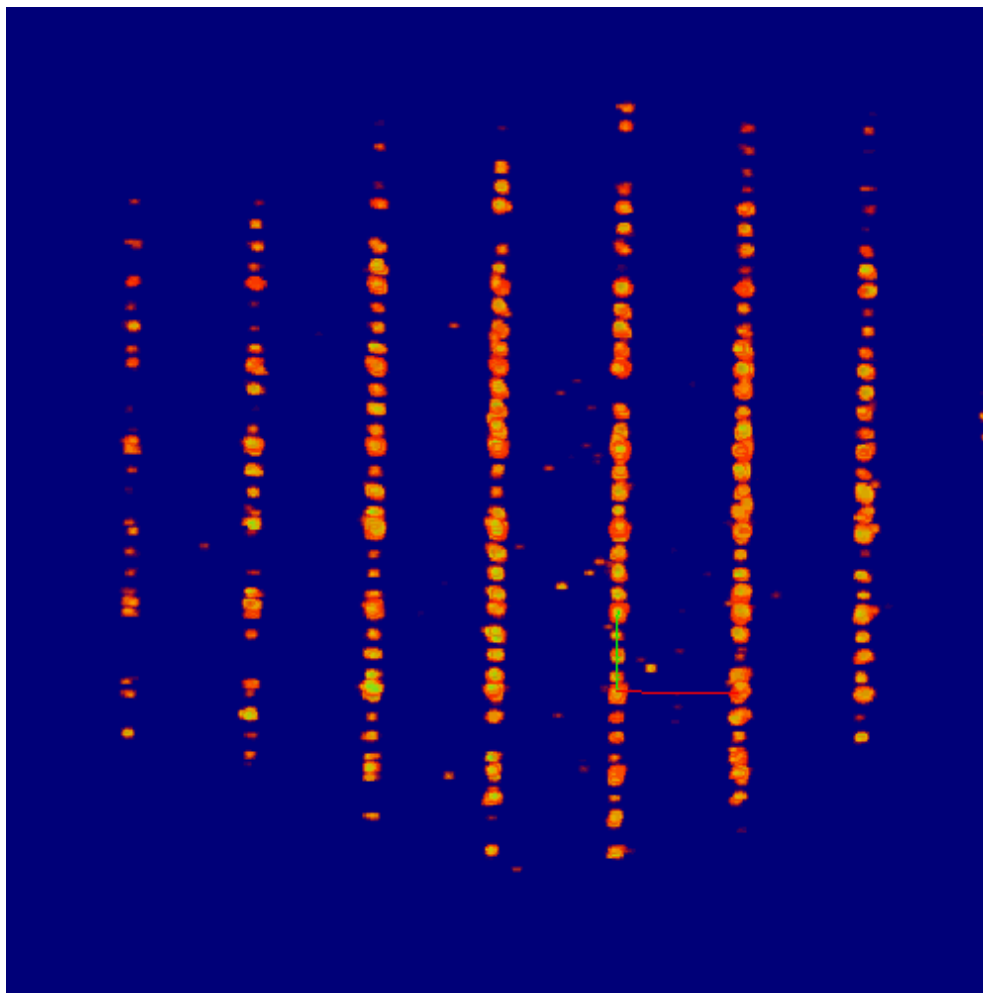
Texture of thin films

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