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
Other diffraction patterns worth saving

Visualization of area detector scans

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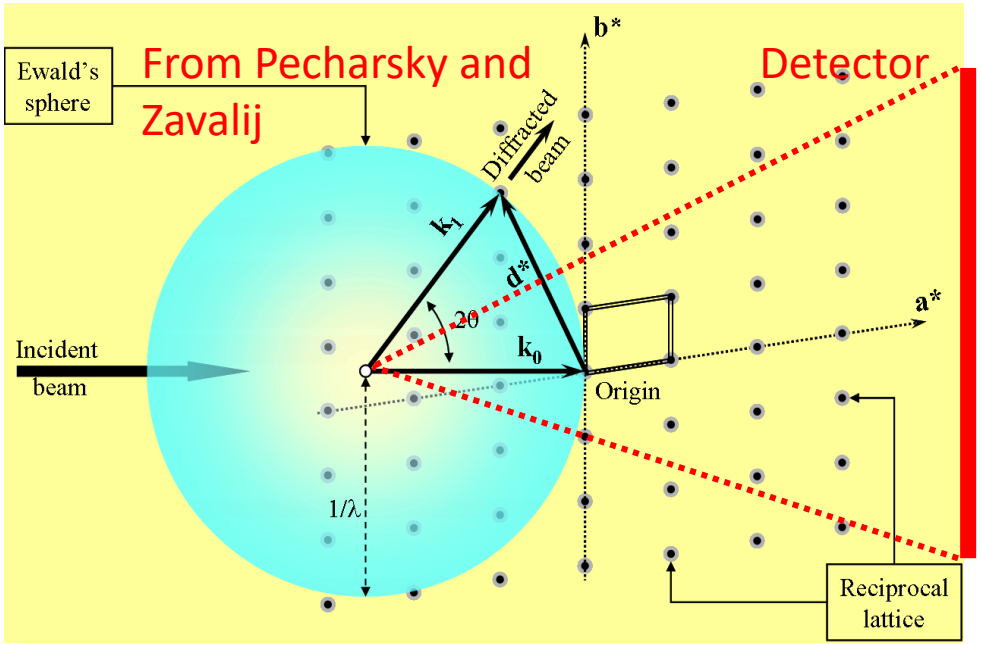
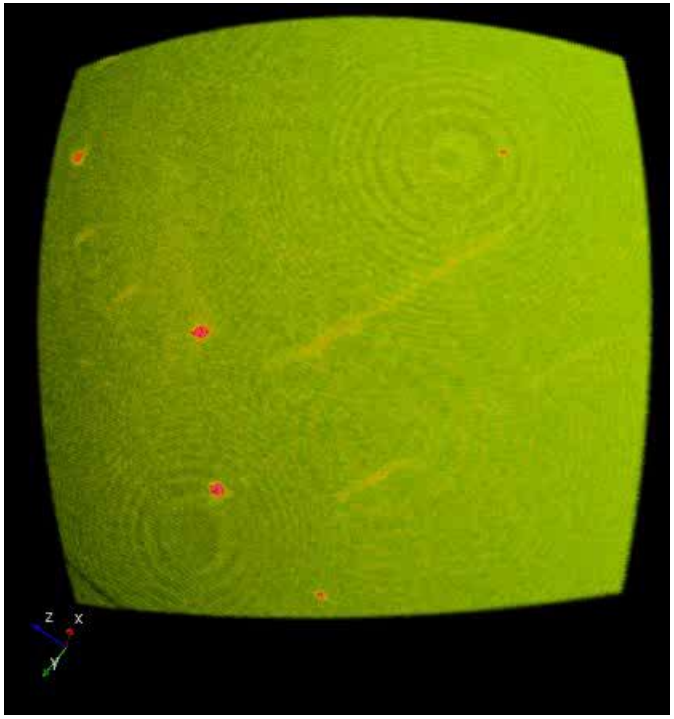
Rotate the sample in the beam and collect 2D frames.

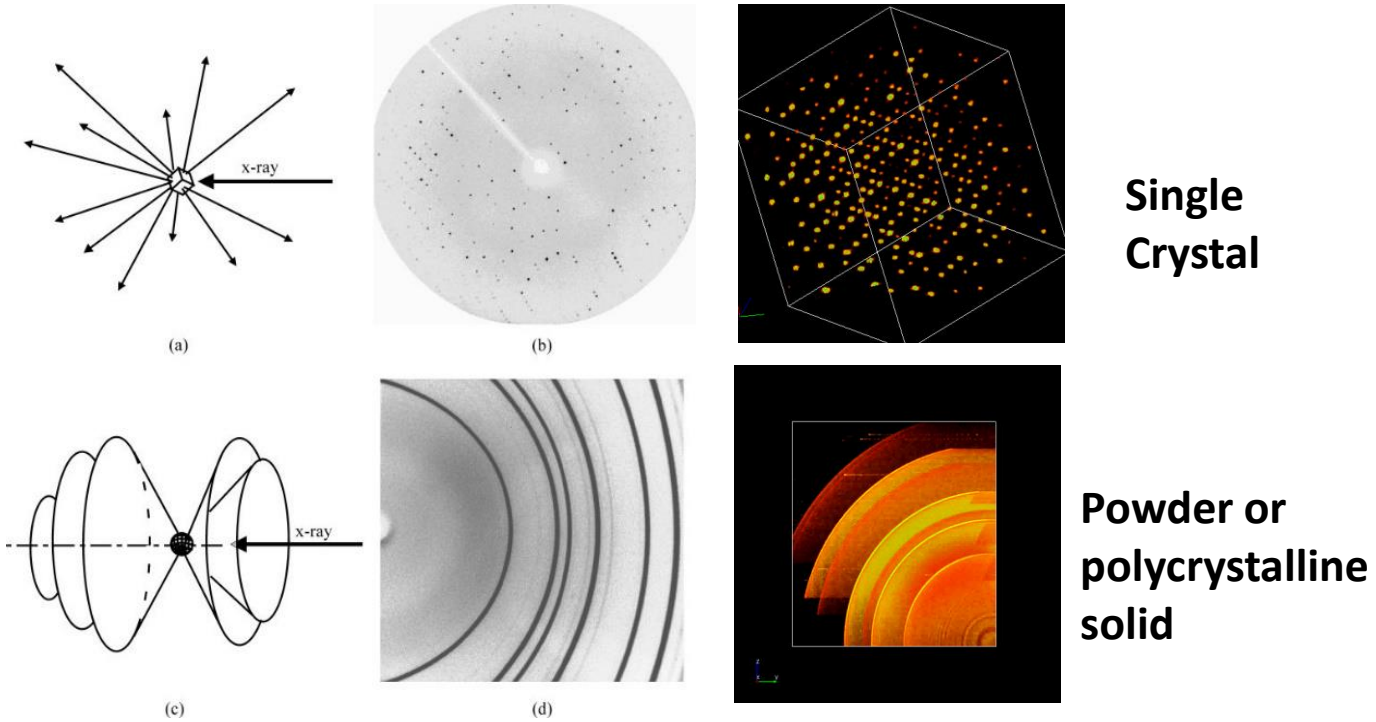




The 2D images can be mapped into reciprocal space – onto the surface of Ewald's Sphere

SCD - 2D image + scan –> 3D Int vs 2θ

XRD³ - 2D image + scan –> 3D Int vs 2θ



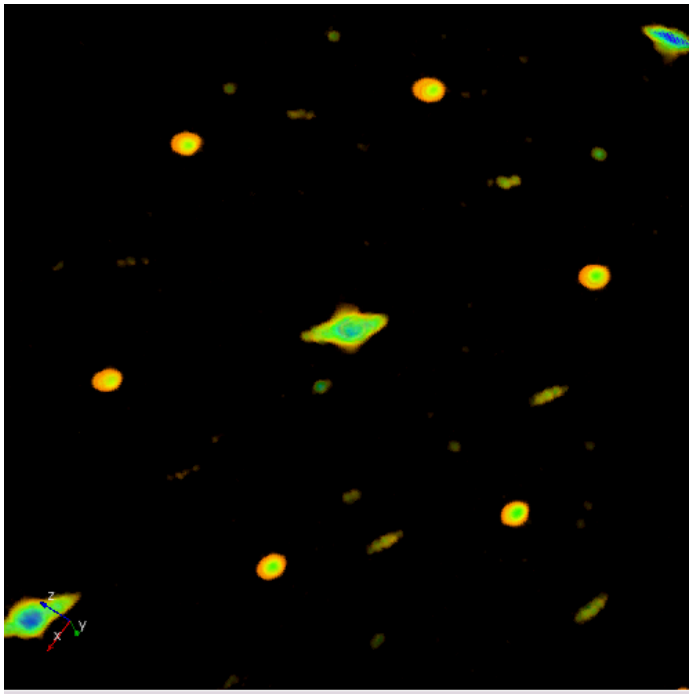
Single Crystal

Powder or polycrystalline solid

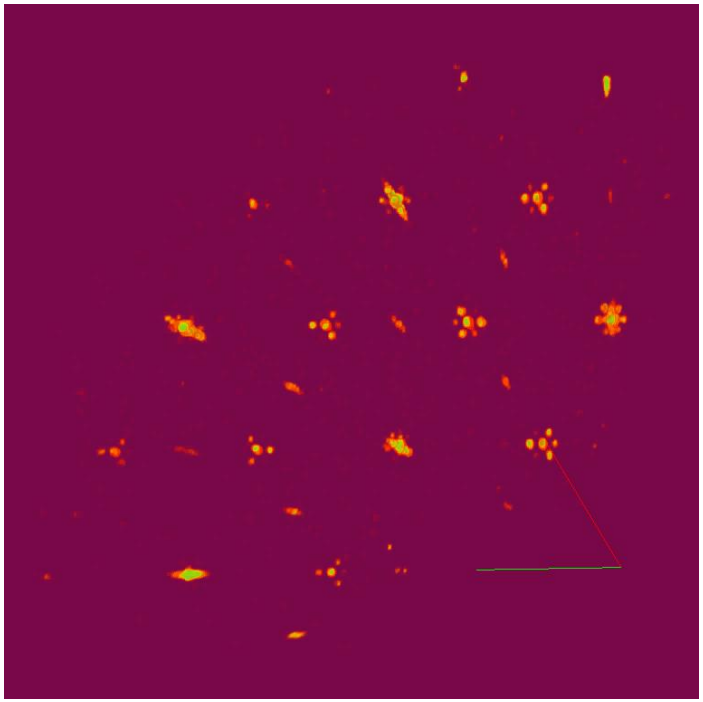
From Bob He's book: Two-Dimensional X-Ray Diffraction

