Diffuse scattering as seen with PILATUS detector

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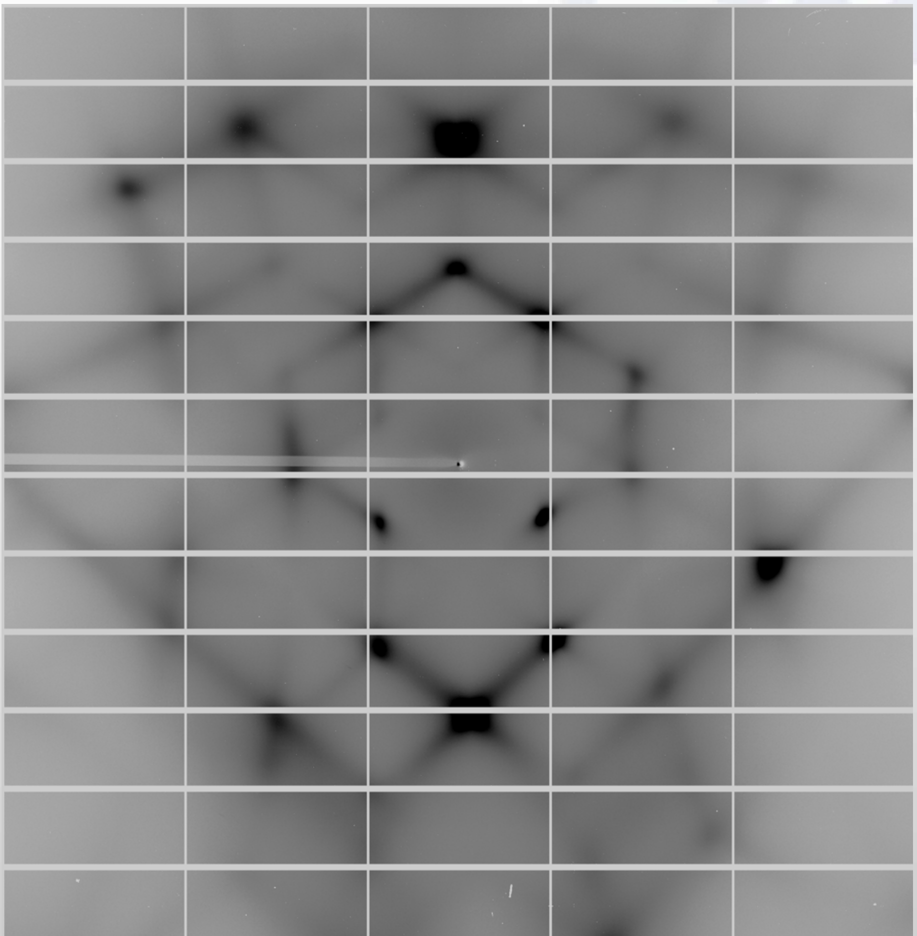
Thermal diffuse scattering in silicon



raw image taken with
PILATUS 6M detector

area detectors -> revival of TDS since 1999

*M. Holt, Z. Wu, H. Hong, P. Zschack, P. Jemian, J. Tischler, H. Chen, T.-C. Chiang Phys. Rev. Lett. **83**, 3317 (1999)*

fitting of single images with lattice dynamics model

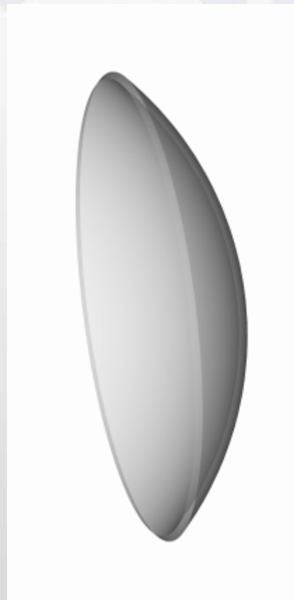
new age with pixel detectors?