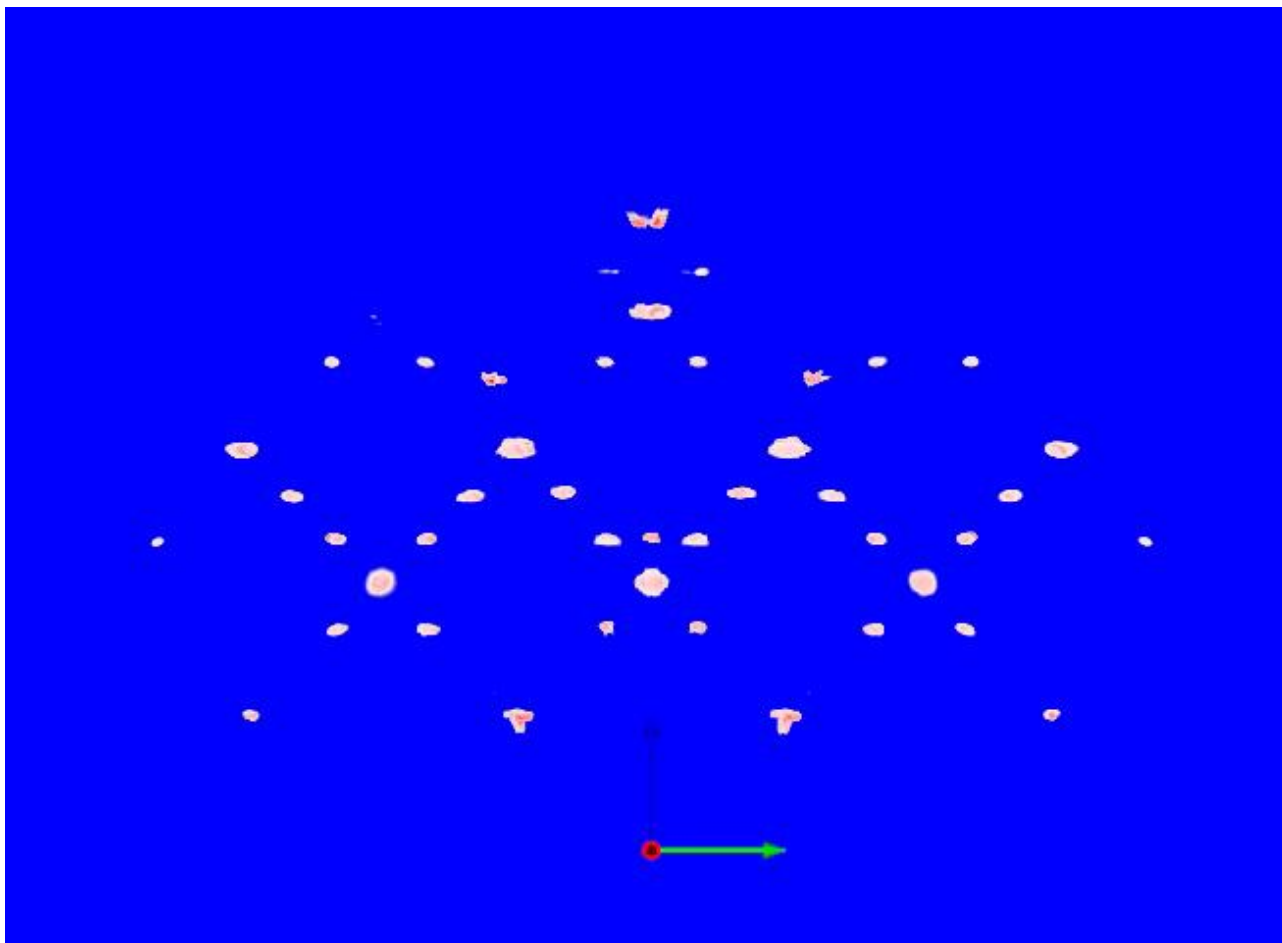
Small Molecule Twinned Crystal