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

Y.J. Kim, Toronto



80C

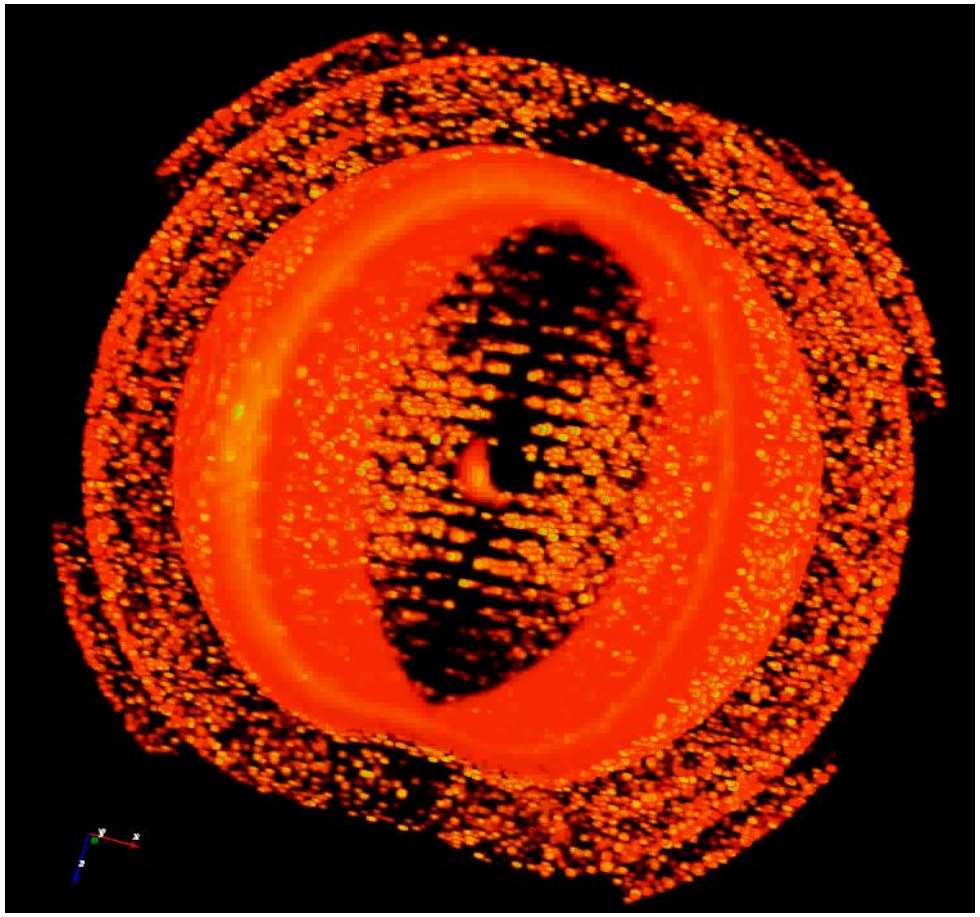


173C

Protein Single Crystal

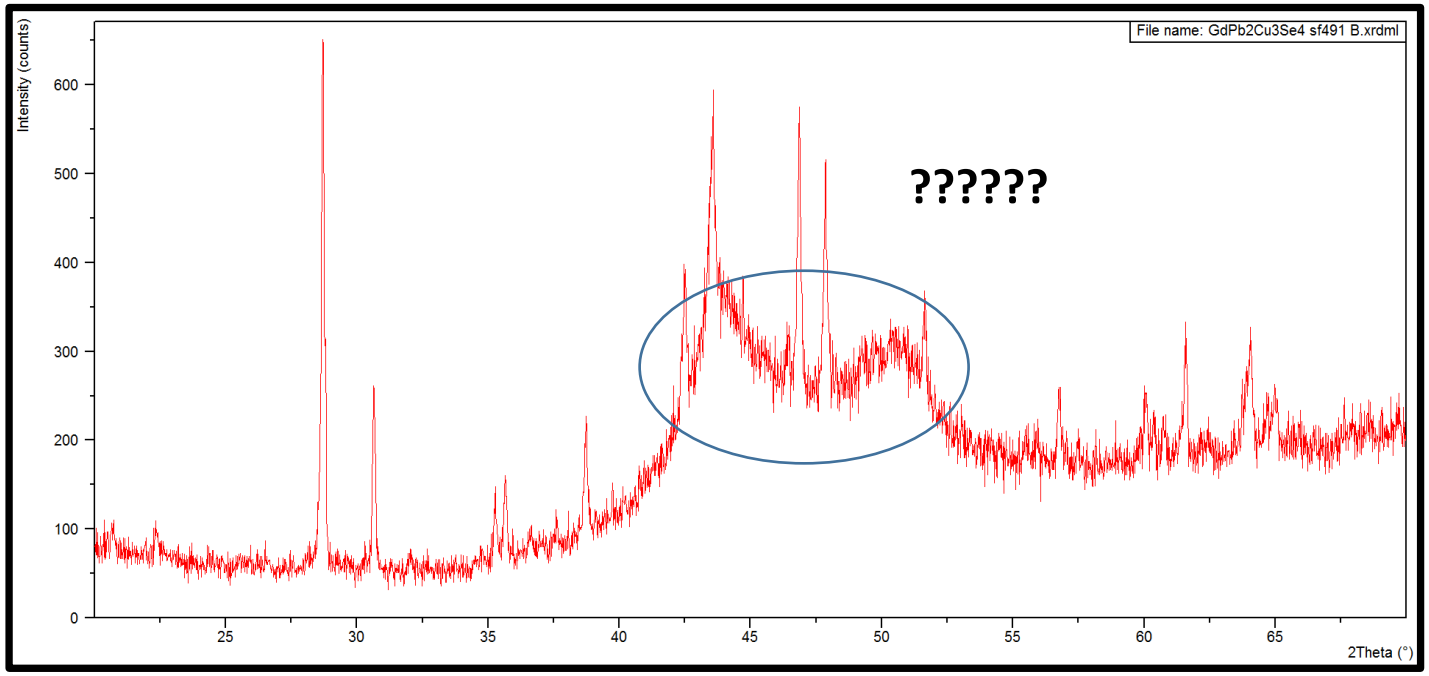
Alba Guarne
Tamiza Nanji

Rigaku
R-Axis4++
Image Plate



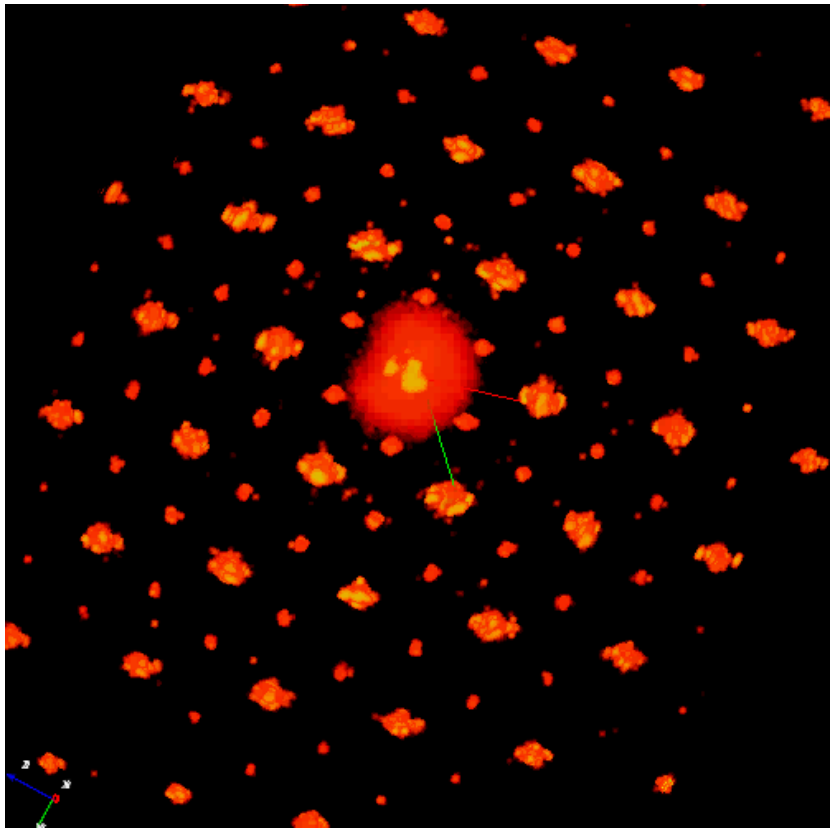
$GdPb_2Cu_3Se_4$ 1200°C for 4 hrs (Plates)

