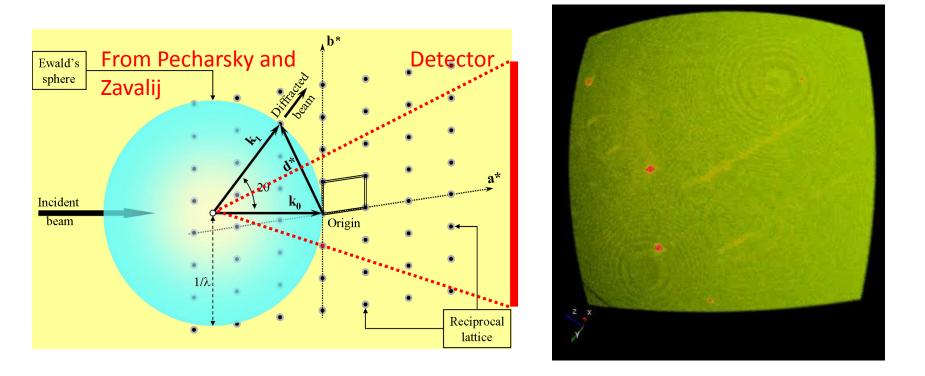
Use of raw data for diffraction space visualization: What are we missing in an integrated HKL file?

Jim Britten McMaster University Canada

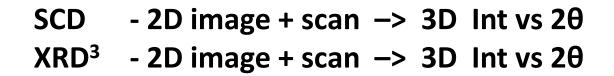
Outline

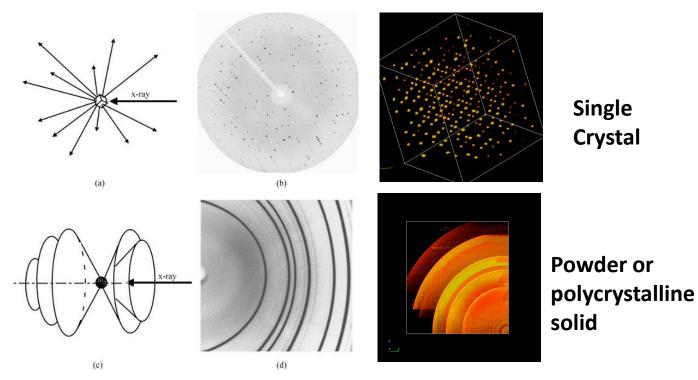
Visualization of area detector scans Supercells Incommensurate scattering Diffuse scattering Twinning Texture of thin films Teaching Crystallography

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



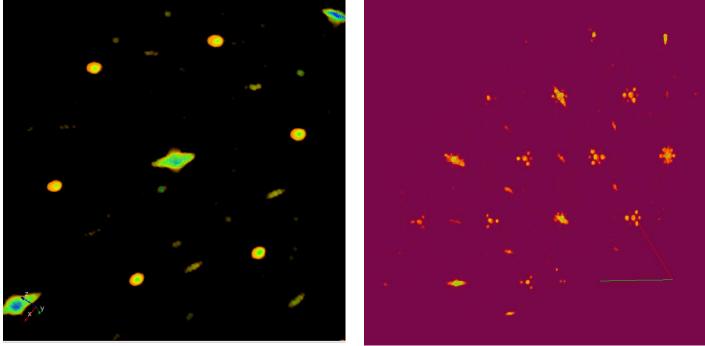
The 2D images can be mapped into reciprocal space – onto the surface of Ewald's Sphere