FULL reciprocal space can be explored in few minutes

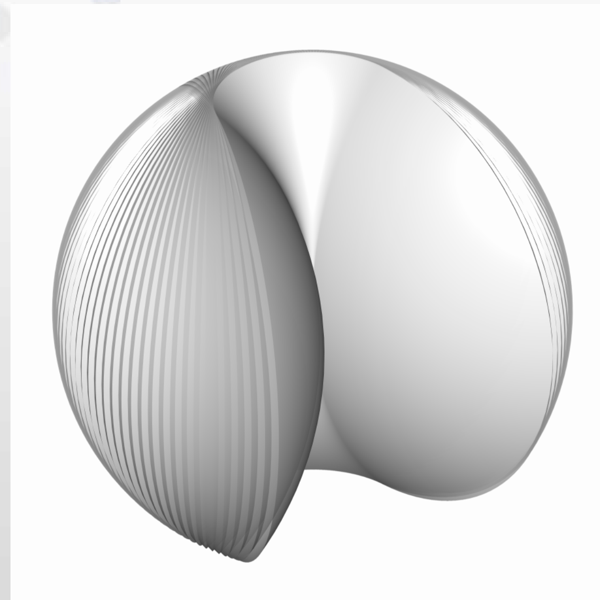
Towards 3D representation

flat image
CBF

sphere



space filling



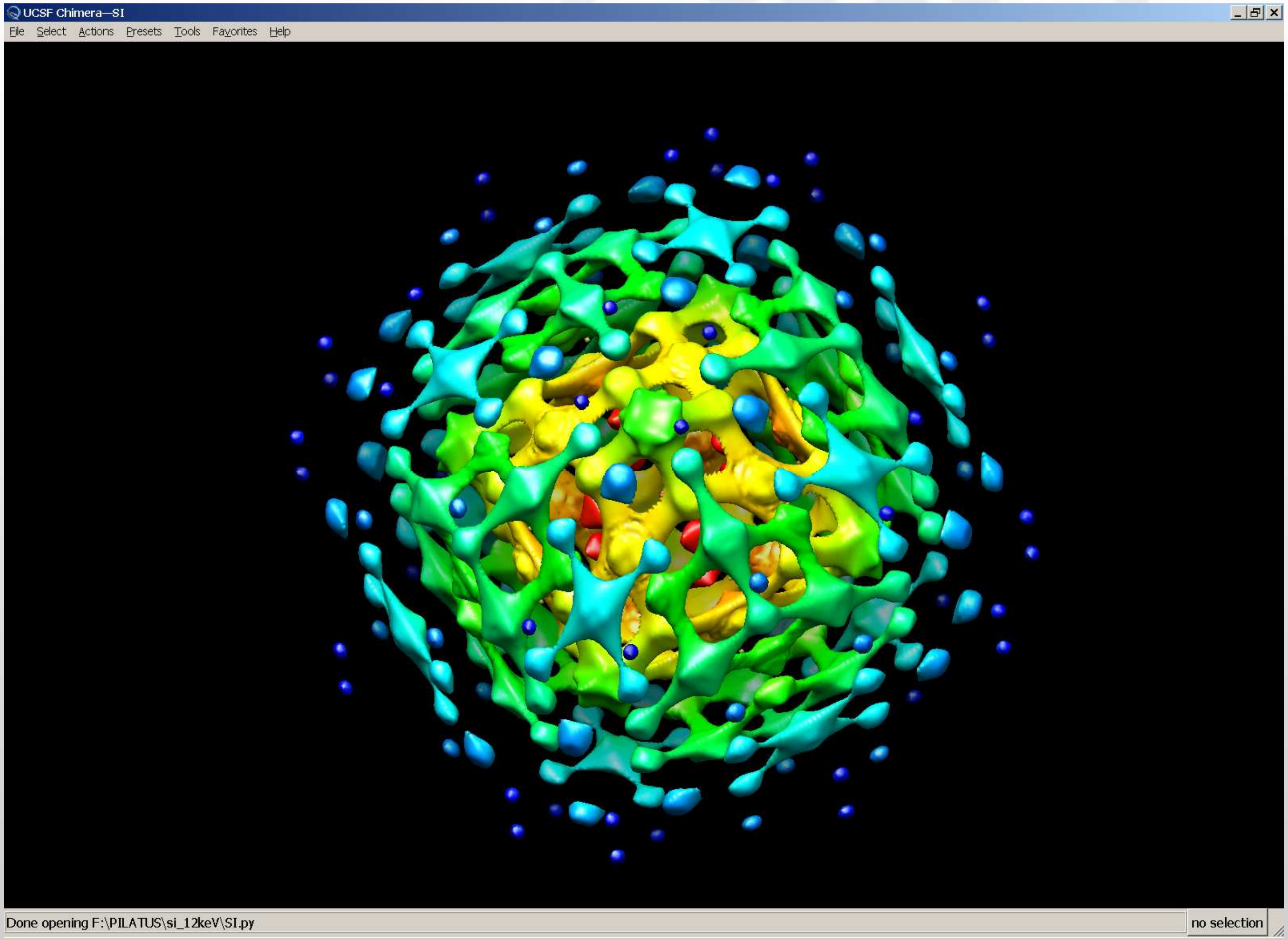
masking, corrections, UB matrix retrieval, application of symmetry elements, etc.

