Coherent X-ray Diffractive imaging, Applications and limitations

S. Marchesini, H.N. Chapman, S.P. Hau-Riege, A. Noy, A. Szöke, H. Szöke, E. Ingermann

H. He, M. R. Howells, R. A. Rachel

U. Weierstall, J.C.H. Spence

T. Beetz

- Coherent Diffractive imaging
- Phase-retrieval problem
    - -Phase retrieval by projections
    - -Examples
- Experiment at the Advanced Light Source
- Radiation Damage Limit
- Atomic-resolution imaging biological macromolecules
- Comparison of techniques

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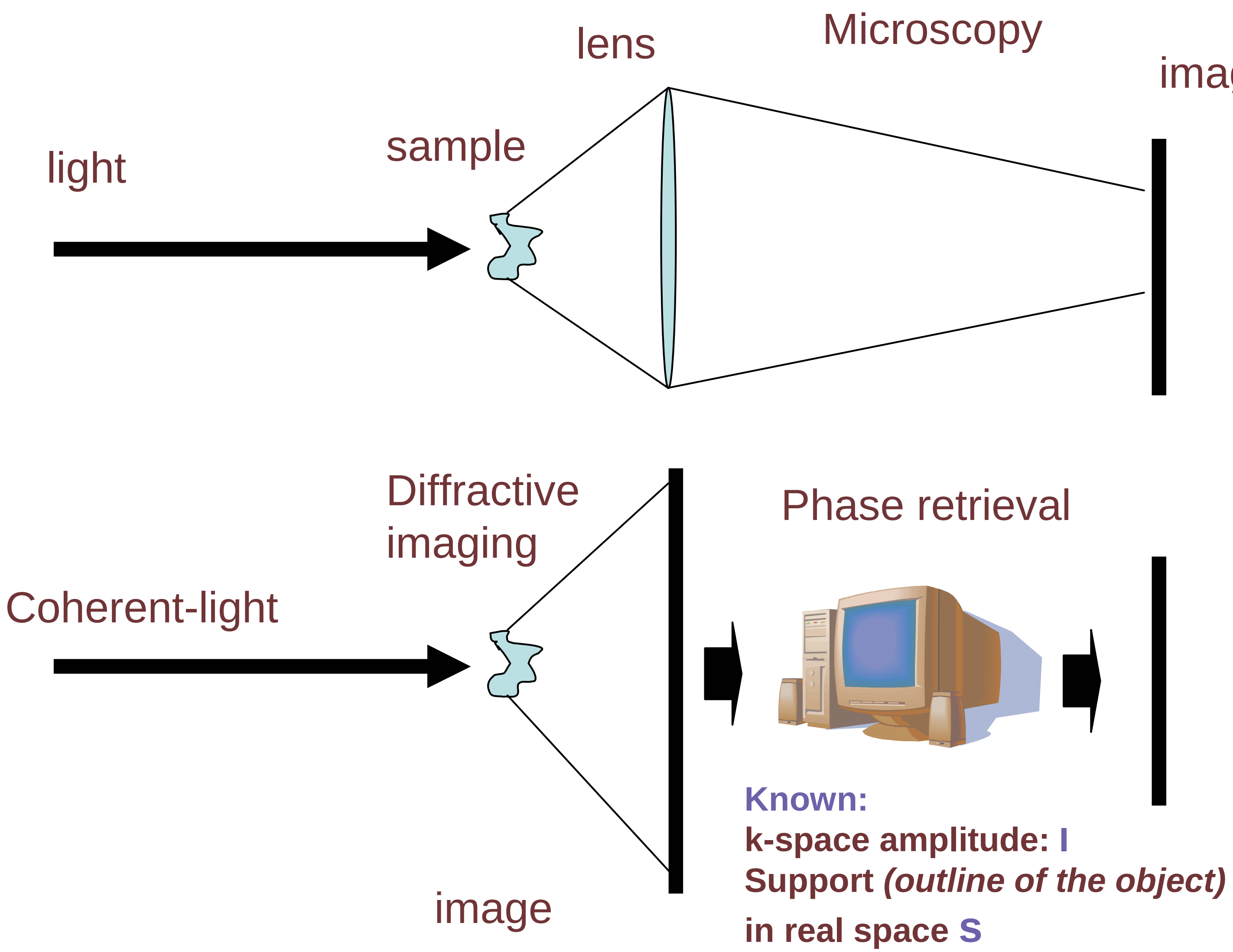
UCRL-PRES-201069