XRD pattern from Panalytical X'Pert Pro Diffractometer, Cu $K\alpha_1$



$GdPb_2Cu_3Se_4$

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



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

Visualization of area detector scans

Supercells

Incommensurate scattering

Diffuse scattering

Twinning

Texture of thin films

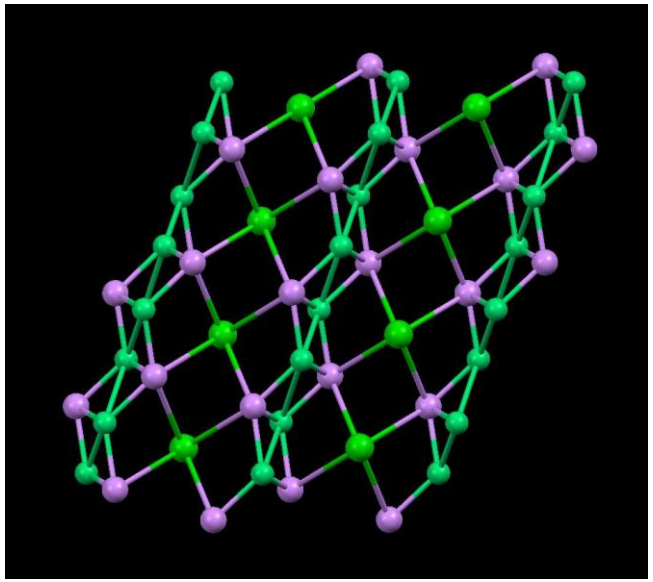
Teaching Crystallography

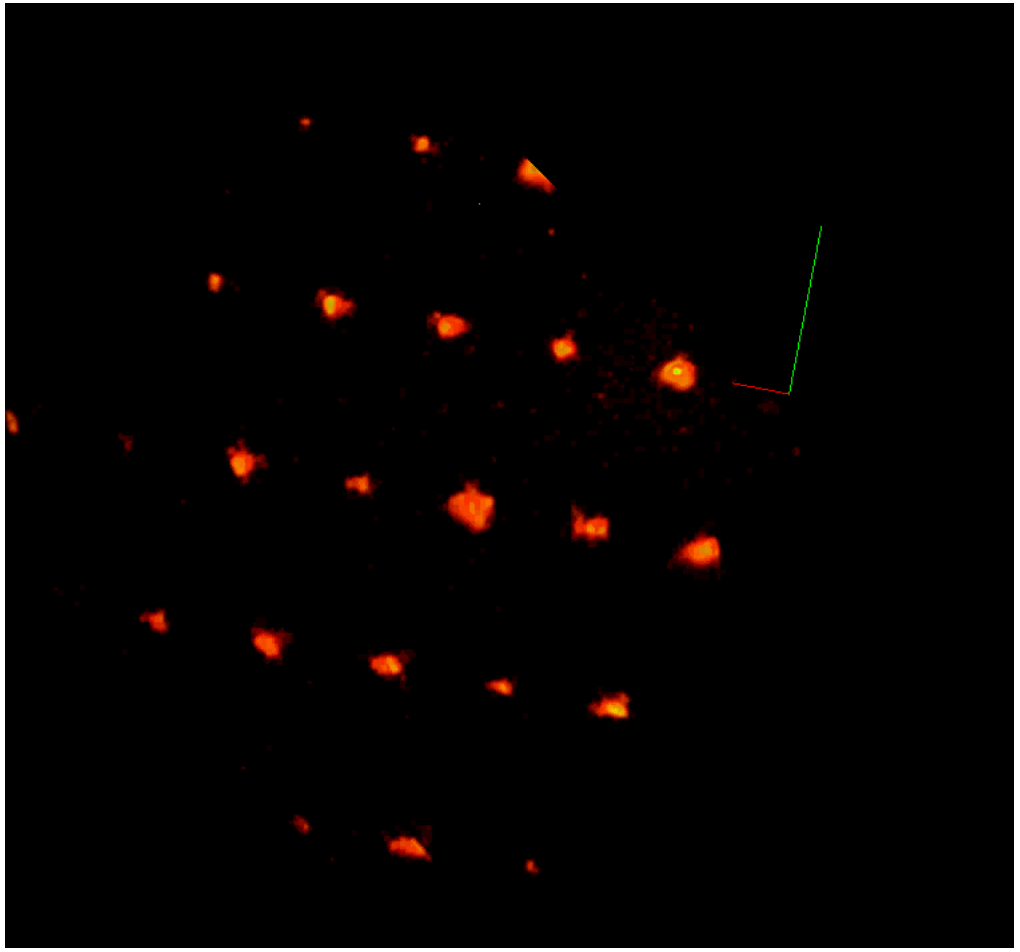
Other diffraction patterns worth saving

Supercell

Athena Safa-Sefat
Yurij Mozharivskij

Ba-As-Ni





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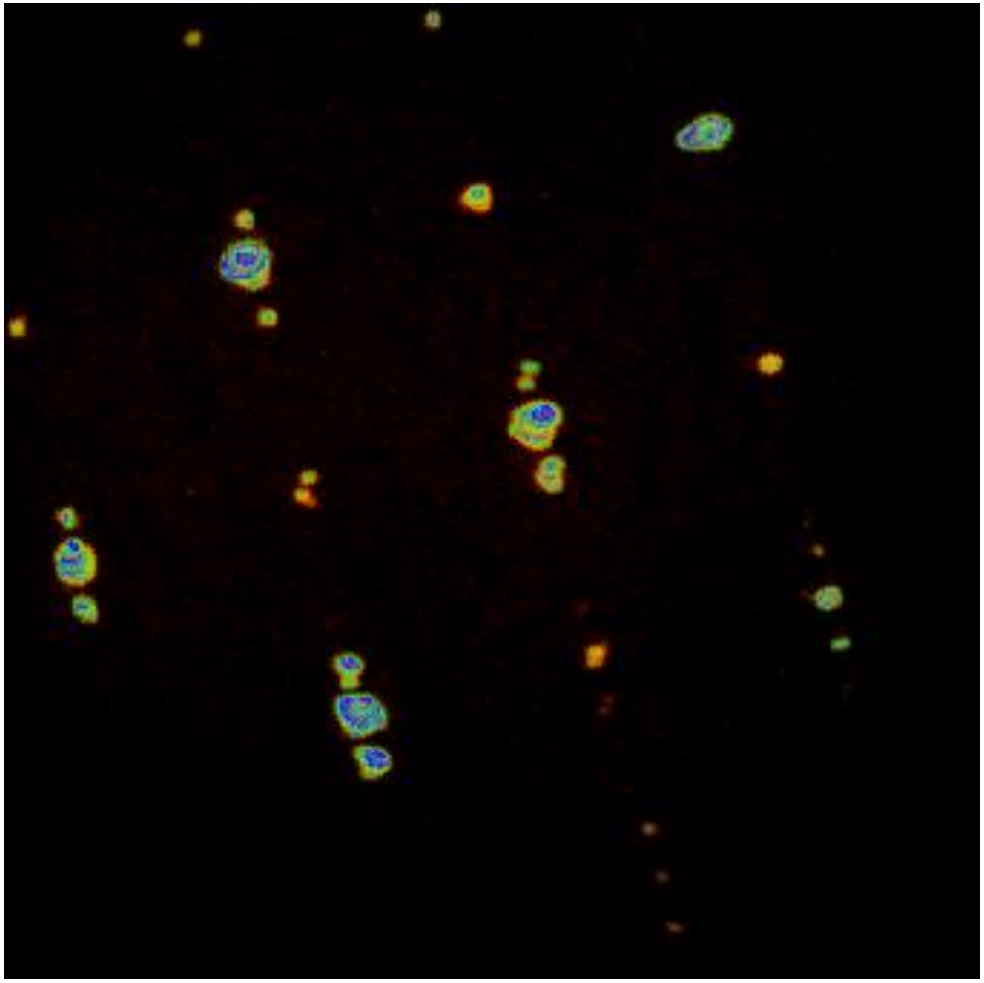
Aperiodic Incommensurate Crystal