CCP4 map format

UCSF Chimera

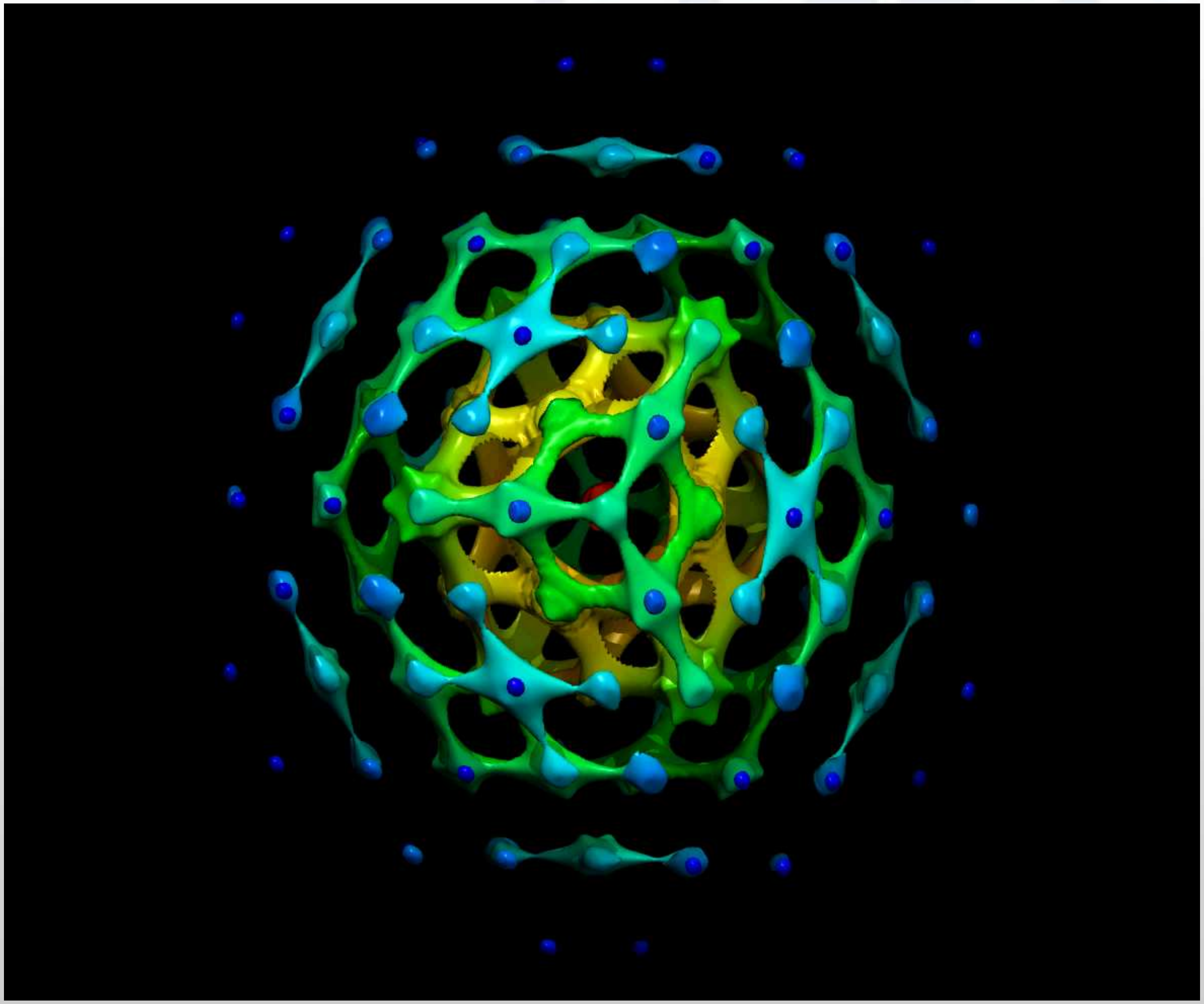
…

3D TDS mapping in silicon



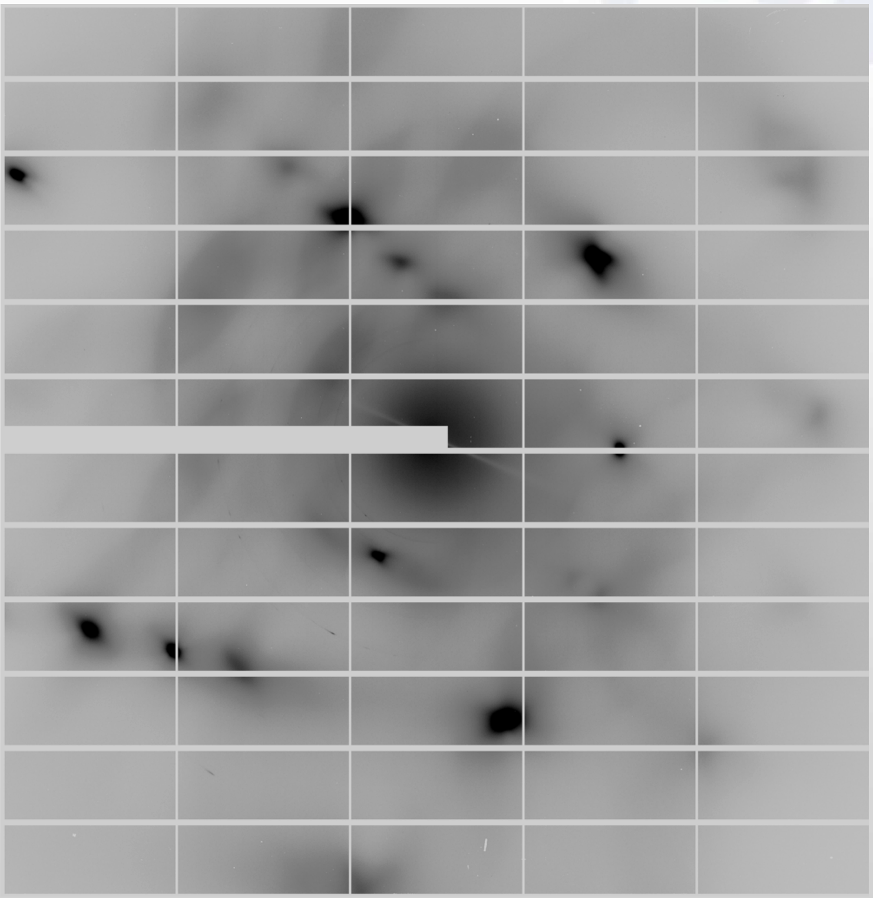
constant TDS intensity surface – phonon contribution only