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



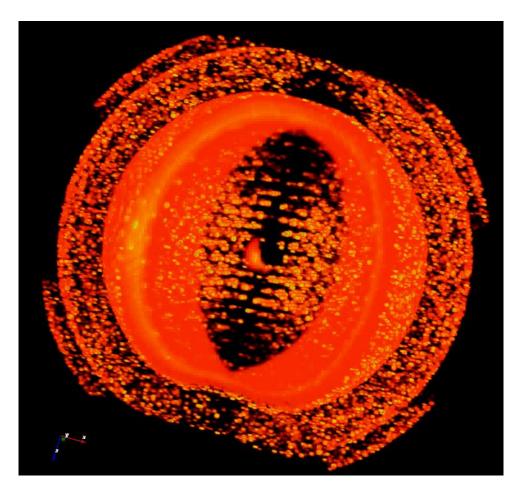


173C

Protein Single Crystal

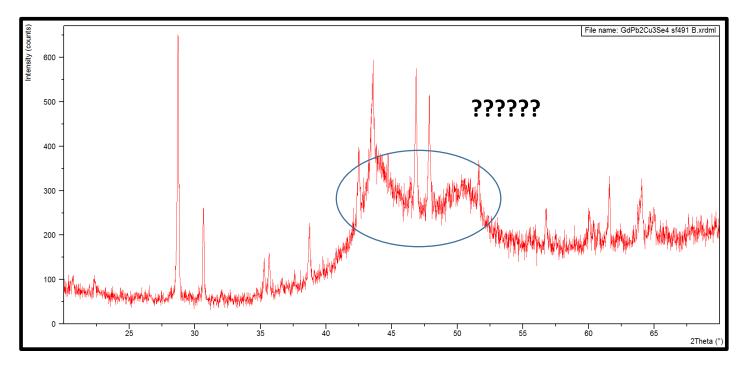
Alba Guarne Tamiza Nanji

Rigaku R-Axis4++ Image Plate



GdPb₂Cu₃Se₄ 1200°C for 4 hrs (Plates)

XRD pattern from Panalytical X'Pert Pro Diffractometer, Cu K α_1

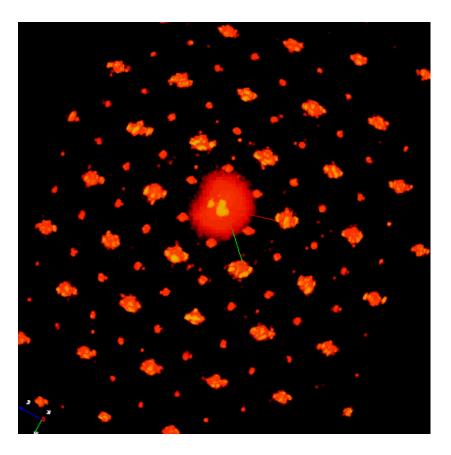


GdPb₂Cu₃Se₄

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



Canadian Centre canadien Light de rayonnement Source synchrotron

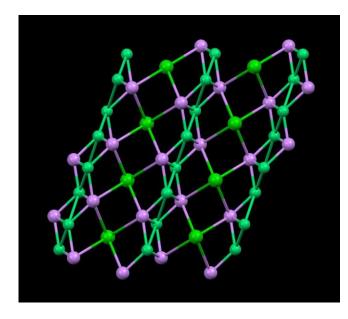


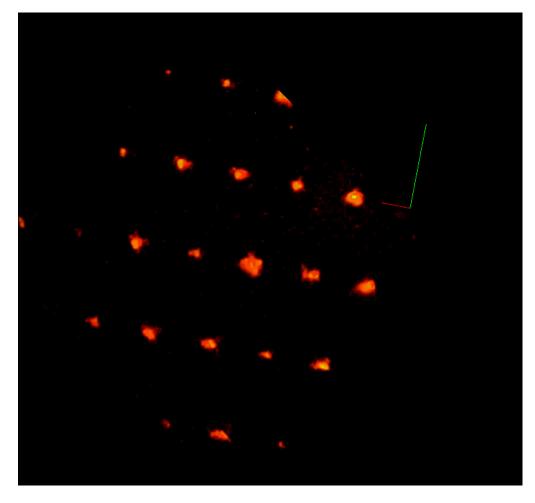
Canadian Macromolecular Crystallography Facility, 08B1-1 (CMCF-BM) Beamline