Bruce Gaulin – Bi Cu Oxide Superconductor

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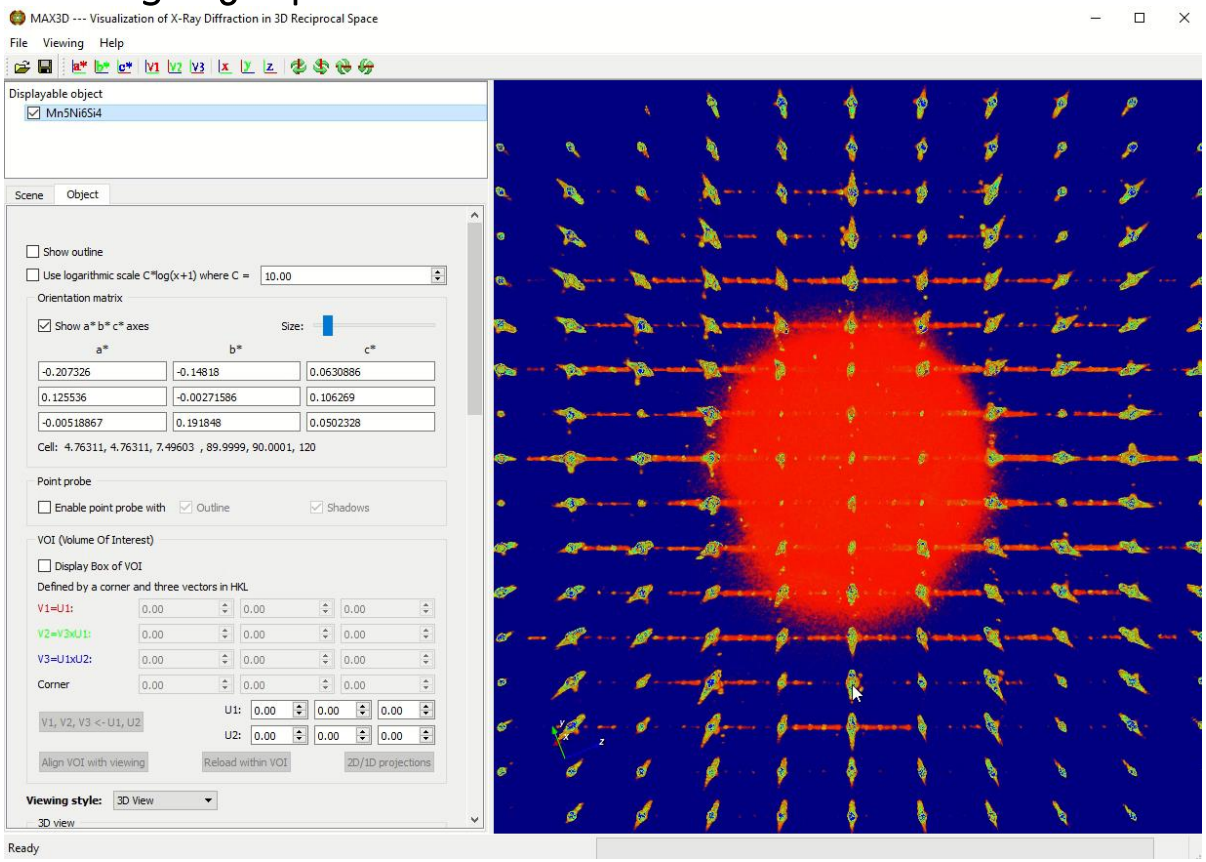
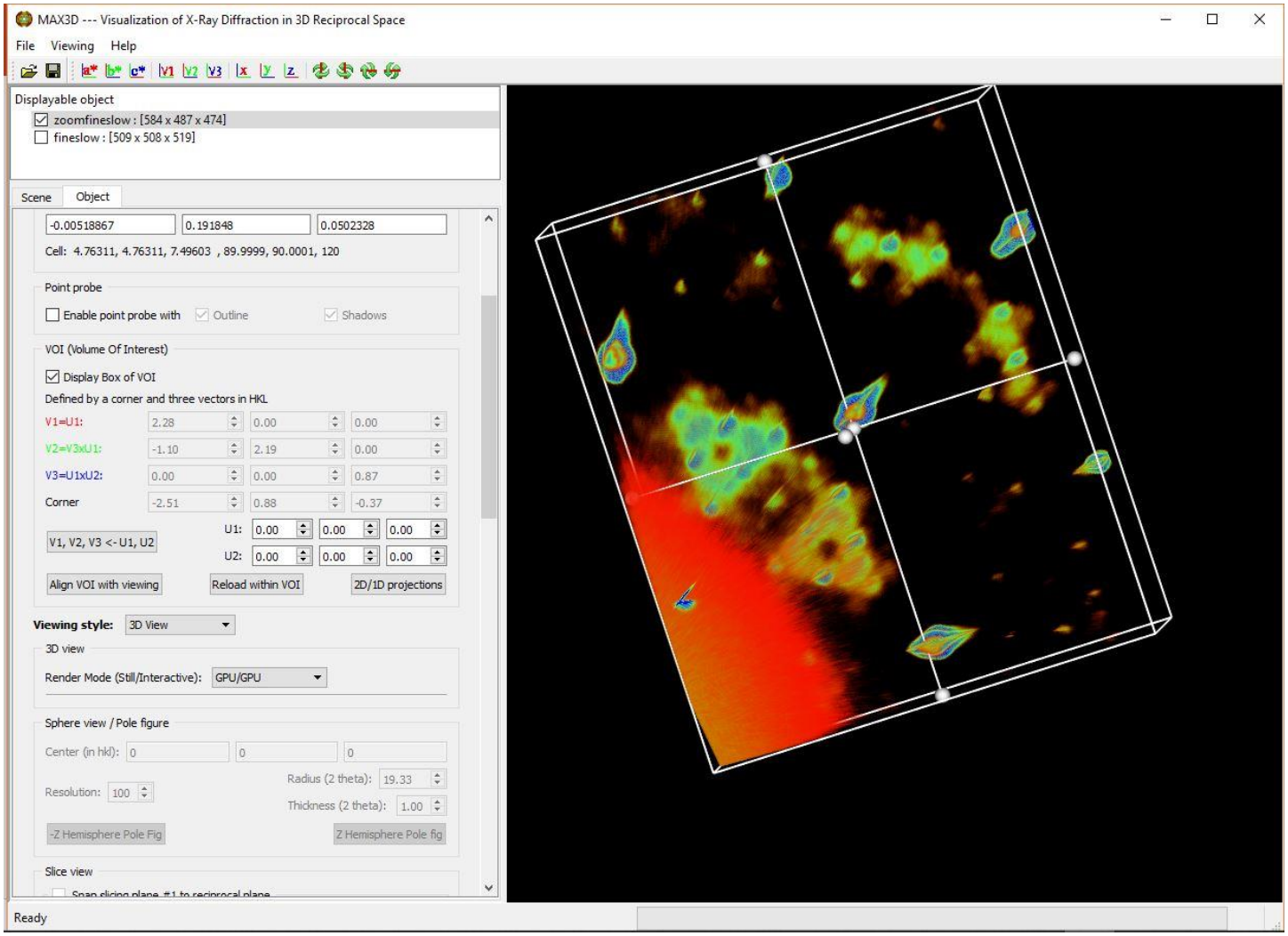
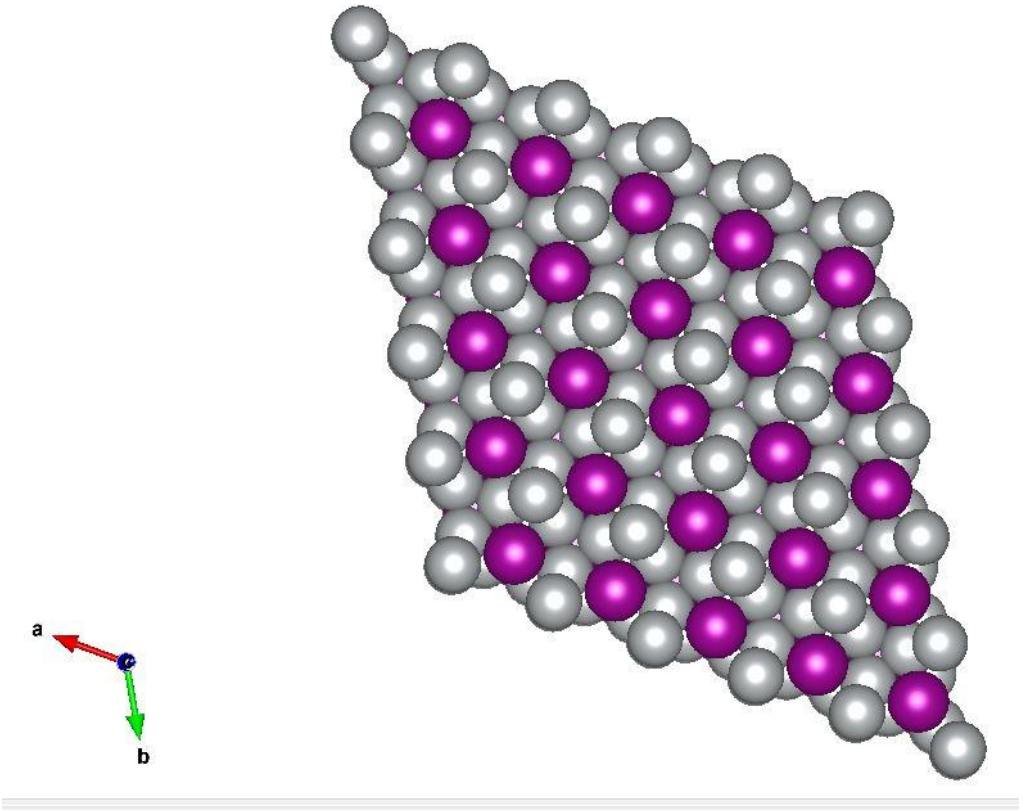
$Mn_5Ni_6Si_4$; Marek Niewczas, Sheikh Ahmed