3D TDS mapping in silicon

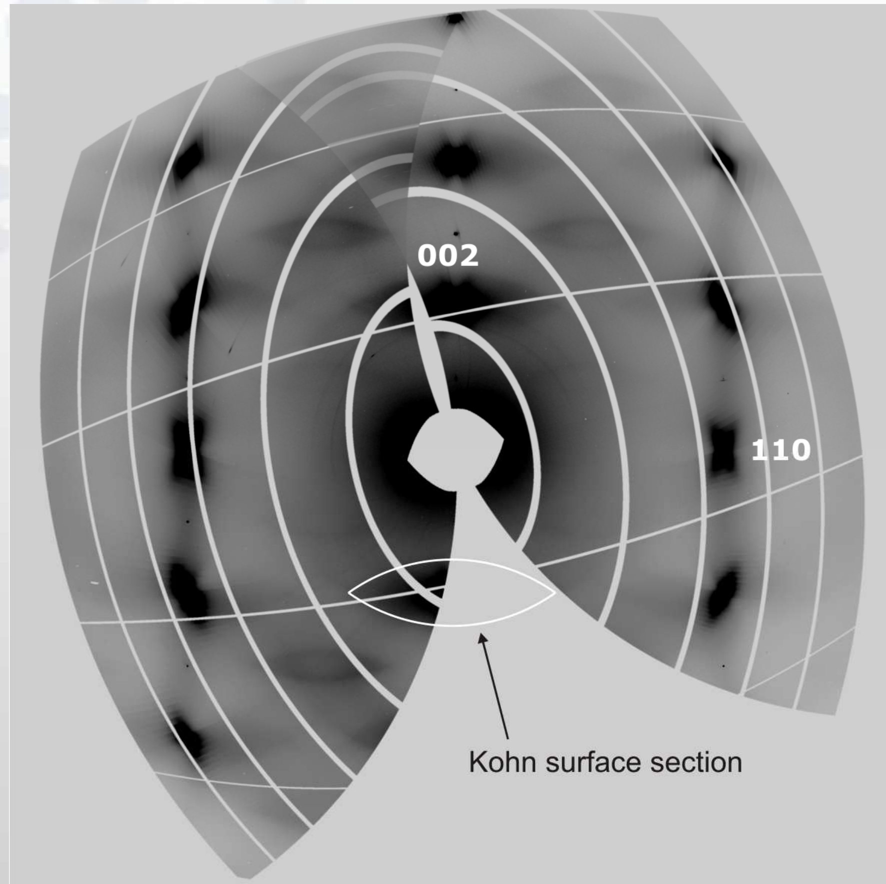


rendering performed
with POV-Ray software

Kohn surface visualization in zinc metal



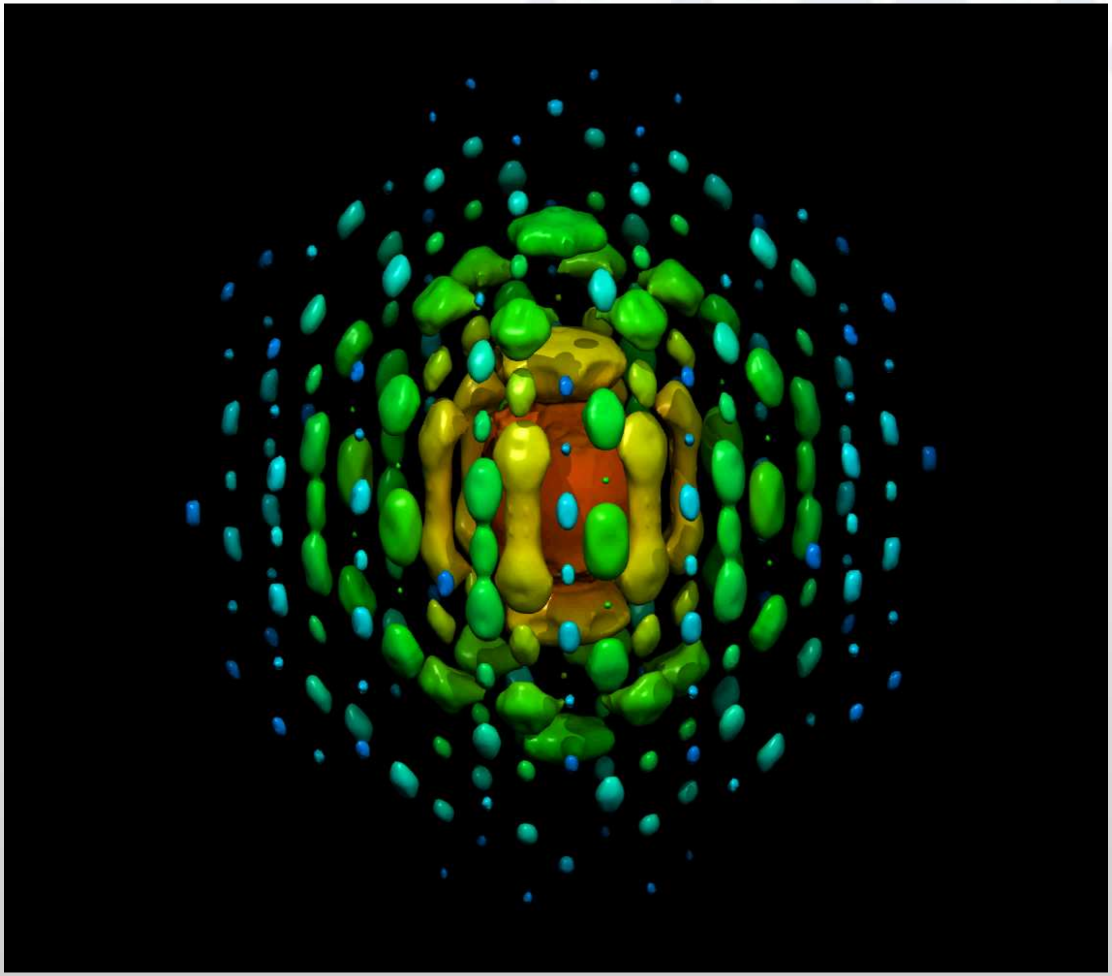
raw image