Bruker Smart
Apex2 CCD



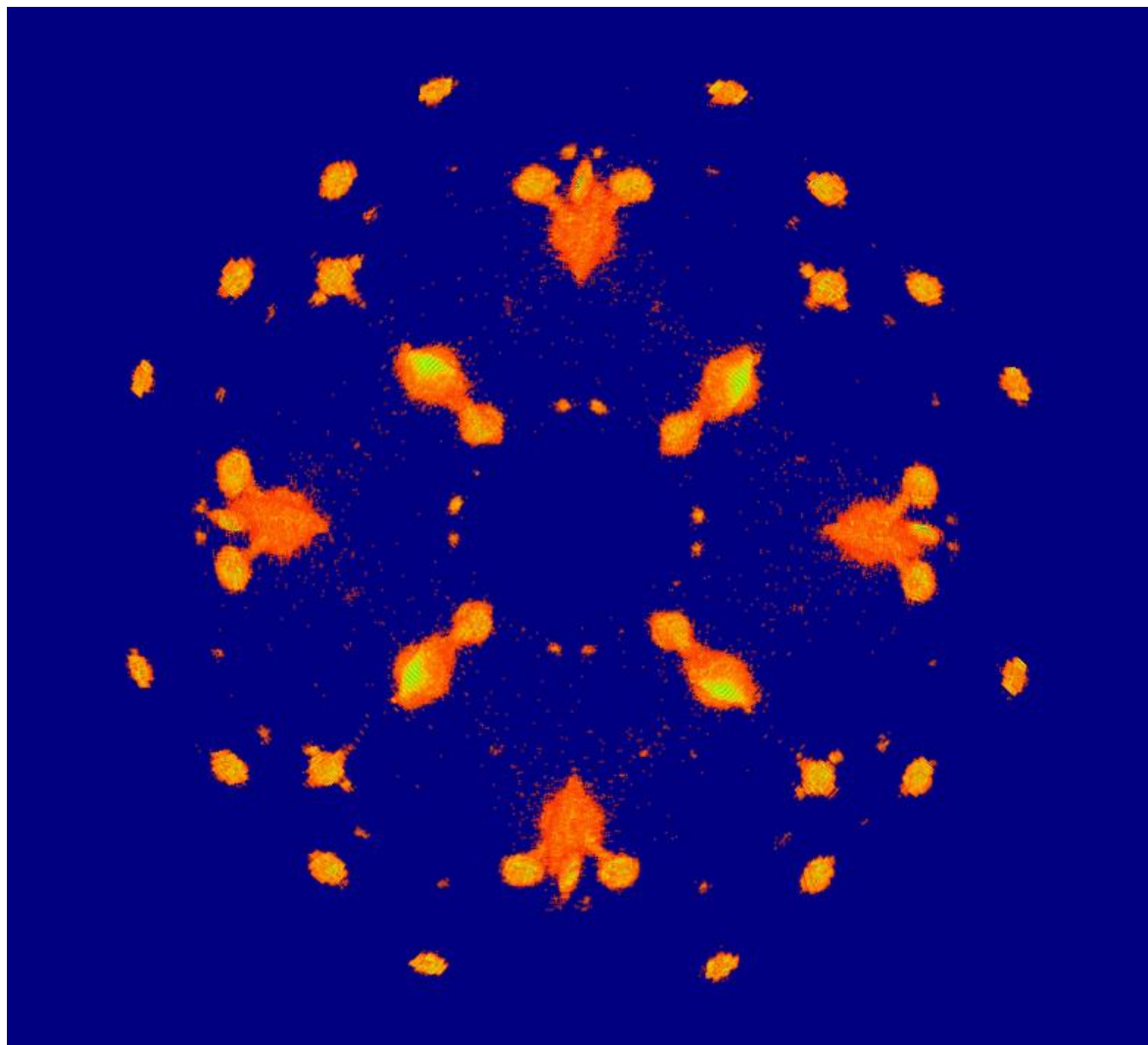
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3D diffraction pattern from thin film of $\text{InAs}_{(1-x)}\text{Sb}_x$ nanowires (isolate (111) reflections)