Coherent Diffractive imaging

phase-retrieval problem

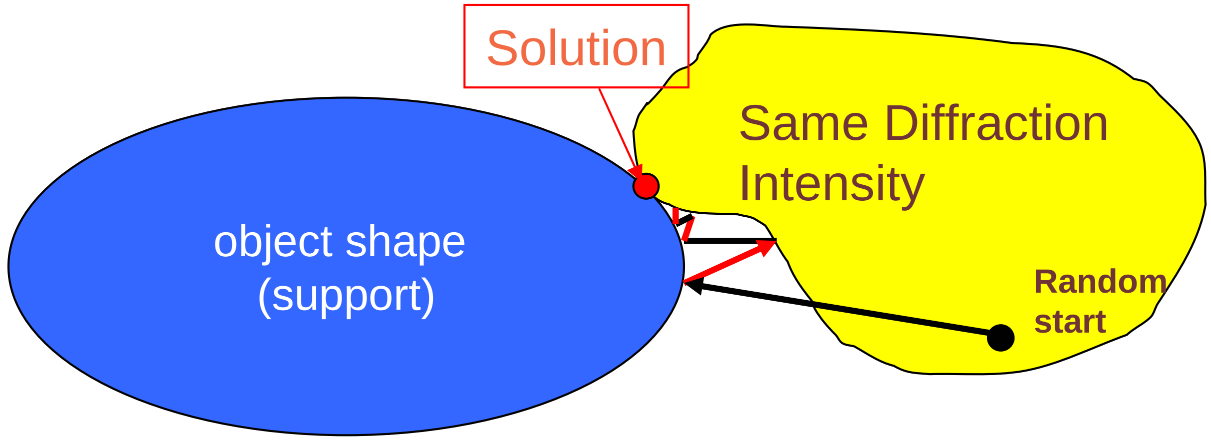


- depth of field limit
- lens-limited
- direct

- No depth of field limit
- No lens-limited
- Computer-limited

Phase retrieval by projections

By projecting back and forth between feasibility sets, we can find the common solution (intersection of two sets)



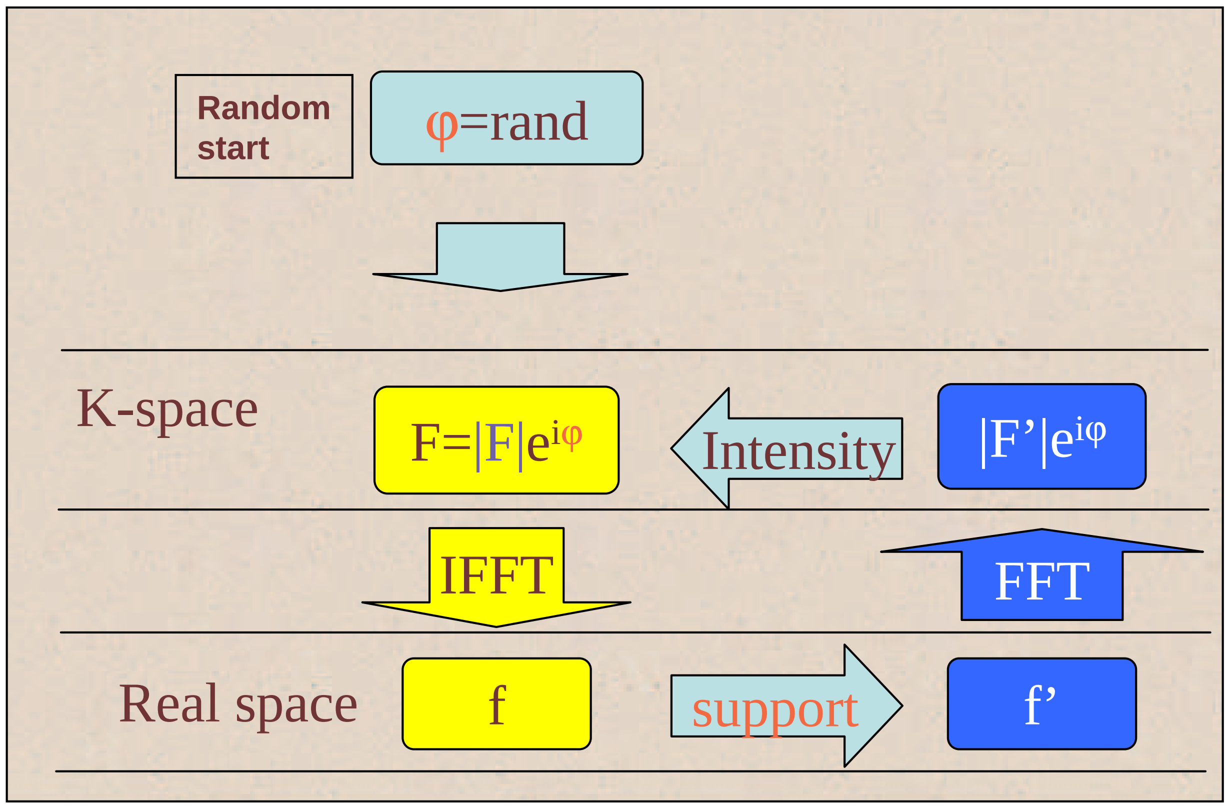
Known:

- **k-space amplitude: |F|**
- **Support *s* in real space: f=0 for s=0**

Unknown:

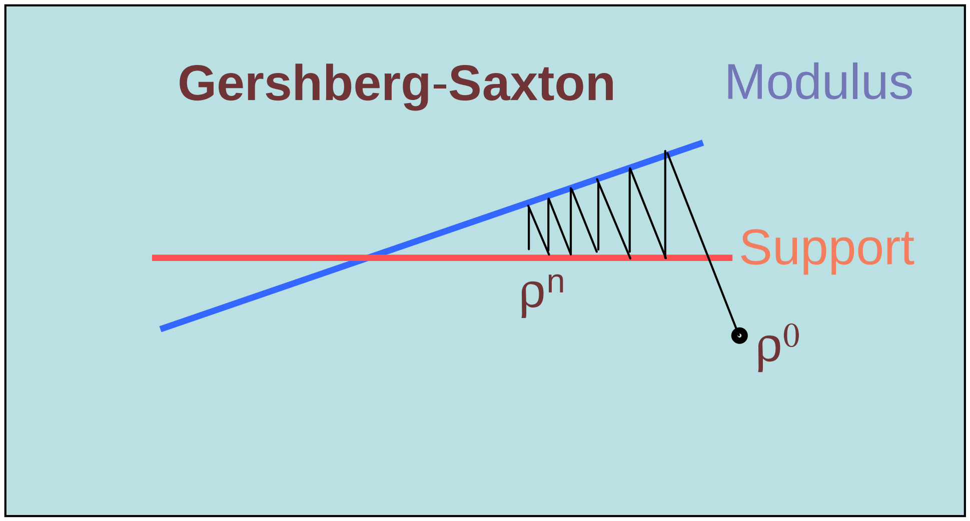
- **Phase in k-space φ**
- **Image inside the support**