RS reconstruction with Crysalis software

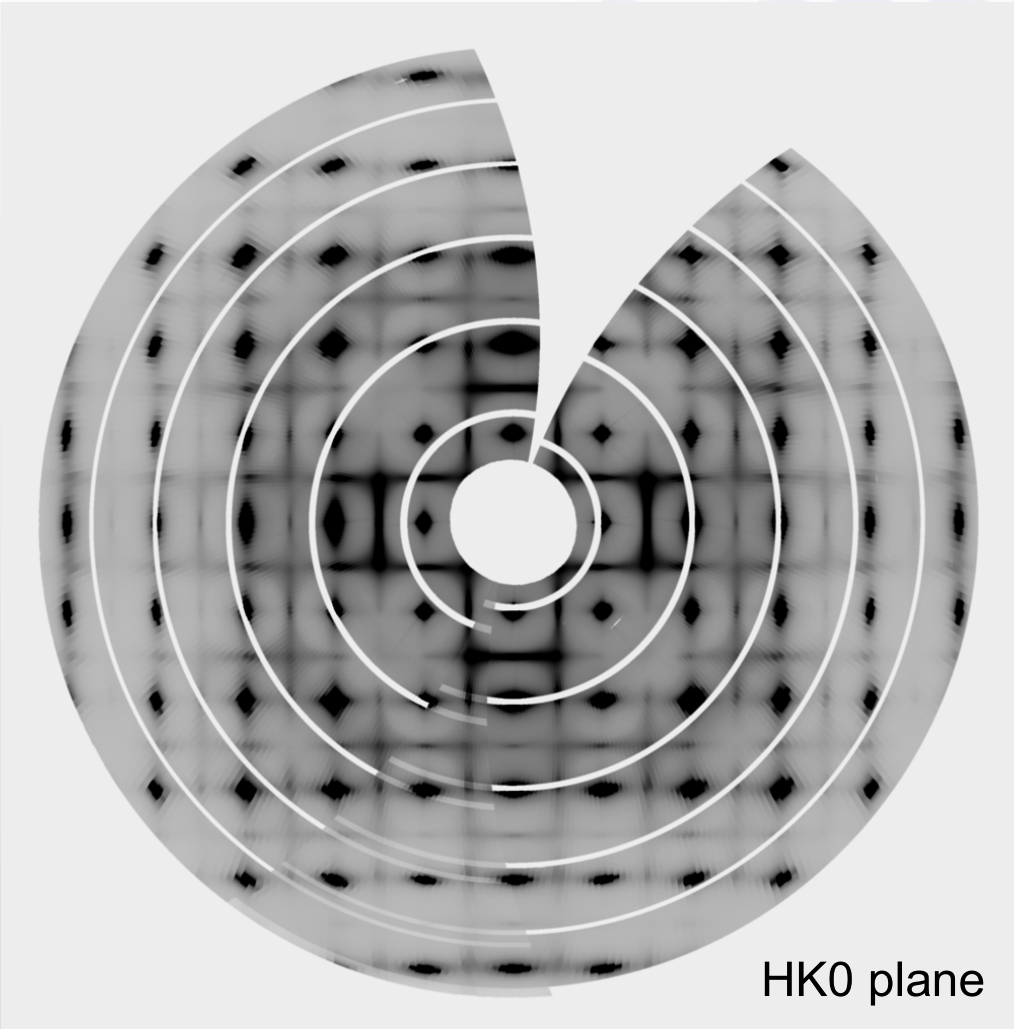
PILATUS: strong suppression of fluorescence!

… and 3D TDS representation



elastic contribution can be neglected (proven by IXS)