(220) and
(311) shells

Diffuse lines
connect twins



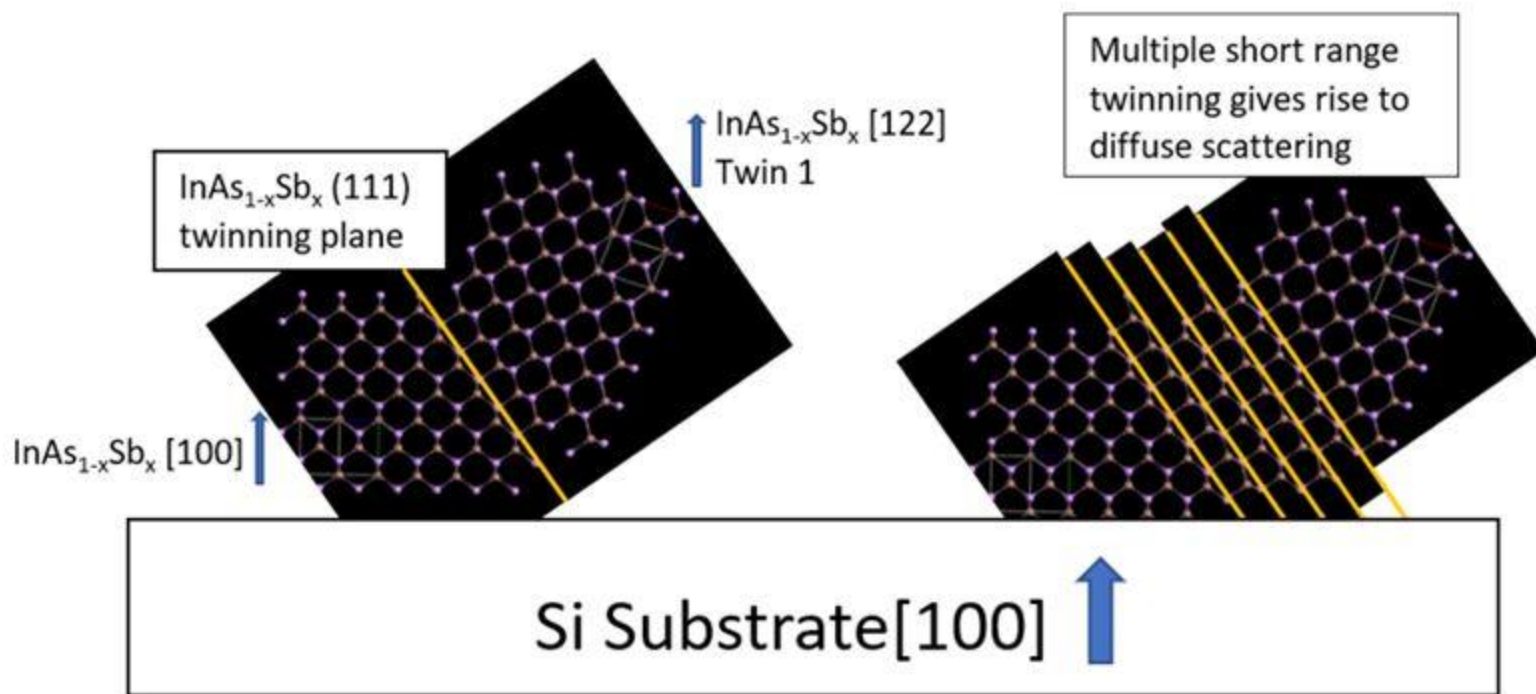


Figure 3. Twinning by 180° (or $\pm 60^\circ$) rotation about the [111] face of $\text{InAs}_{1-x}\text{Sb}_x$. Regions of multiple layer twinning account for the diffuse scattering observed in the 3D diffraction pattern. Twin planes are indicated by yellow lines.