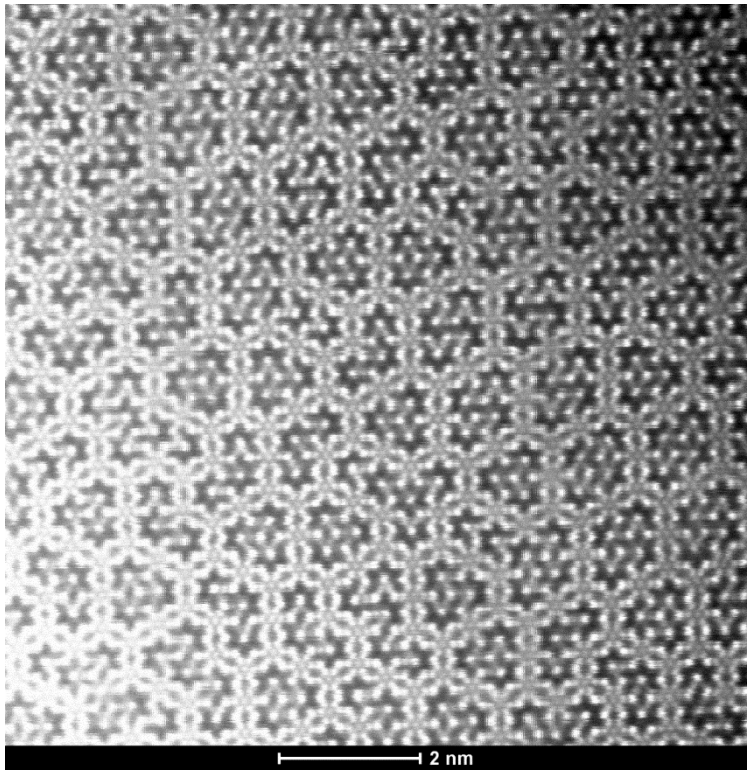


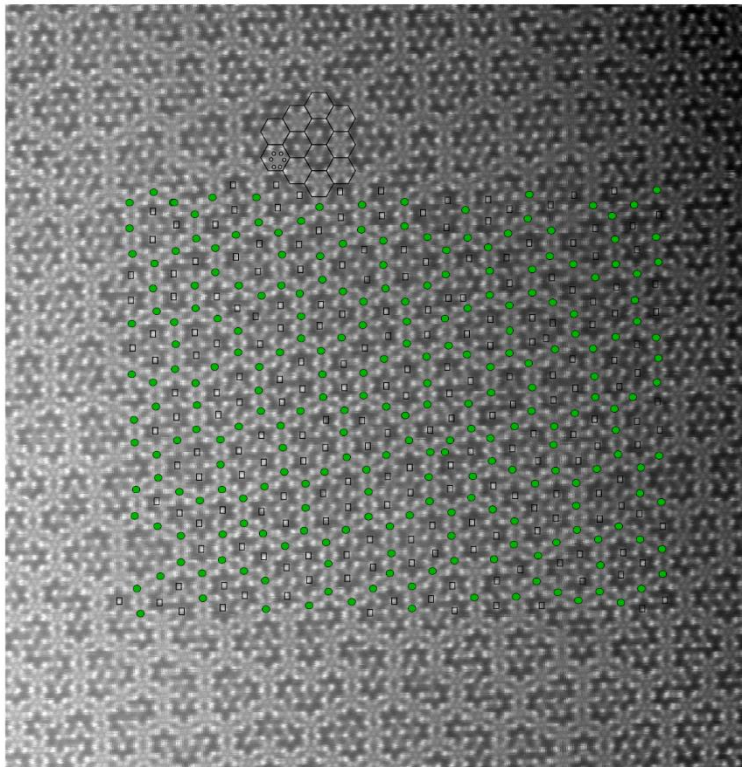

MAX3D --- Visualization of X-Ray Diffraction in 3D Reciprocal Space
File
Viewing
Help
Displayable object
zoomfineslow : [584 x 487 x 474]
fineslow : [509 x 508 x 519]
Scene
Object
-0.00518867
0.191848
0.0502328
Cell: 4.76311, 4.76311, 7.49603 , 89.9999, 90.0001, 120
Point probe
Enable point probe with
Outline
Shadows
VOI (Volume Of Interest)
Display Box of VOI
Defined by a corner and three vectors in HKL
V1=U1:
V2=V3xU1:
V3=U1xU2:
Corner
U1:
U2:
V1, V2, V3 <- U1, U2
Align VOI with viewing
Reload within VOI
2D/1D projections
Viewing style:
3D View
3D view
Render Mode (Still/Interactive):
GPU/GPU
Sphere view / Pole figure
Center (in hkl):
Resolution:
Radius (2 theta):
Thickness (2 theta):
-Z Hemisphere Pole Fig
Z Hemisphere Pole fig
Slice view
Ready

$Mn_5Ni_6Si_4$; Marek Niewczas, Sheikh Ahmed

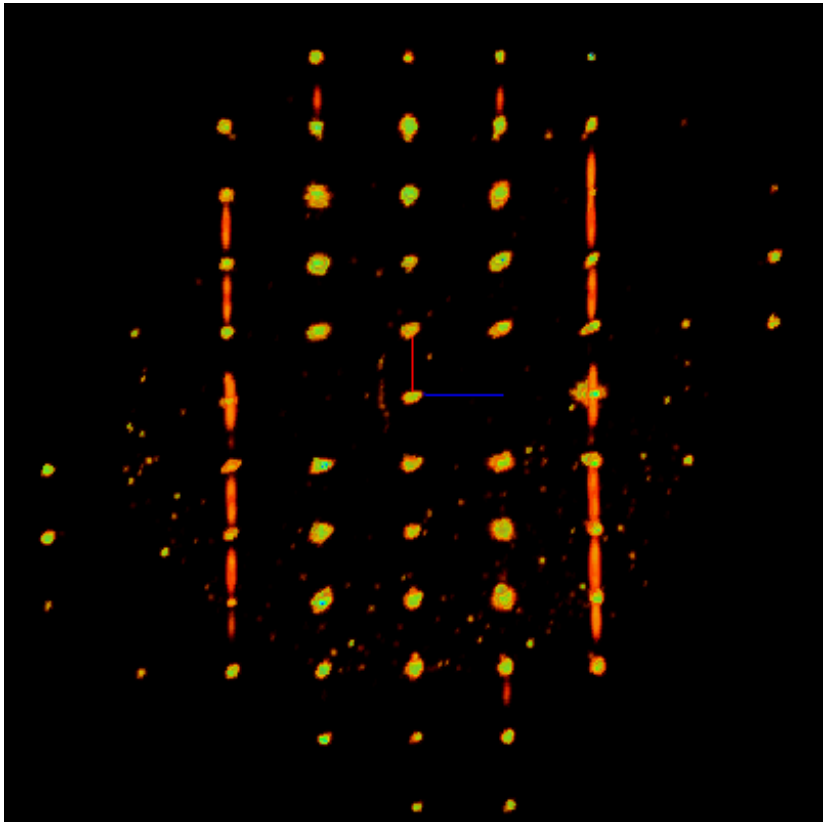


HRTEM





Diffuse Scattering

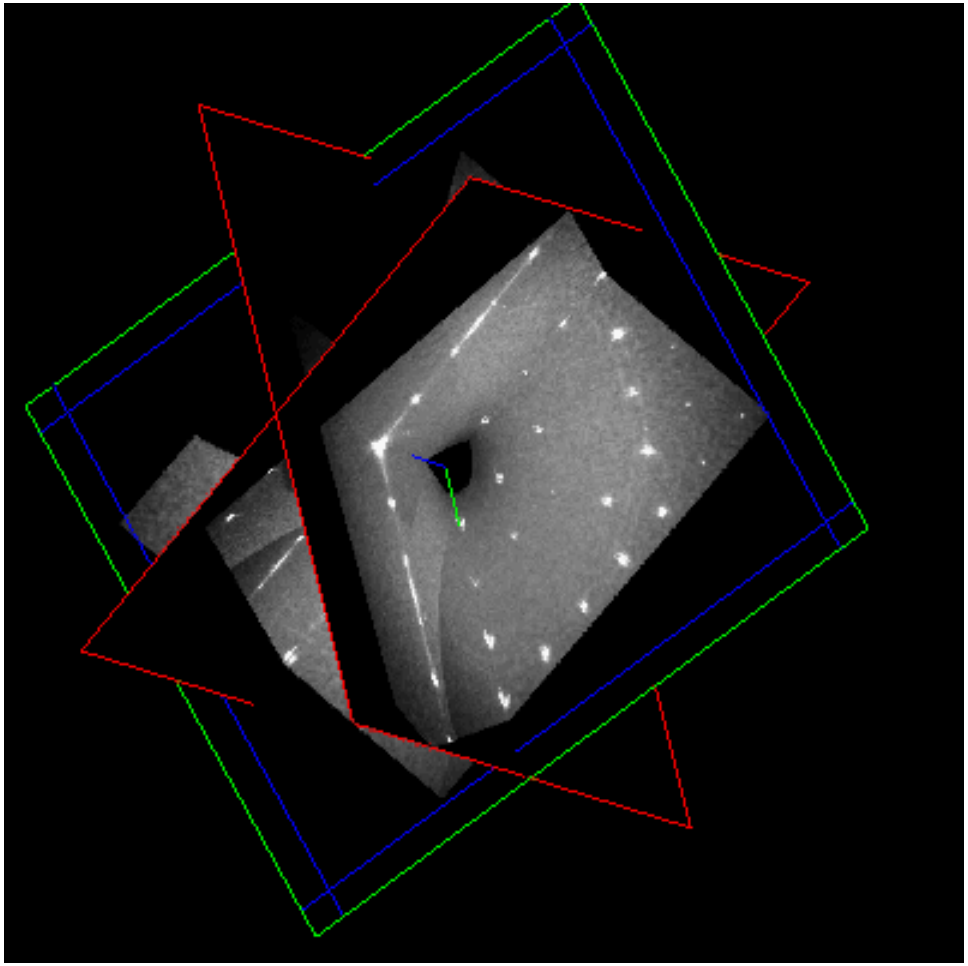


Columns of hexanapthylbenzene are ordered along the stacking axis. The columns have a partial rotational disorder relative to one another.
The refined structure shows a multiple orientations for the napthyls. The configuration of the molecule in the ordered stack cannot be determined.