Prussian blue: correlated disorder



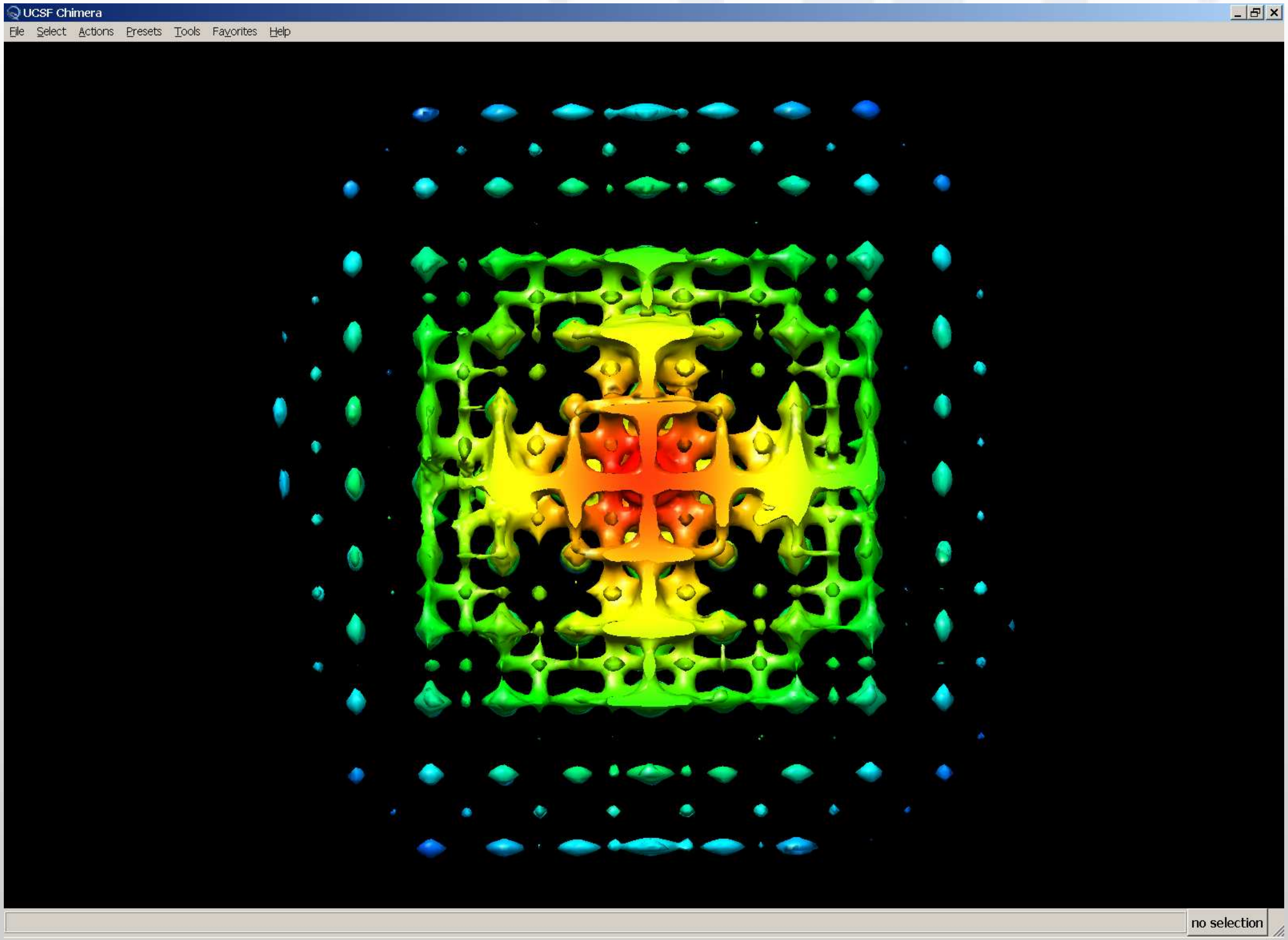
$Mn(II)[Mn(III)(CN)_6]_{2/3} \cdot (6H_2O)_{1/3} \cdot yH_2O$

replacement of $[Mn(CN)_6)]$ by $[6H_2O]$