Supercell

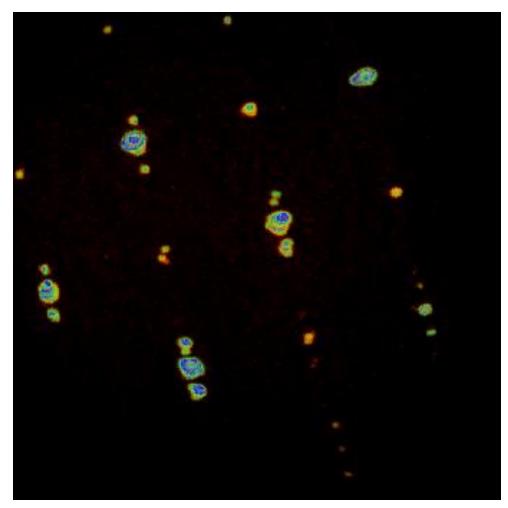
Athena Safa-Sefat Yurij Mozharivskij

Ba-As-Ni





Aperiodic Incommensurate Crystal



Bruce Gaulin – Bi Cu Oxide Superconductor When should small molecule crystallographers

$Mn_5Ni_6Si_4$; Marek Niewczas, Sheikh Ahmed

DAX3D --- Visualization of X-Ray Diffraction in 3D Reciprocal Space

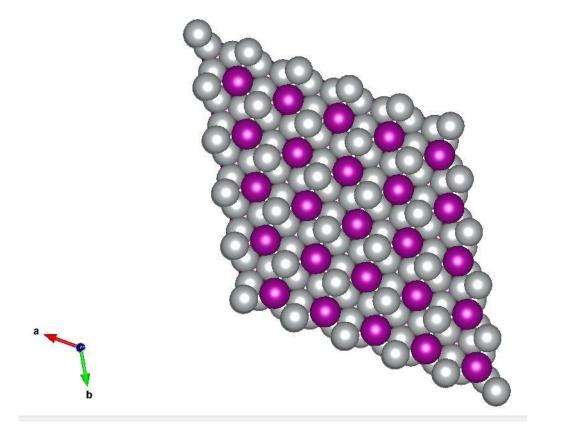
File Viewing Help

– 🗆 🗙

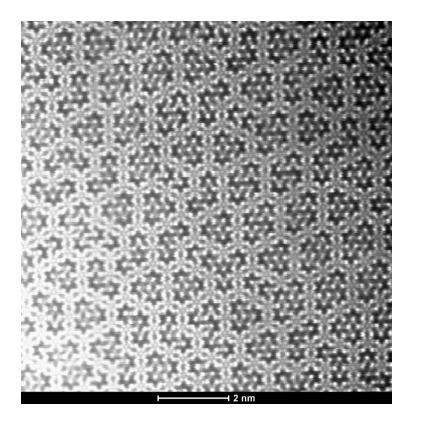
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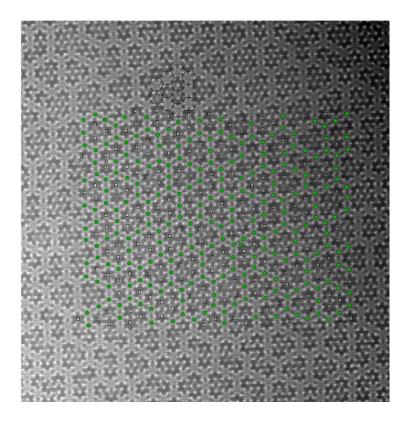
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Mn₅Ni₆Si₄ ; Marek Niewczas, Sheikh Ahmed