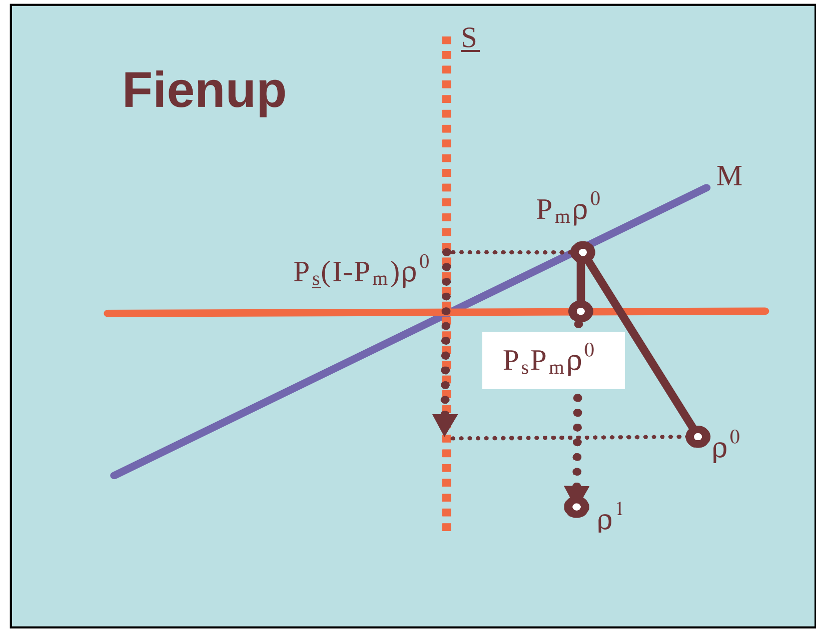
f=? For s=1

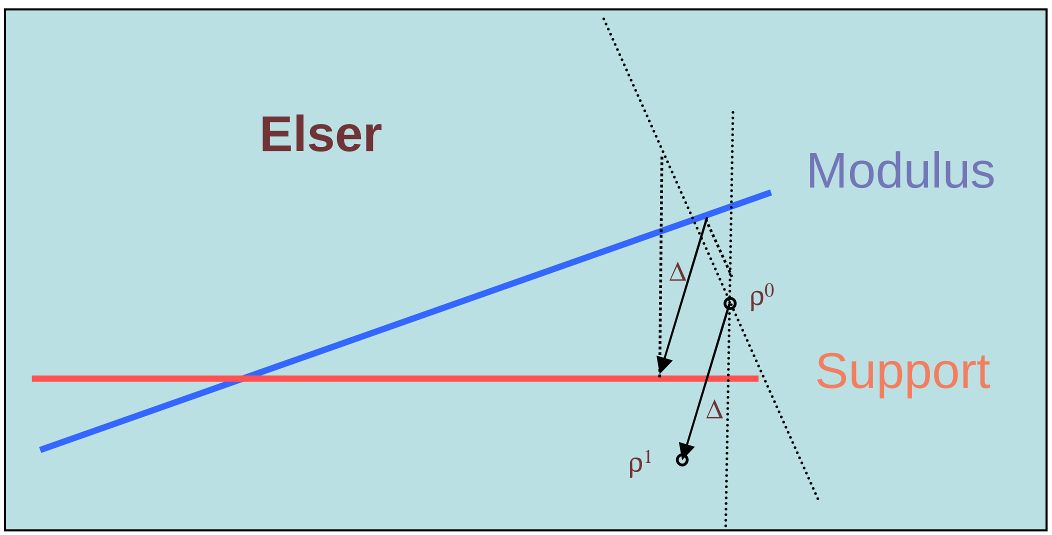


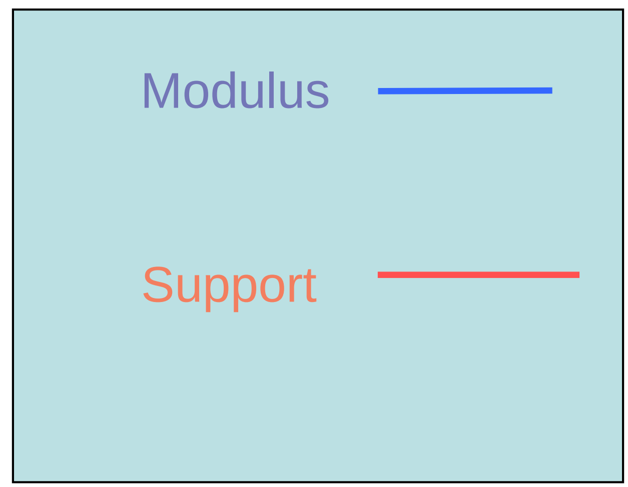
Projection algorithms

By projecting back and forth between feasibility sets, we can find the common solution (intersection of two sets)