not fully random!

inelastic contribution
to the strong diffuse
features is negligible

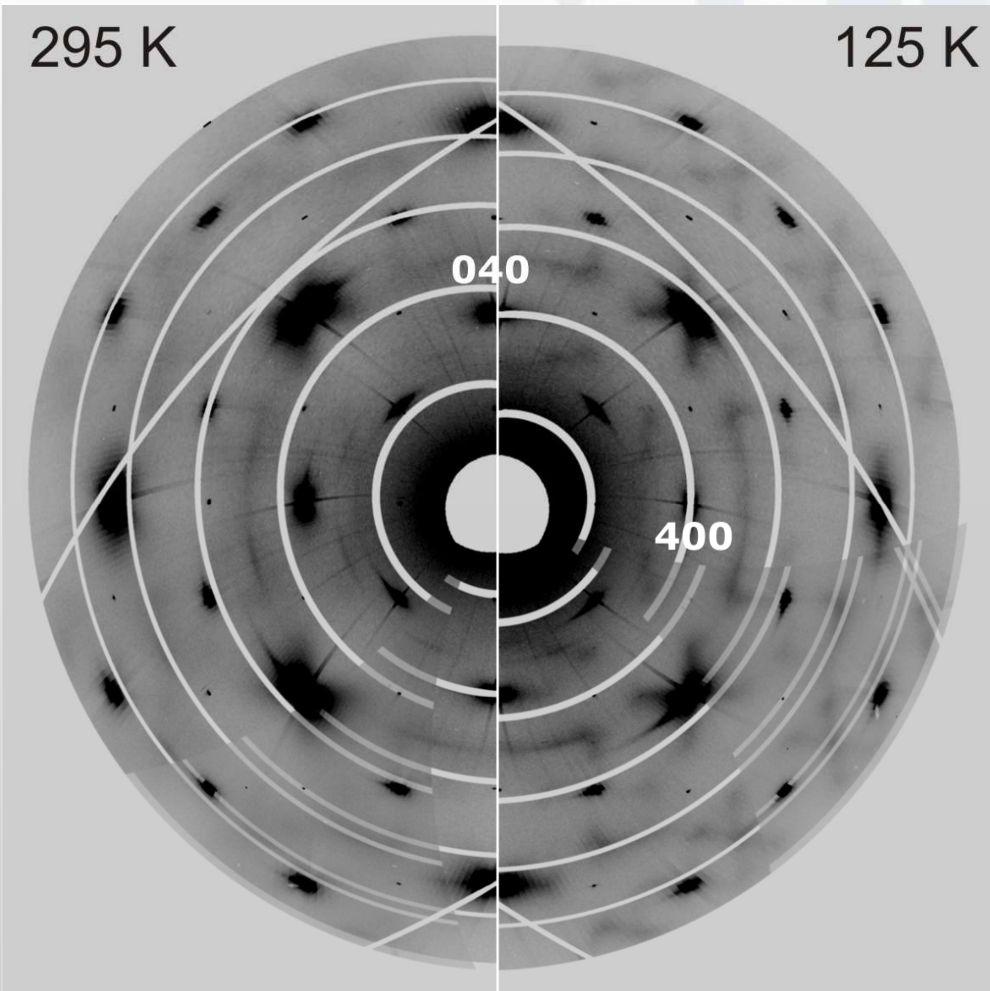
Step towards 3D pair distribution function?