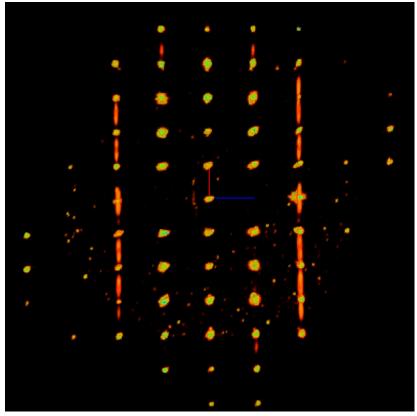


HRTEM





Diffuse Scattering

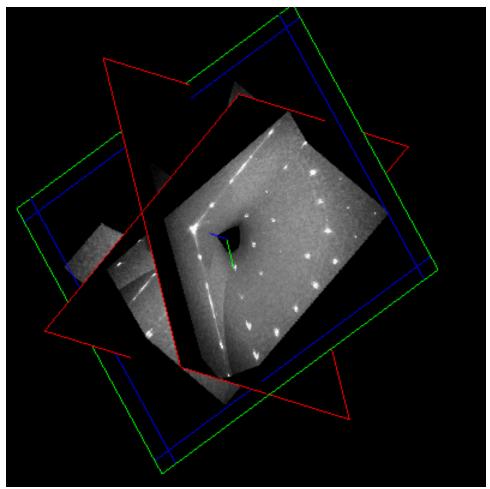


Columns of hexanapthylbenzene are ordered along the stacking axis. The columns have a partial rotational disorder relative to one another. The refined structure shows a multiple orientations for the napthyls. The configuration of the molecule in the ordered stack cannot be determined.