Goosney, Jarvis, Britten, Lapierre, Infrared Physics and Technology

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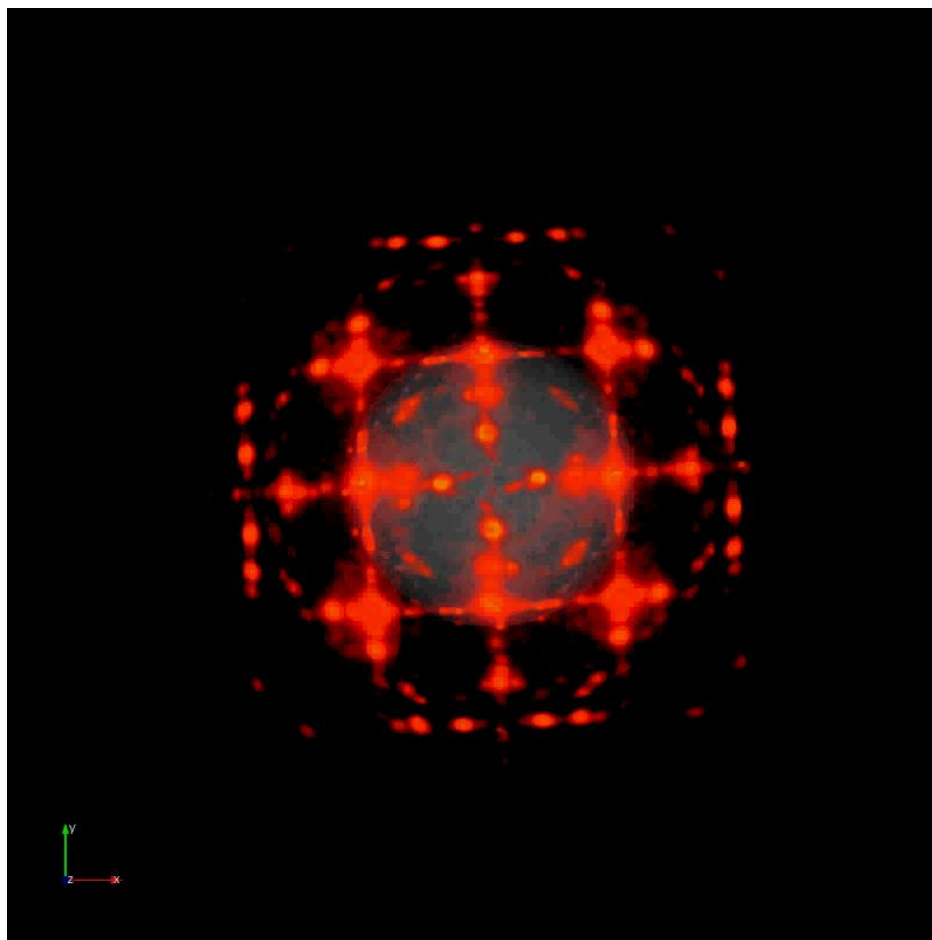
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Multiple (8) Orientations of GaAs NW's on Si Substrate

Ray LaPierre,
Vicky Jarvis,
McMaster



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Everything you have seen here and more . . .