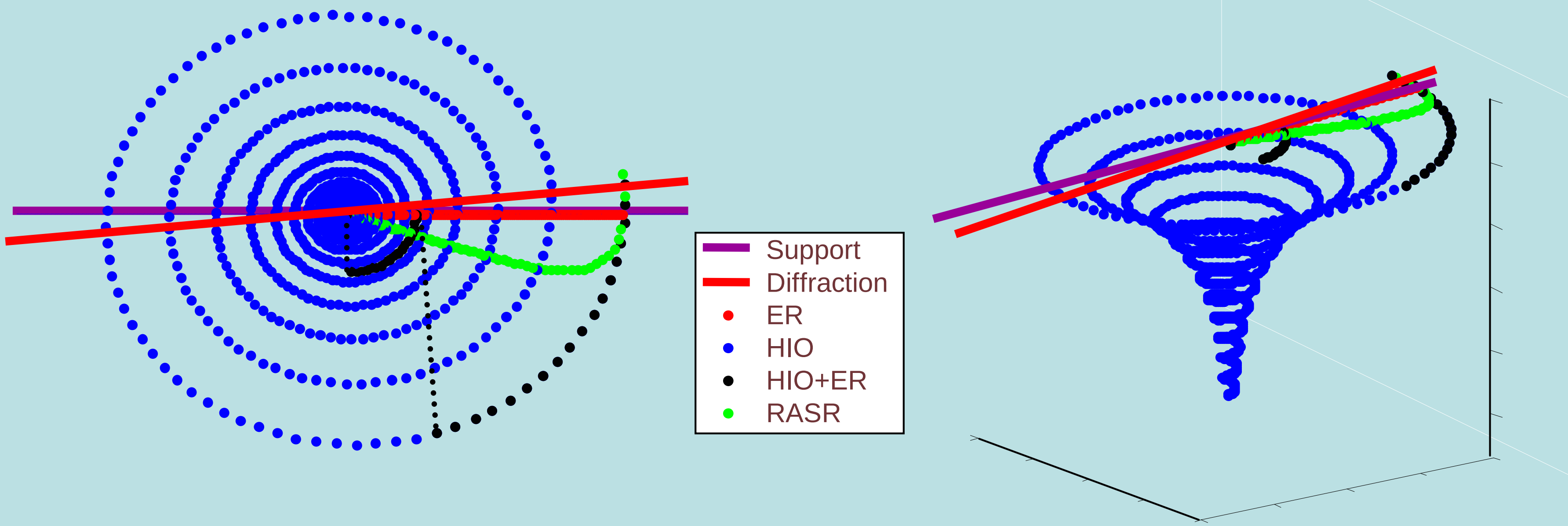




Example:

find the intersection of two lines

when the two lines do not intersect



Comparison of various algorithms

How some algorithm escape local minima

•(ER) R. Gerchberg, W. Saxton, Optik 35, 237 (1972).
•(HIO) J. R. Fienup, J.R. (1982) . Appl. Optics, 21, 2758-2769
•(Diff. Map) V. Elser, J. Opt. Soc. Am. A 20, 40-55 (2003)
•(ASR,HPR, RASR) H. Bautschke, P.L. Combettes & D. R. Luke, (2002) . J. Opt. Soc. Am., 19, 1344-1345

Many error metrics

- real space error (stuff outside support)
- reciprocal space error, (R_{fact})
- difference between reconstructions

Reciprocal space error

$$R^n = \frac{\sum_{\mathbf{k}} \left\| \tilde{\rho}_{obs}(\mathbf{k}) \right| - \left| \tilde{\rho}^n(\mathbf{k}) \right\|^2}{\sum_{\mathbf{k}} \left| \tilde{\rho}_{obs}(\mathbf{k}) \right|^2}$$