Pioneering work:

P. Schaub, T. Weber, W. Steurer
Phil. Mag. **87**, 18 (2007)

Magnetite: old mistery of phase transition



phase transition: 122 K

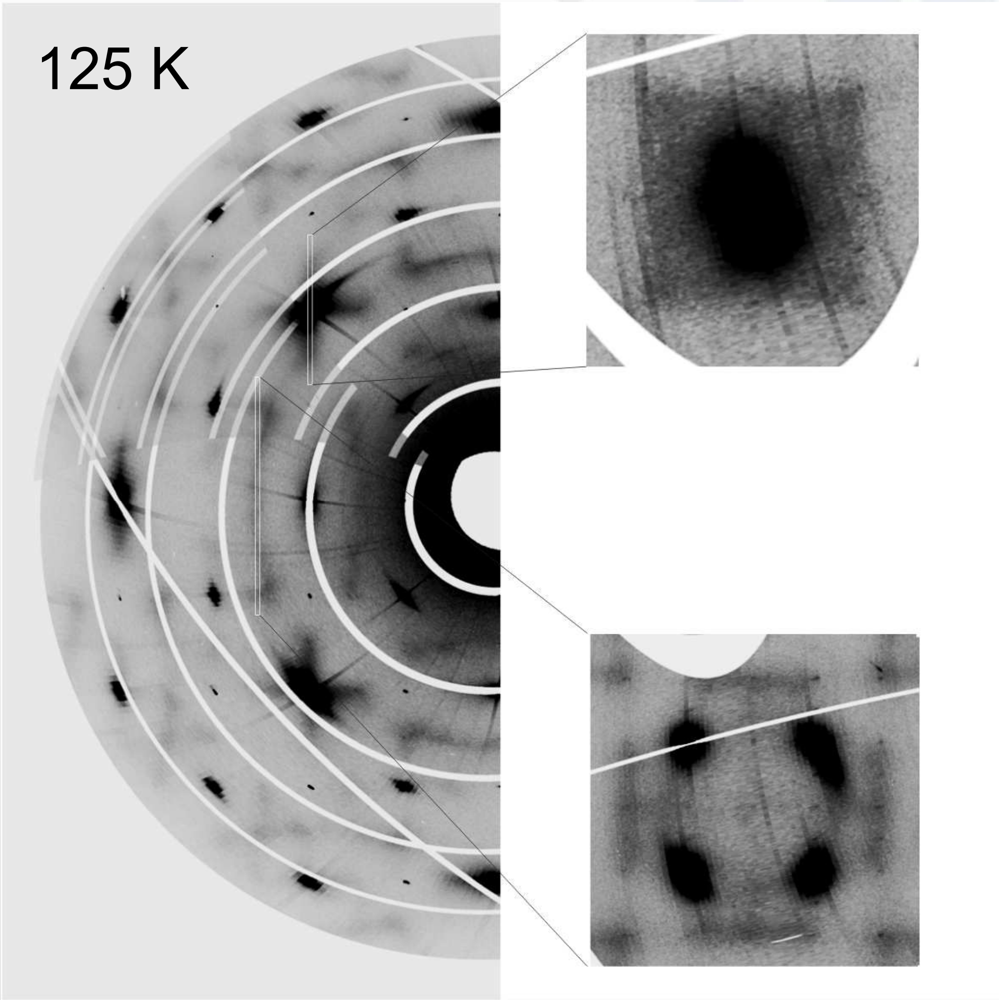
disorder?

polarons?

phonons?

we need a roadmap for IXS!

Magnetite: old mistery of phase transition



new features in diffuse scattering are revealed

NB: some maxima of diffuse scattering are not commensurate with basic lattice