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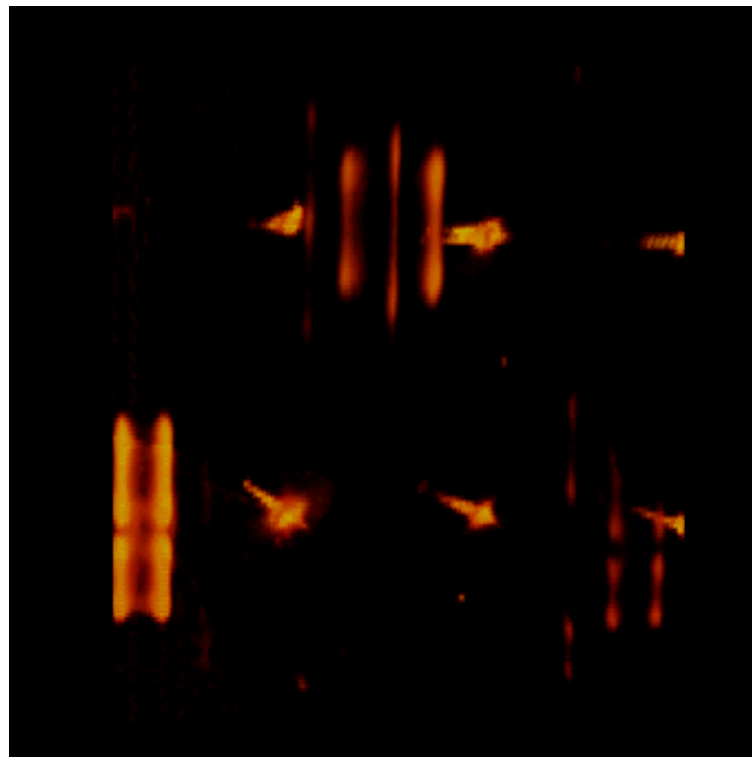
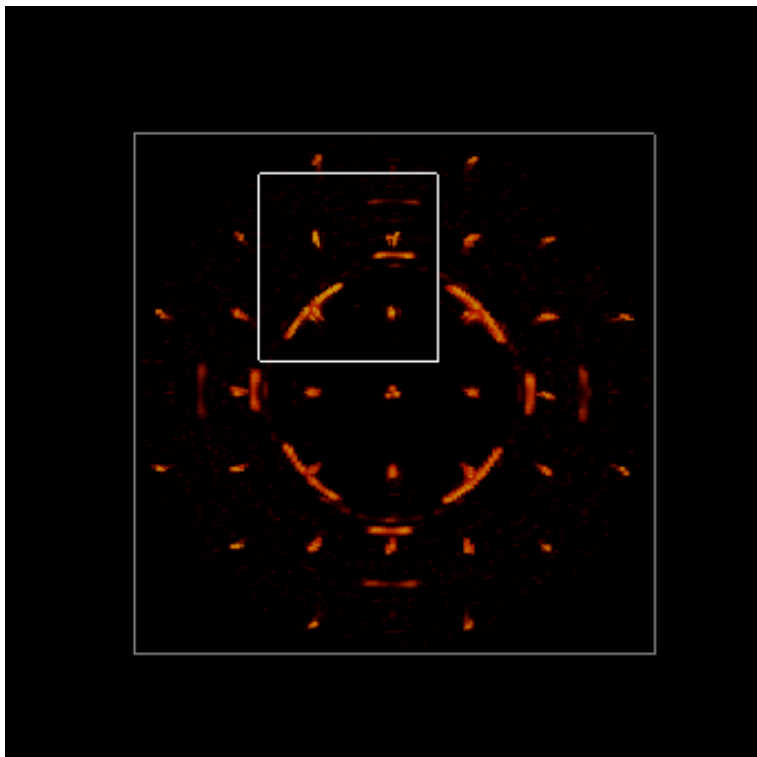
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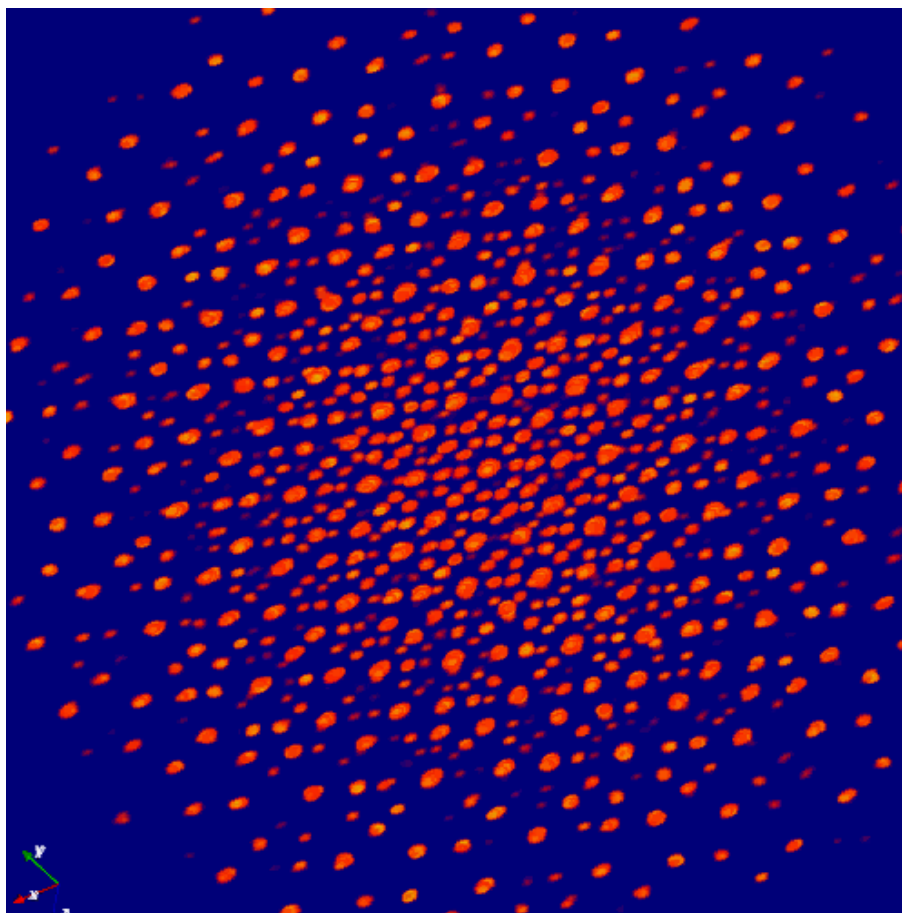
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Follow Phase Changes