Real space error

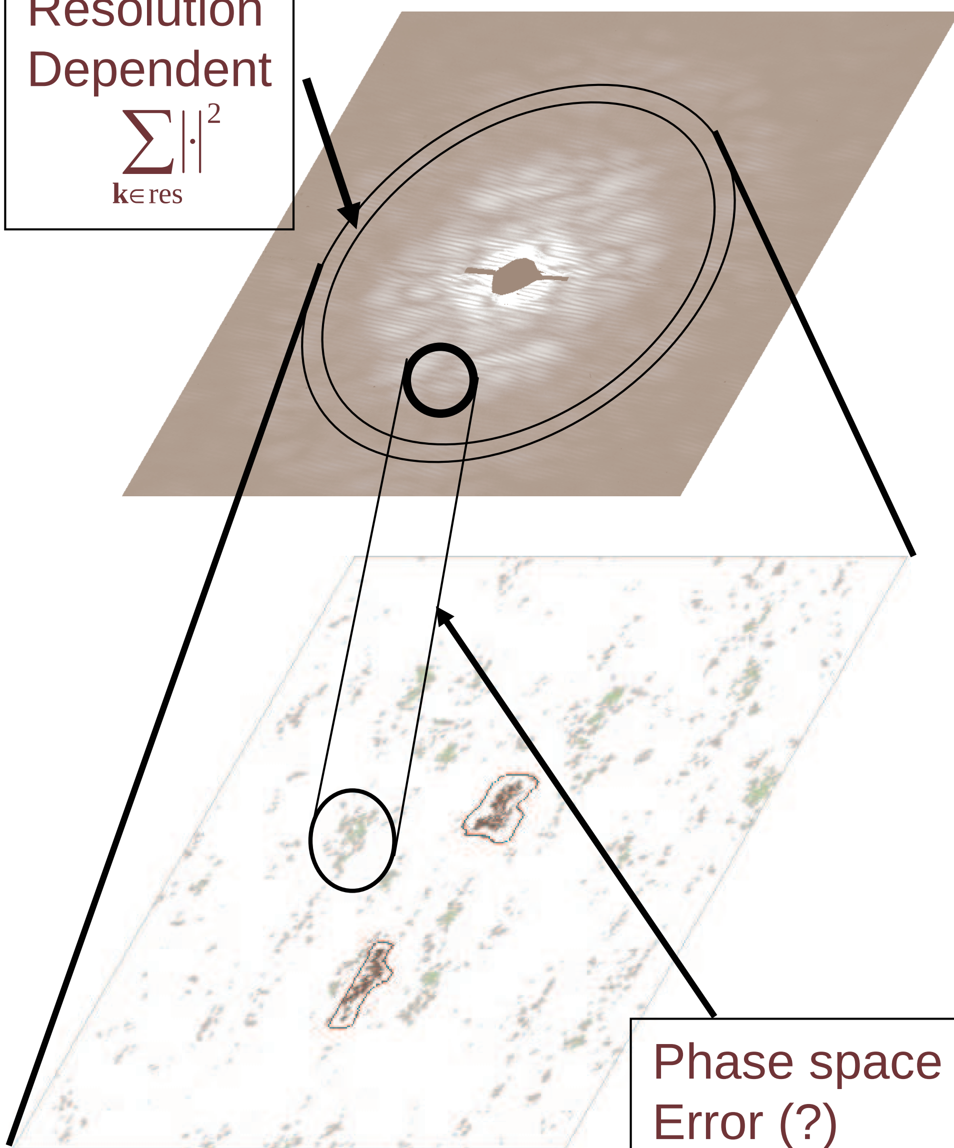
$$\varepsilon_{\mathrm{s}}^n = \frac{\sum_{\mathbf{x}} \left| \mathbf{P}_{\mathrm{s}} \rho^n(\mathbf{x}) - \rho^n(\mathbf{x}) \right|^2}{\sum_{\mathbf{x}} \left| \mathbf{P}_{\mathrm{s}} \rho^n(\mathbf{x}) \right|^2}$$

Error between reconstructions

$$\varepsilon^{1,2} = \frac{\left\| \rho^1 - \rho^2 \right\|^2}{\left\| \frac{1}{2}\left(\rho^1 + \rho^2\right) \right\|^2}$$

Resolution Dependent

$$\sum_{\mathbf{k} \in \mathrm{res}} \left| \cdot \right|^2$$



Phase space Error (?)

Parseval

$$\left\| \cdot \right\|^2 = \sum_{\mathbf{x}} \left| \cdot \right|^2 = \frac{1}{N} \sum_{\mathbf{k}} \left| \tilde{\cdot} \right|^2$$

In the language of projectors and sets

Constraints errors

$$\varepsilon_{\mathrm{m}}^{\mathrm{n}} = \frac{\left\| \mathbf{P}_{\mathrm{m}} \rho^n - \rho^n \right\|^2}{\left\| \mathbf{P}_{\mathrm{m}} \rho^n \right\|^2}$$

$$\varepsilon_{\mathrm{s}}^{\mathrm{n}} = \frac{\left\| \mathbf{P}_{\mathrm{s}} \rho^n - \rho^n \right\|^2}{\left\| \mathbf{P}_{\mathrm{s}} \rho^n \right\|^2}$$

Phase problem not unique!

One family of homometric structures (Hoseman and Bagchi, Acta Cryst 7, p. 237 (1954))
may be generated using the result that…..

Homometric structures.

$$\rho_1(r) = l(r) * m(r)$$

and

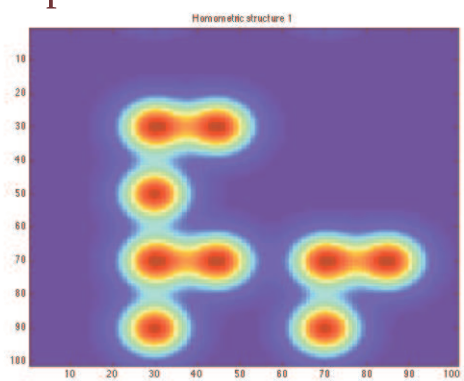
$$\rho_2(r) = l(r) * m^*(-r)$$

$$have \;\; same \;\; Fourier \;\; modulus \;\; |R(u)|, \;\; since$$

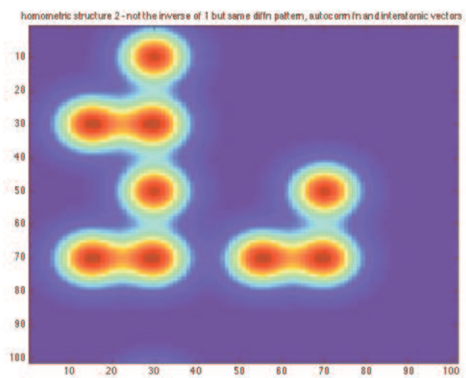
$$R_1(u) = L(u)M(u) \;\; and \;\; R_2(u) = L(u)M^*(u)$$

If l(r) is a lattice and m(r) a molecule, then m, m* are enants, but ρ_1, ρ_2 are not enants.