Hexanapthylbenzene. Laura Harrington, Mike McGlinchey

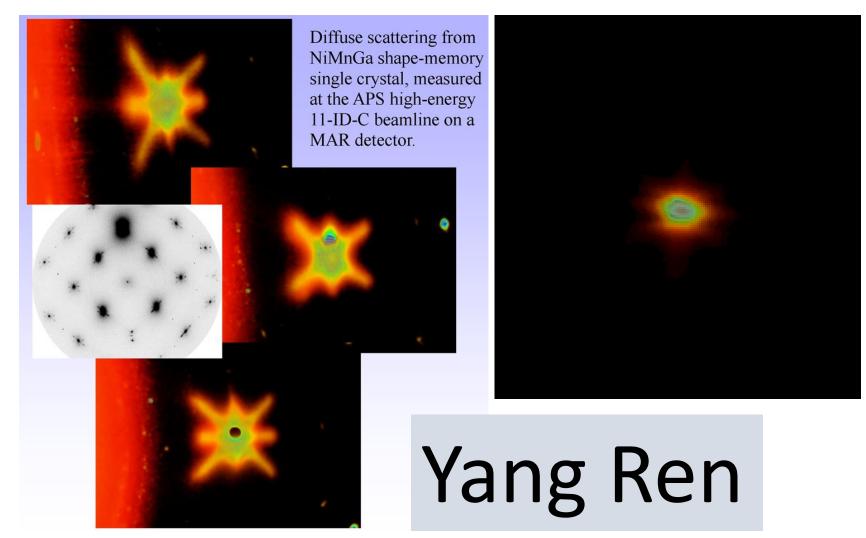
19

Diffuse Scattering

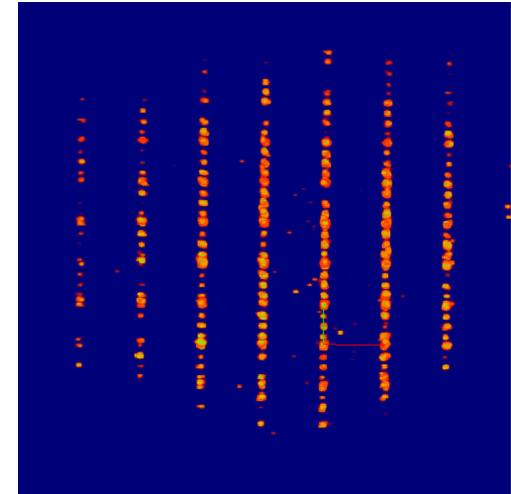


Hexanapthylbenzene. Laura Harrington, Mike McGlinchey

Diffuse Scattering

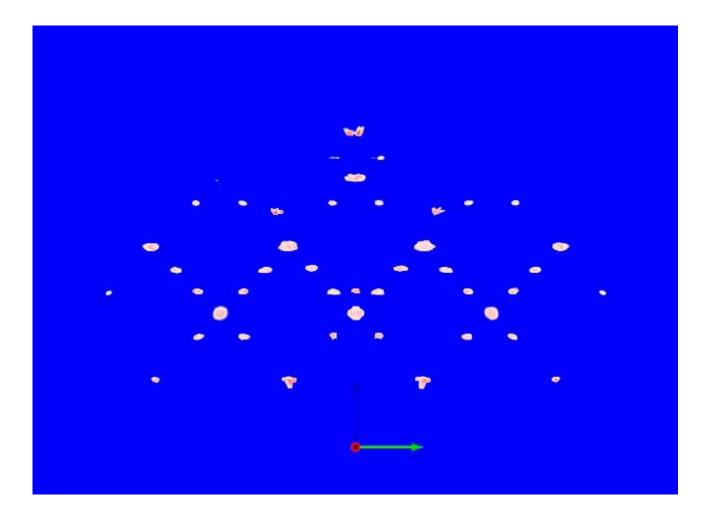


Small Molecule Twinned Crystal



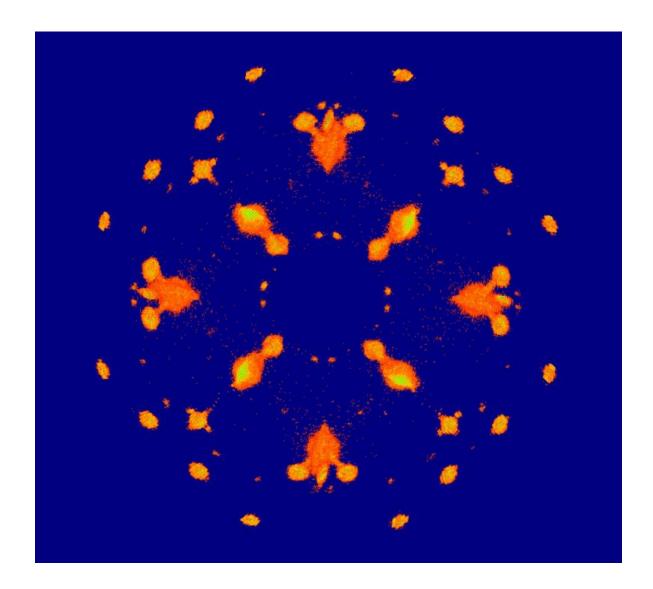
Bruker Smart Apex2 CCD

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



(220) and (311) shells

Diffuse lines connect twins



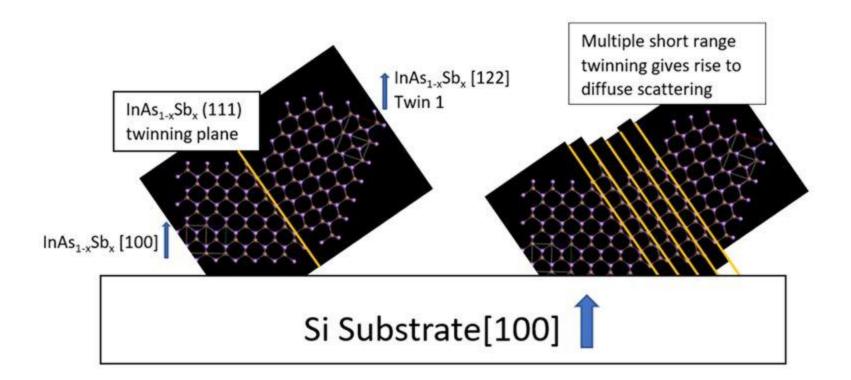
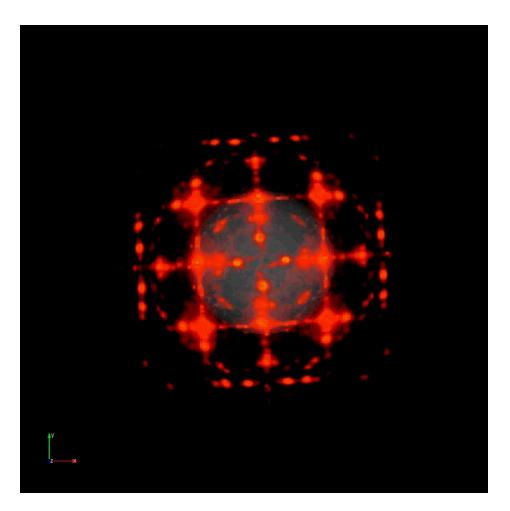