Hexanapthylbenzene. Laura Harrington, Mike McGlinchey

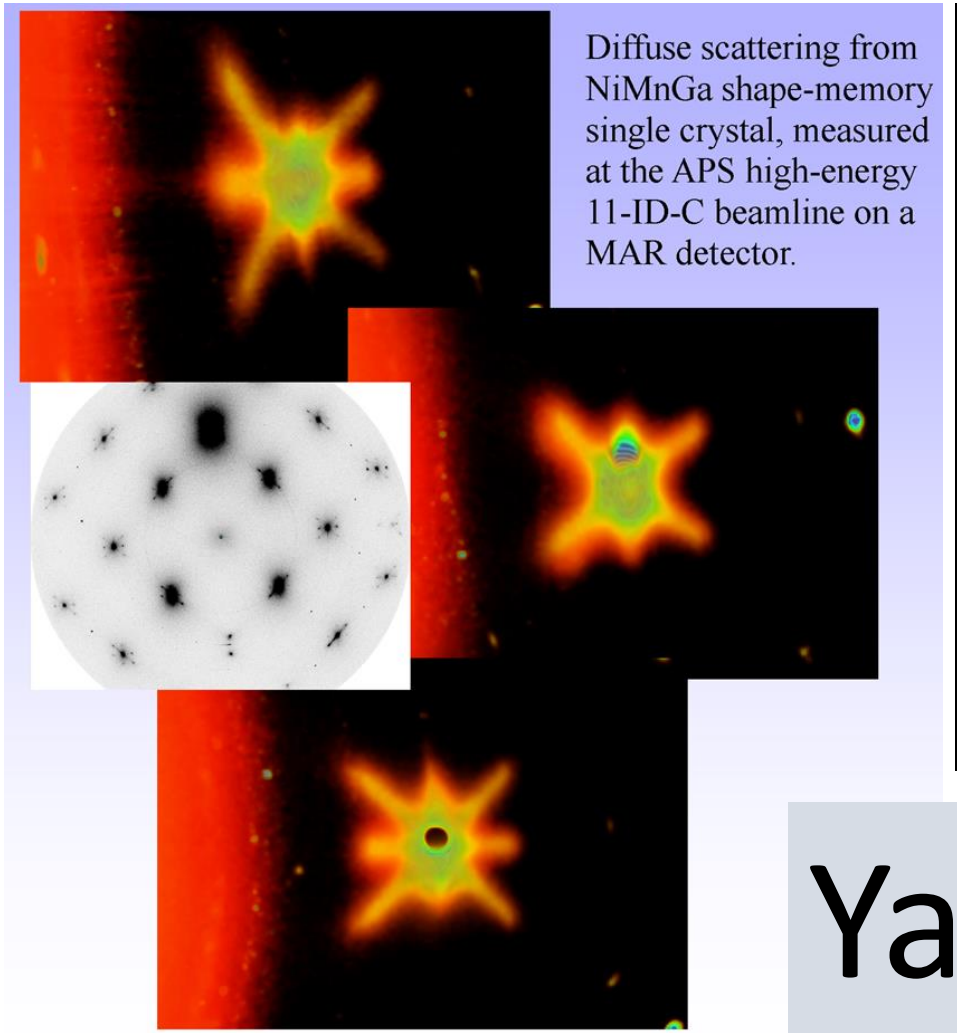
19

Diffuse Scattering

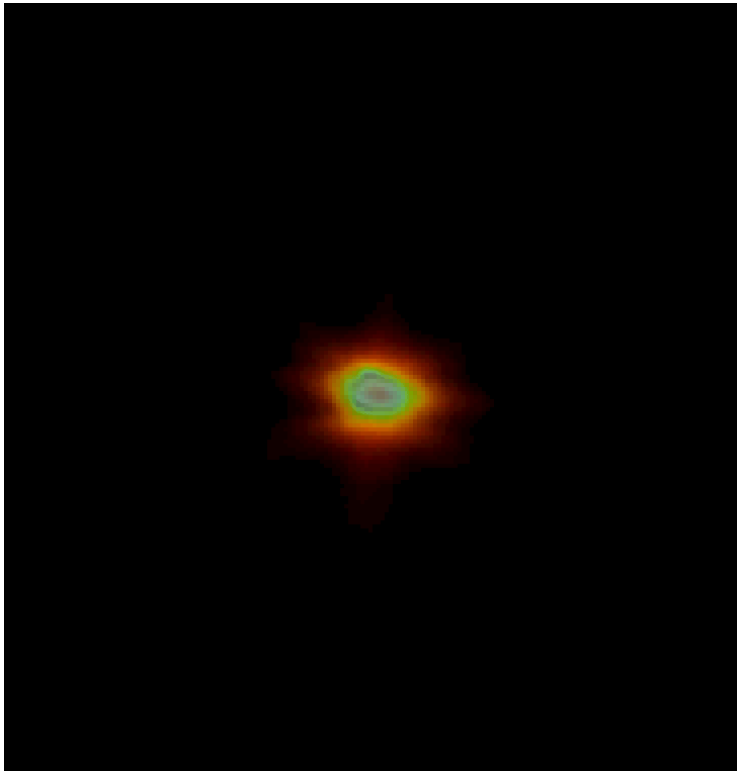


Hexanapthylbenzene. Laura Harrington, Mike McGlinchey

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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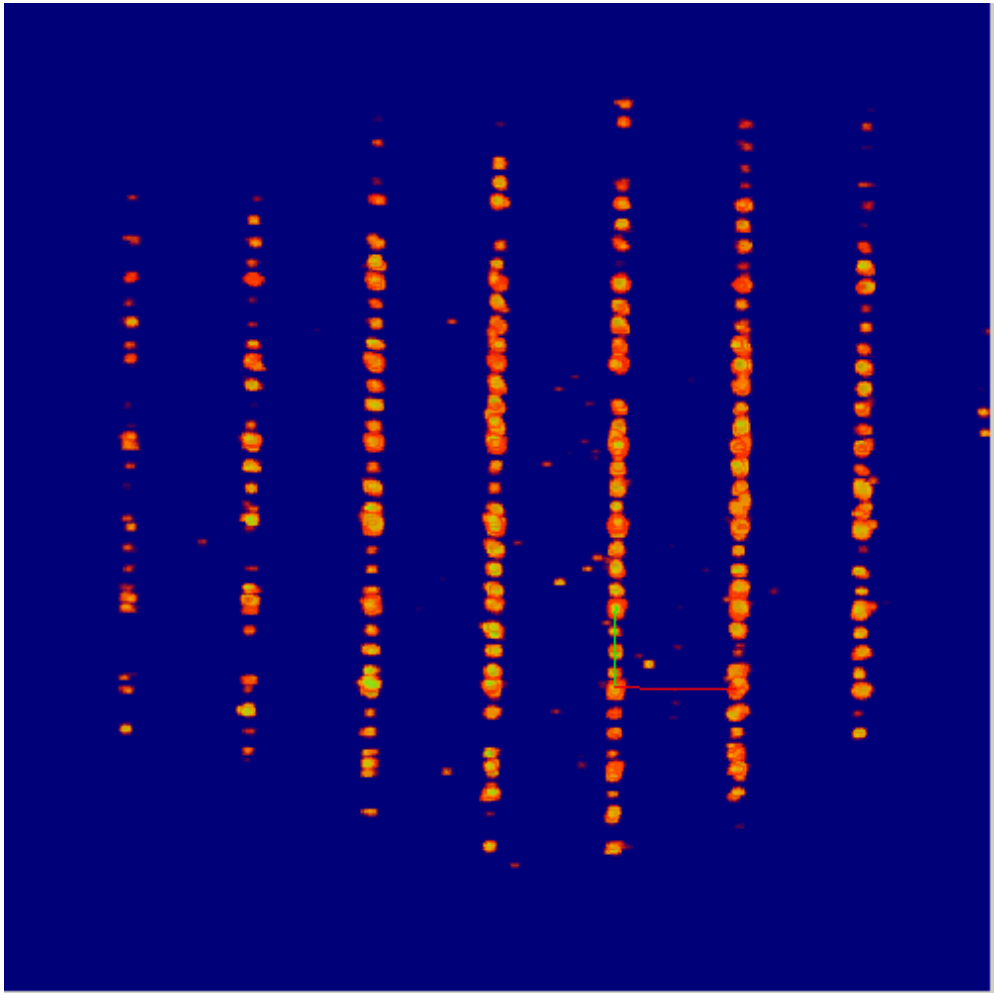
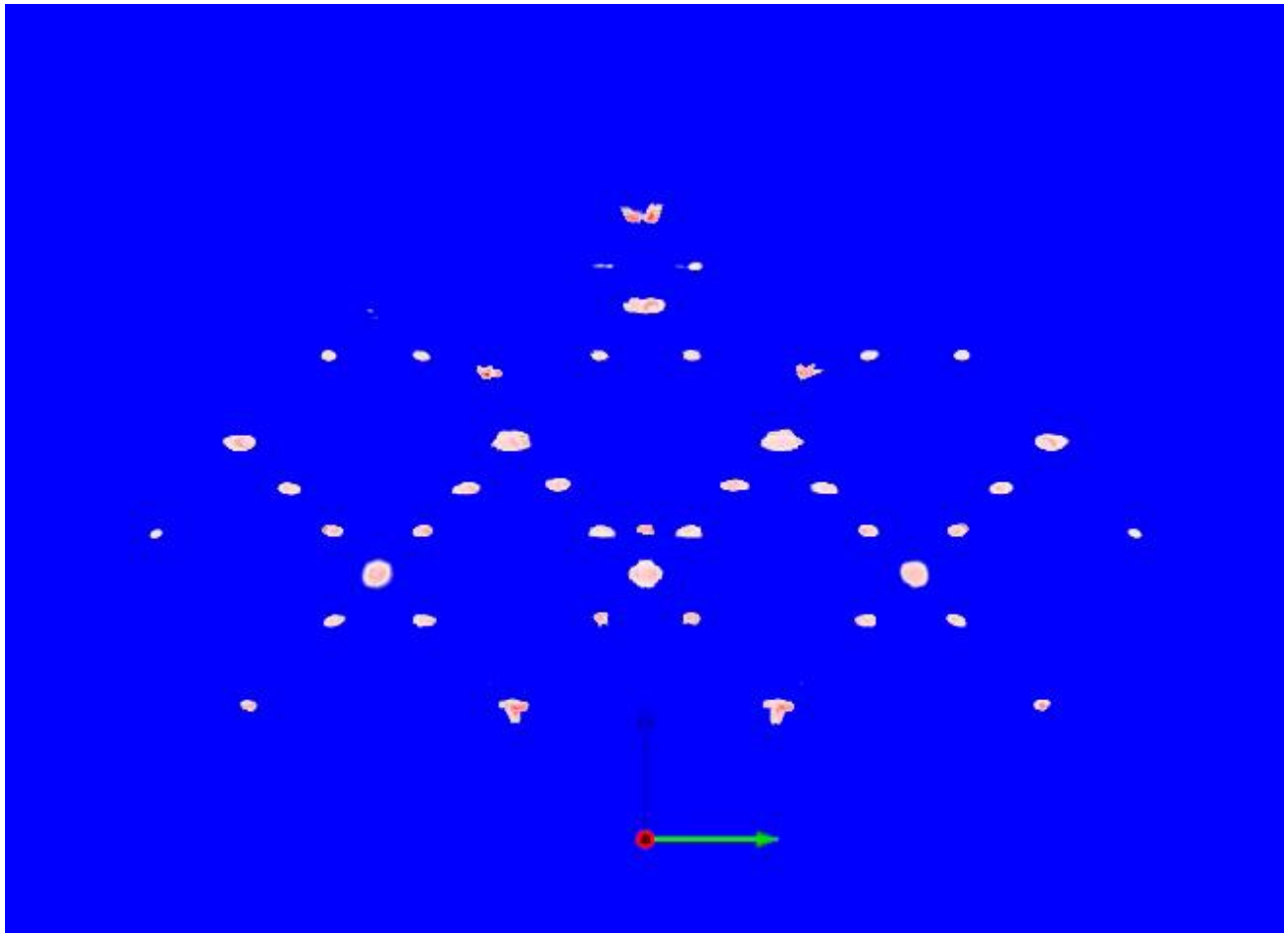
Small Molecule Twinned Crystal