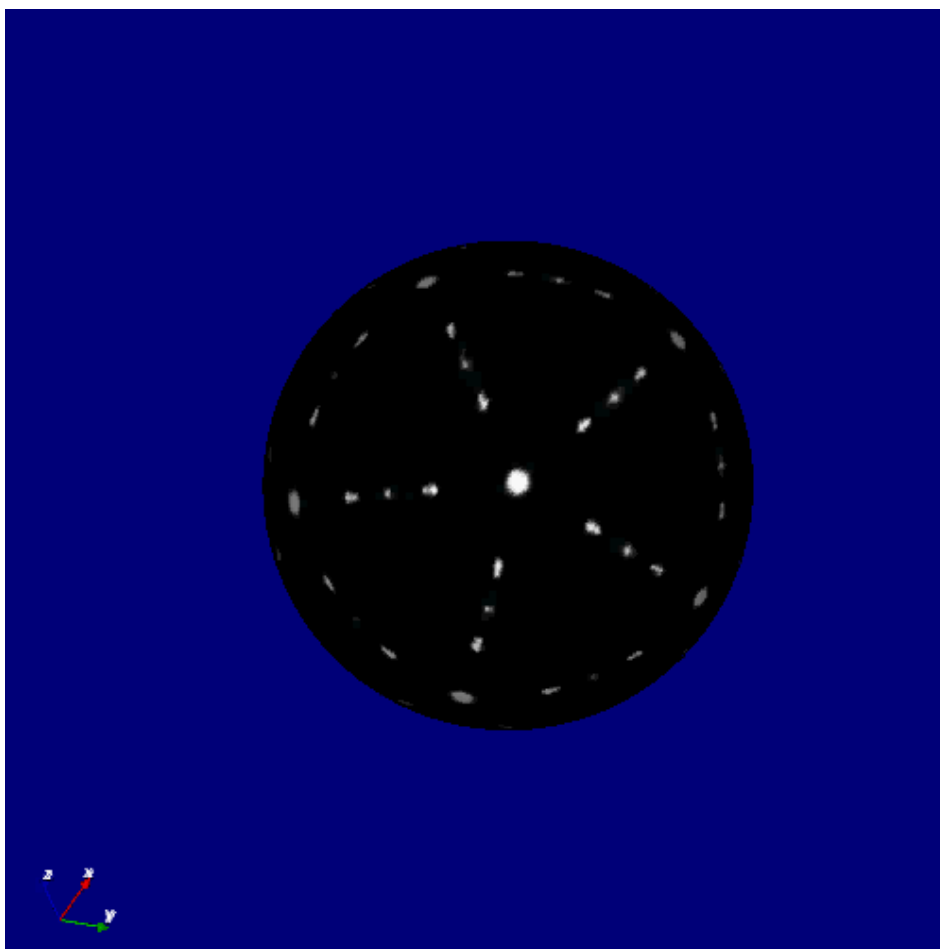
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What do we do with beautiful single crystal data from a quasicrystal?



$\text{Al}_{70}\text{Pd}_{21}\text{Mn}_9$ - Geetha Balakrishnan, University of Warwick
Nathan Armstrong, Tom Timusk, McMaster

$\text{Al}_{70}\text{Pd}_{21}\text{Mn}_9$ - Geetha Balakrishnan, University of Warwick
Nathan Armstrong, Tom Timusk, McMaster



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Software:

MAX3D : Jim Britten and Weiguang Guan,
McMaster University, Canada

Thank you for your attention.