Figure 3. Twinning by 180° (or $\pm 60^{\circ}$) rotation about the [111] face of $InAs_{1-x}Sb_x$. Regions of multiple layer twinning account for the diffuse scattering observed in the 3D diffraction pattern. Twin planes are indicated by yellow lines.

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

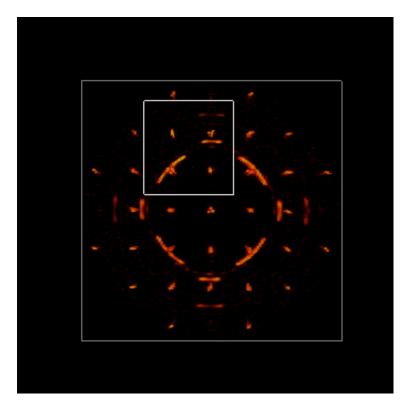
Multiple (8) Orientations of GaAs NW's on Si Substrate

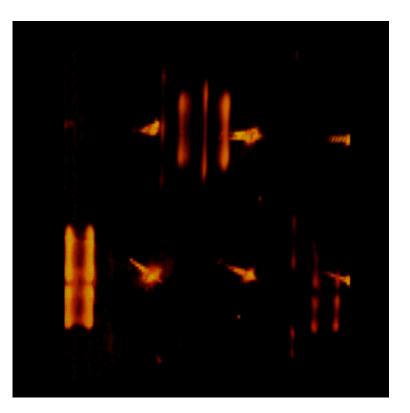
Ray LaPierre, Vicky Jarvis, McMaster



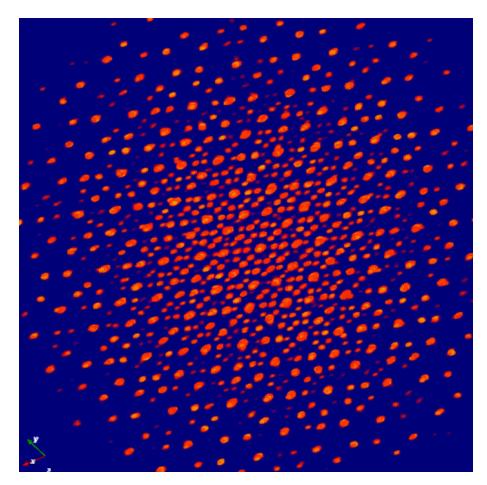
Everything you have seen here and more . . .

Follow Phase Changes



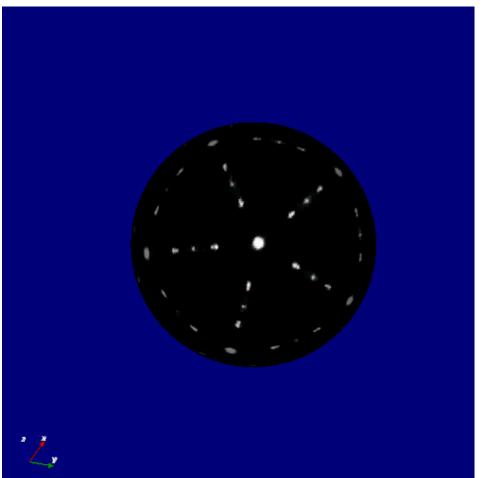


What do we do with beautiful single crystal data from a quasicrystal?



Al₇₀Pd₂₁Mn₉ - Geetha Balakrishnan, University of Warwick Nathan Armstrong, Tom Timusk, McMaster

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



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

Thank you for your attention.