Bruker Smart Apex2 CCD

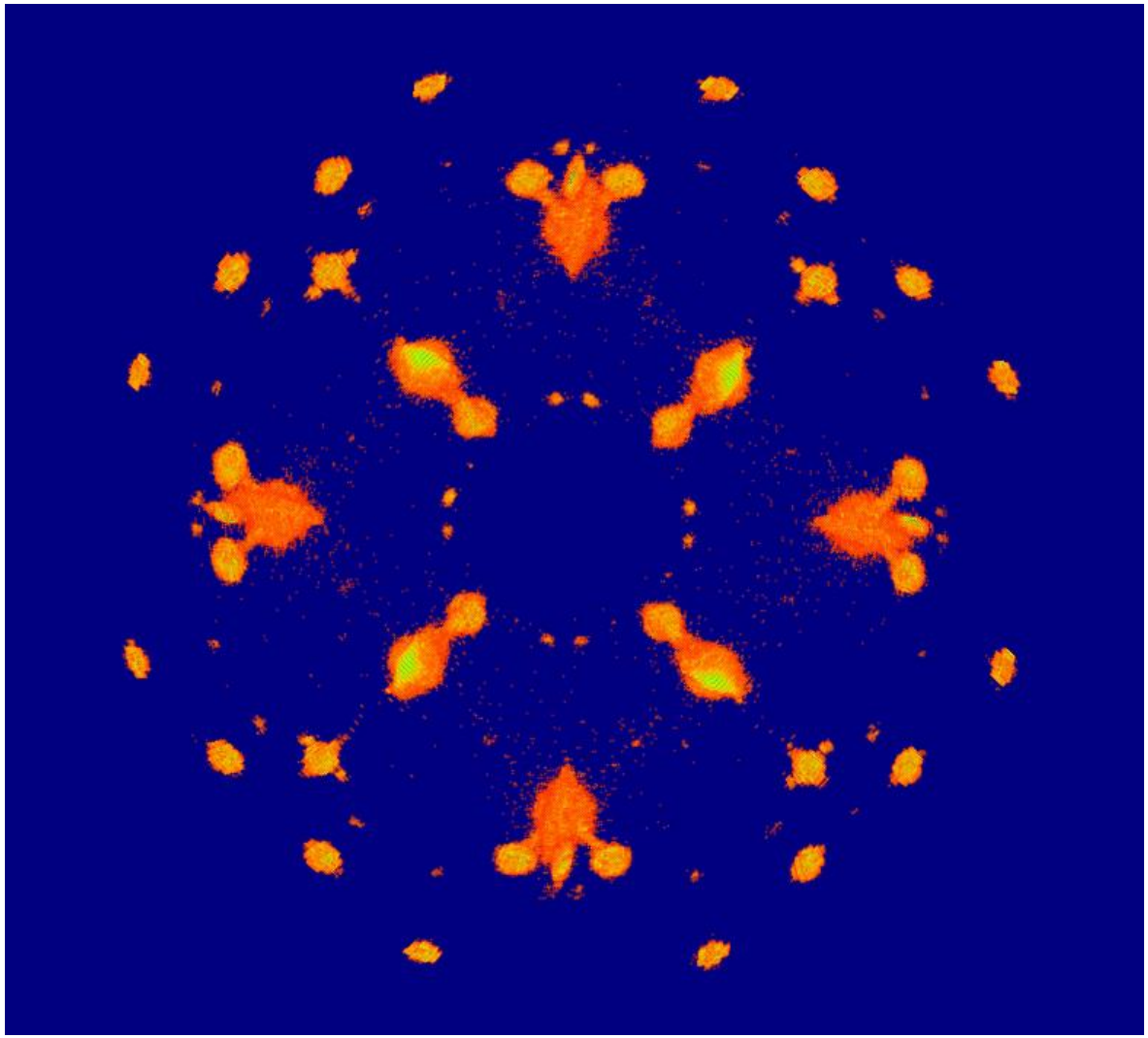


3D diffraction pattern from thin film of $InAs_{(1-x)}Sb_x$ nanowires (isolate (111) reflections)



(220) and
(311) shells

Diffuse lines
connect twins



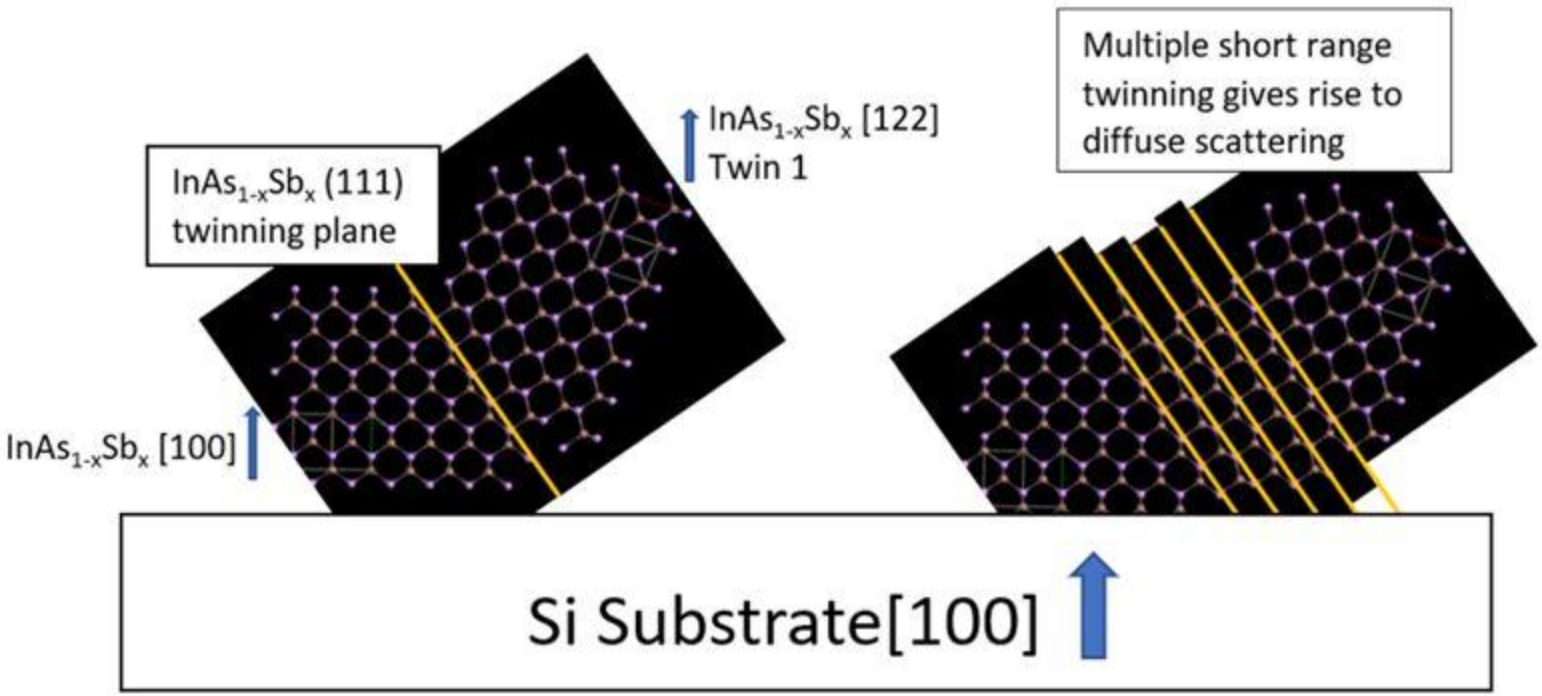


Figure 3. Twinning by 180° (or ±60°) rotation about the [111] face of $InAs_{1-x}Sb_x$. Regions of multiple layer twinning account for the diffuse scattering observed in the 3D diffraction pattern. Twin planes are indicated by yellow lines.

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

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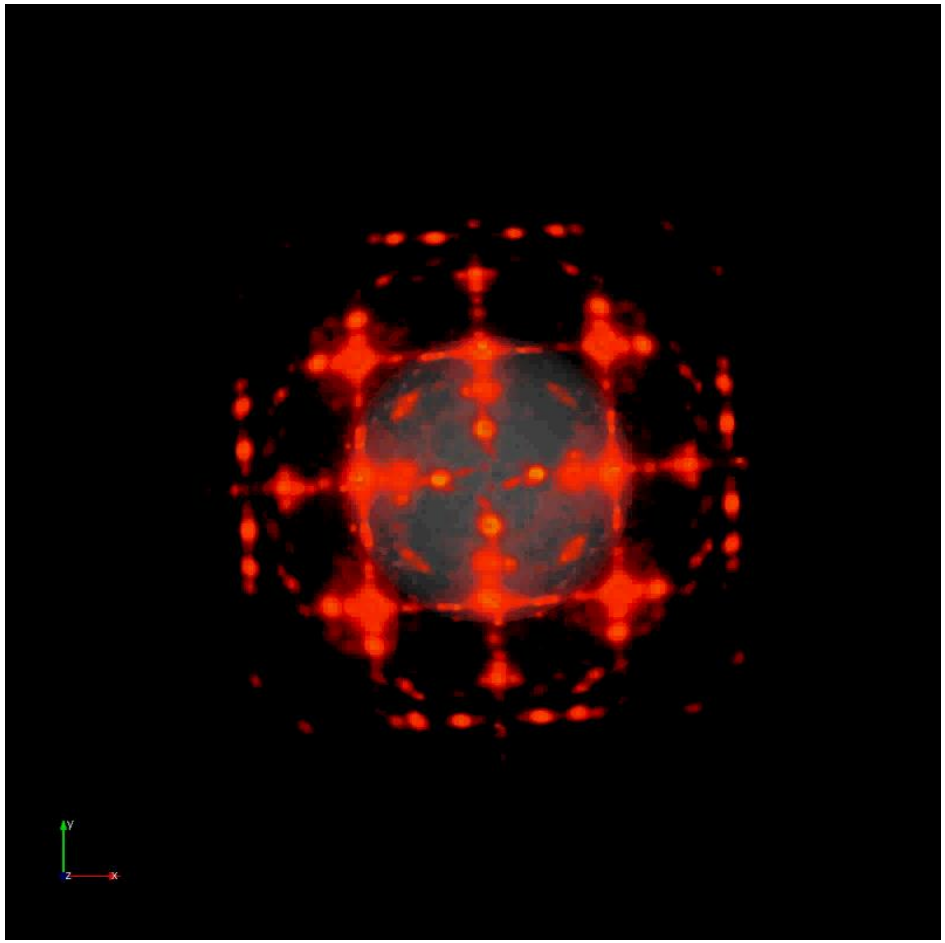
Multiple (8) Orientations of GaAs NW's on Si Substrate

Ray LaPierre,
Vicky Jarvis,
McMaster



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Everything you have seen here and more . . .