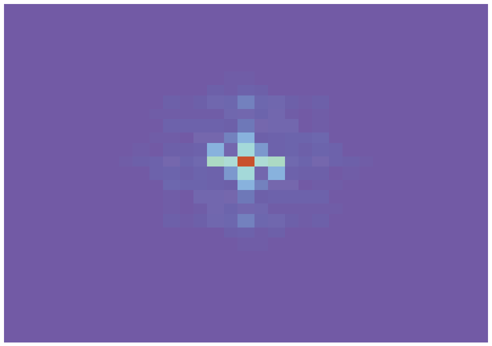
Example:



Homo1



Homo2



Fourier Mod of either

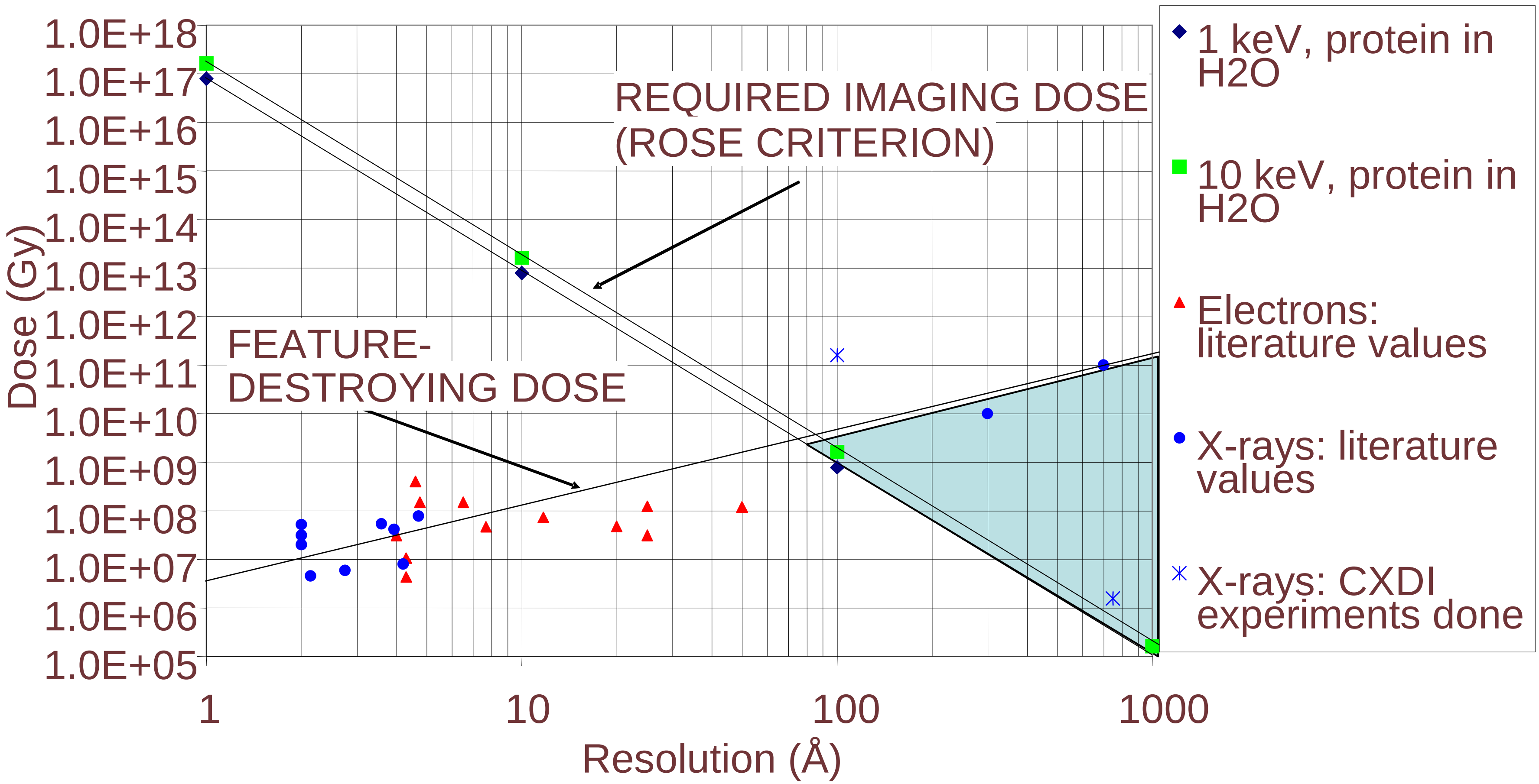
Note: Homo1 is not the inverse (enantiomorph) of Homo2.

Conclusion: HiO could not distinguish these unless tight support provided.