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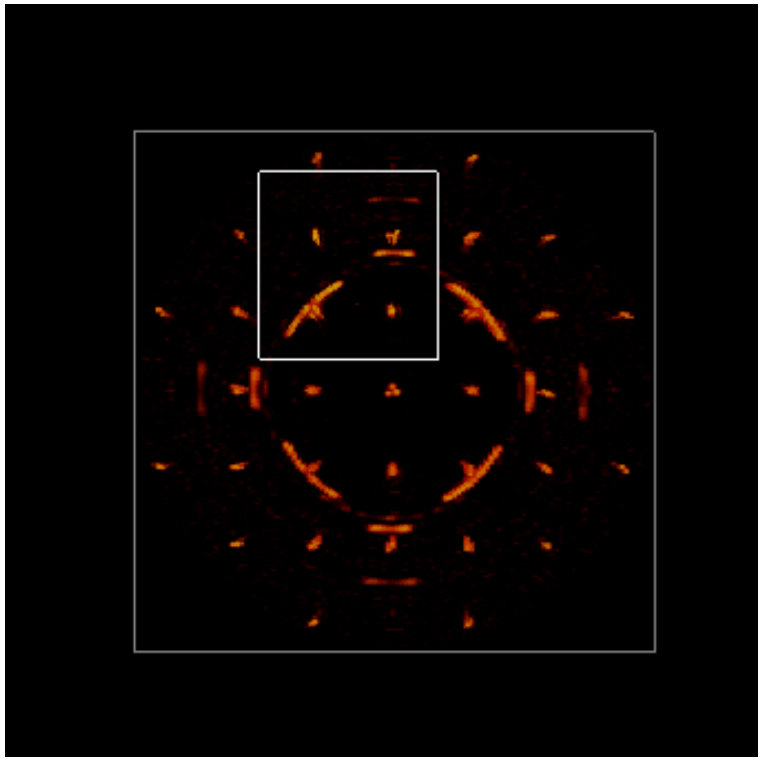
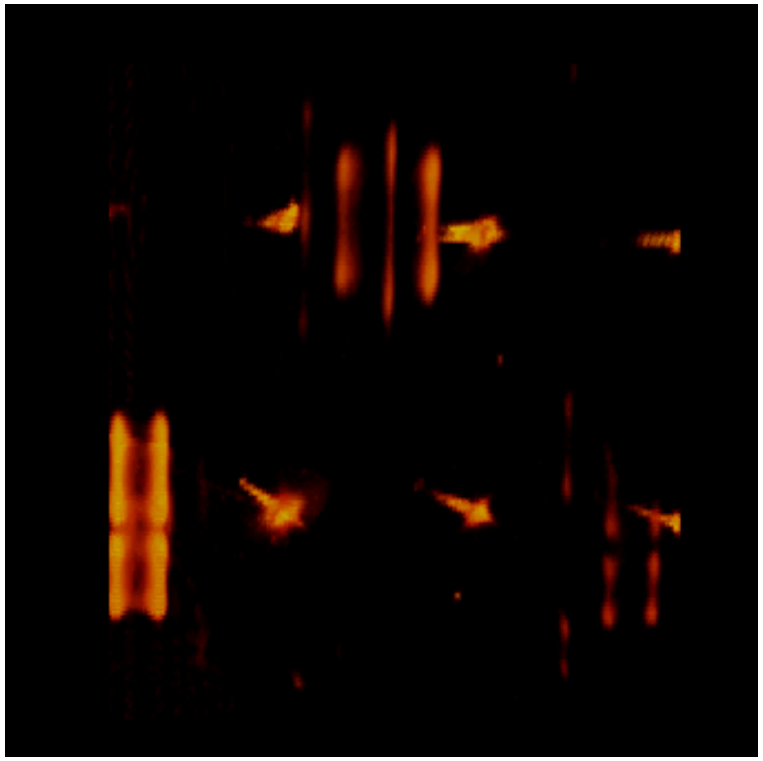
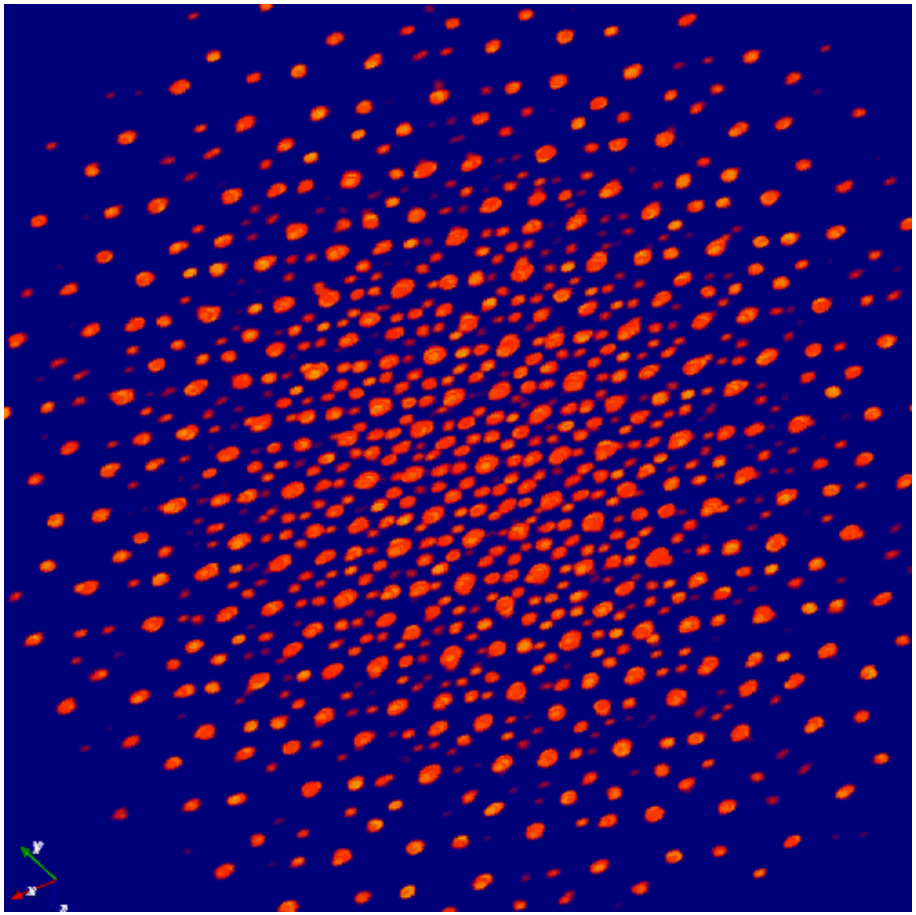
Follow Phase Changes





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



$Al_{70}Pd_{21}Mn_9$ - Geetha Balakrishnan, University of Warwick
Nathan Armstrong, Tom Timusk, McMaster

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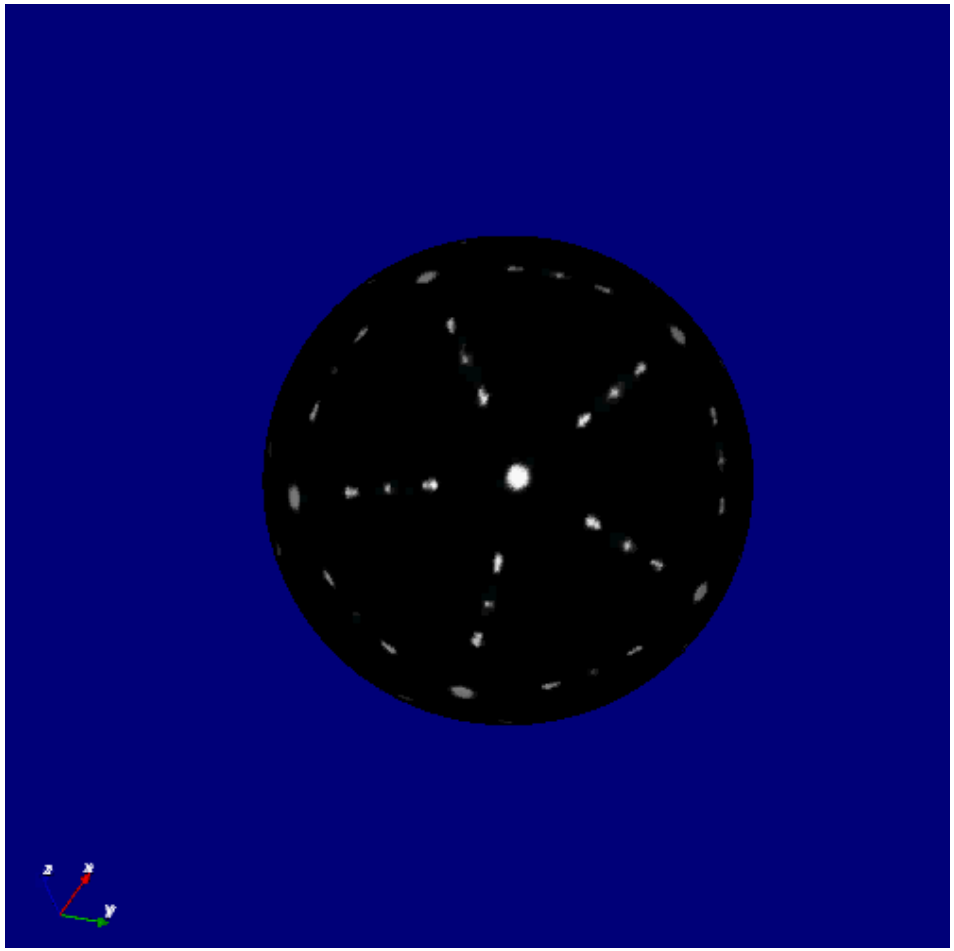
Nathan Armstrong, Tom Timusk, McMaster



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

Thank you for your attention.