Distinguished by Multiple scattering ELNES

RADIATION DAMAGE LIMITED DOSE-RESOLUTION CURVES

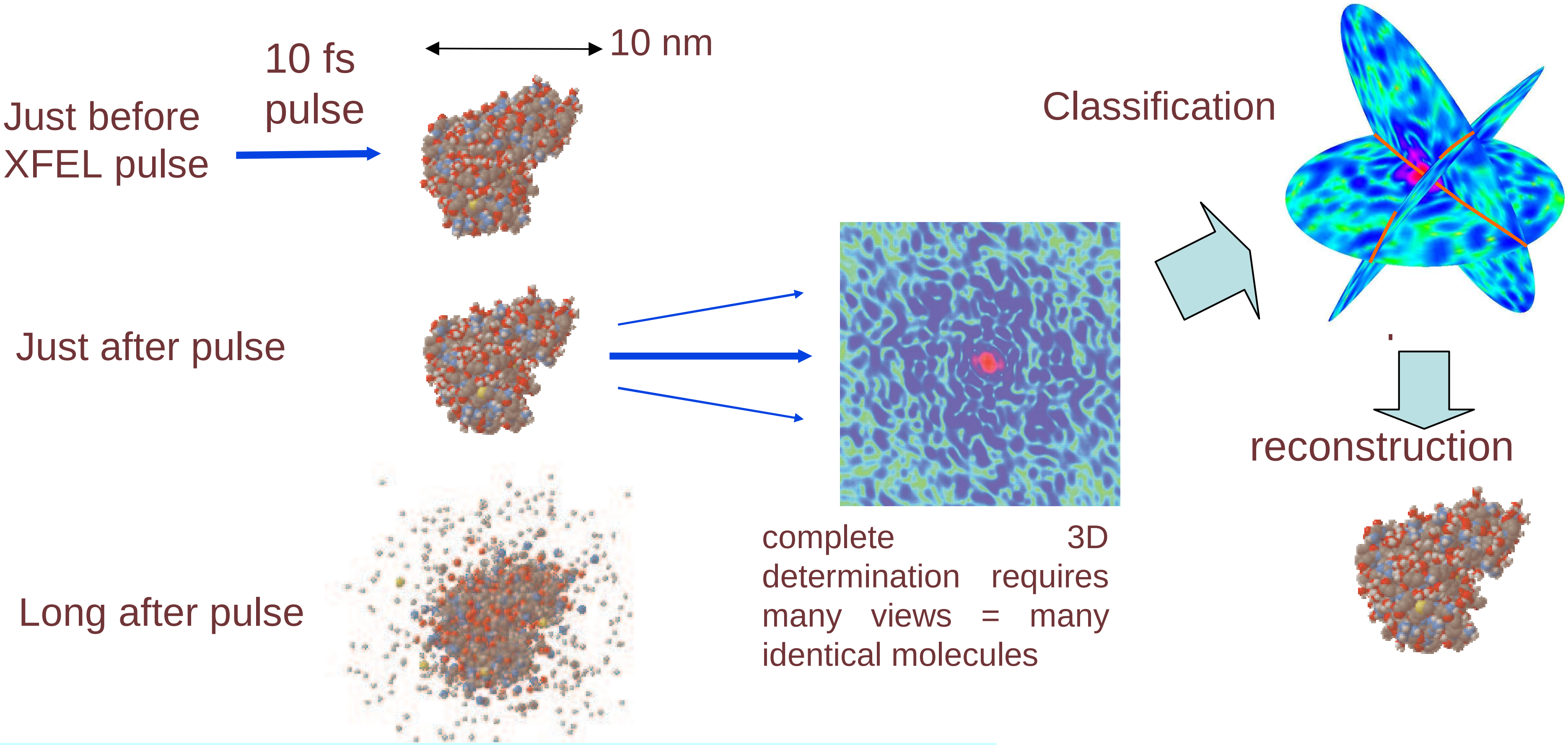
M. R. Howells



Optics Express 11(19), 2344 (2003), [arXiv:physics.optics/0308064]

Atomic-resolution imaging of virtually any biological macromolecule will become possible with XFELs

Diffraction from a single molecule:

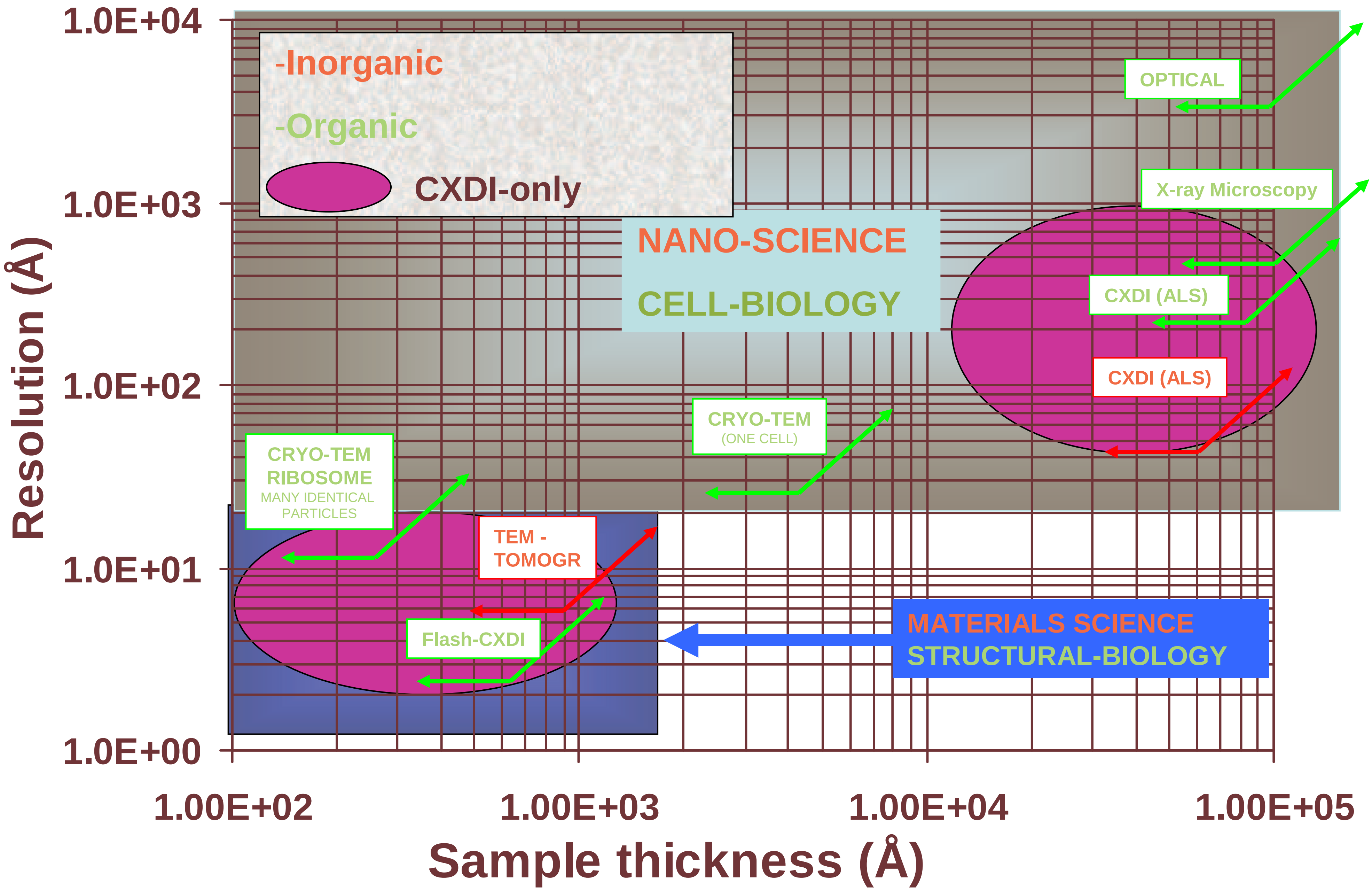


Many critical issues need to be solved:

- details of short-pulse photon-matter interactions
- image reconstruction
- sample manipulation and injection

Planned damage experiments at SPPS (Stanford), and TTF (Hamburg)

Comparison of techniques

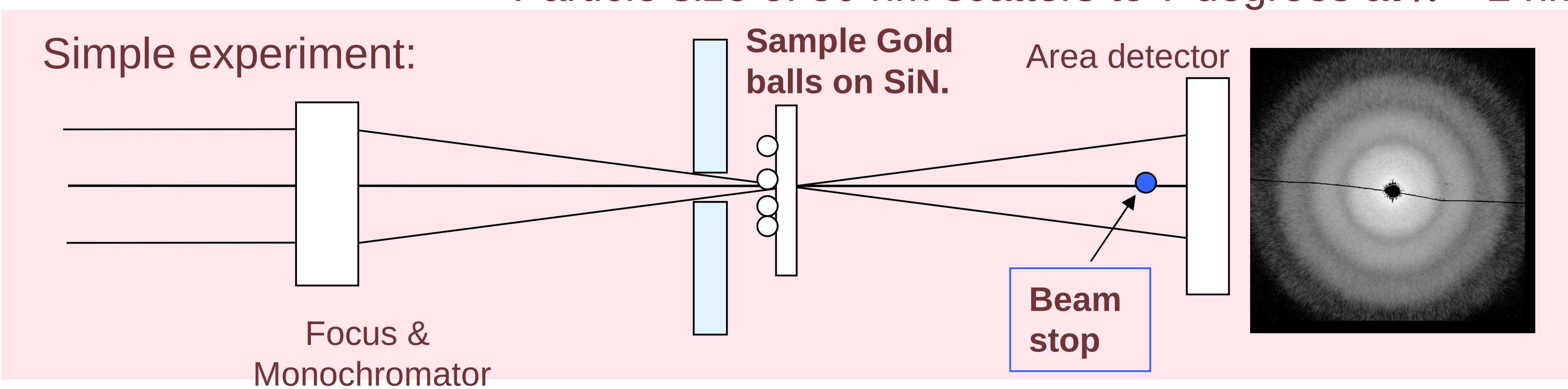


Experiment

Layout of the diffraction chamber

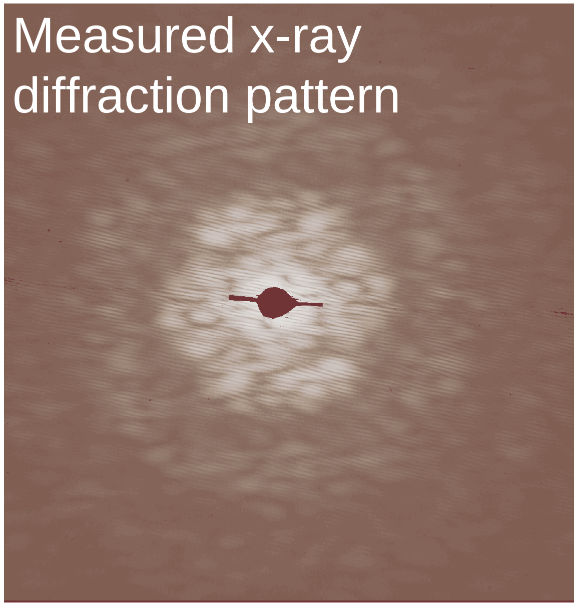
at BL 9.0.1 at Advanced Light Source, LBL

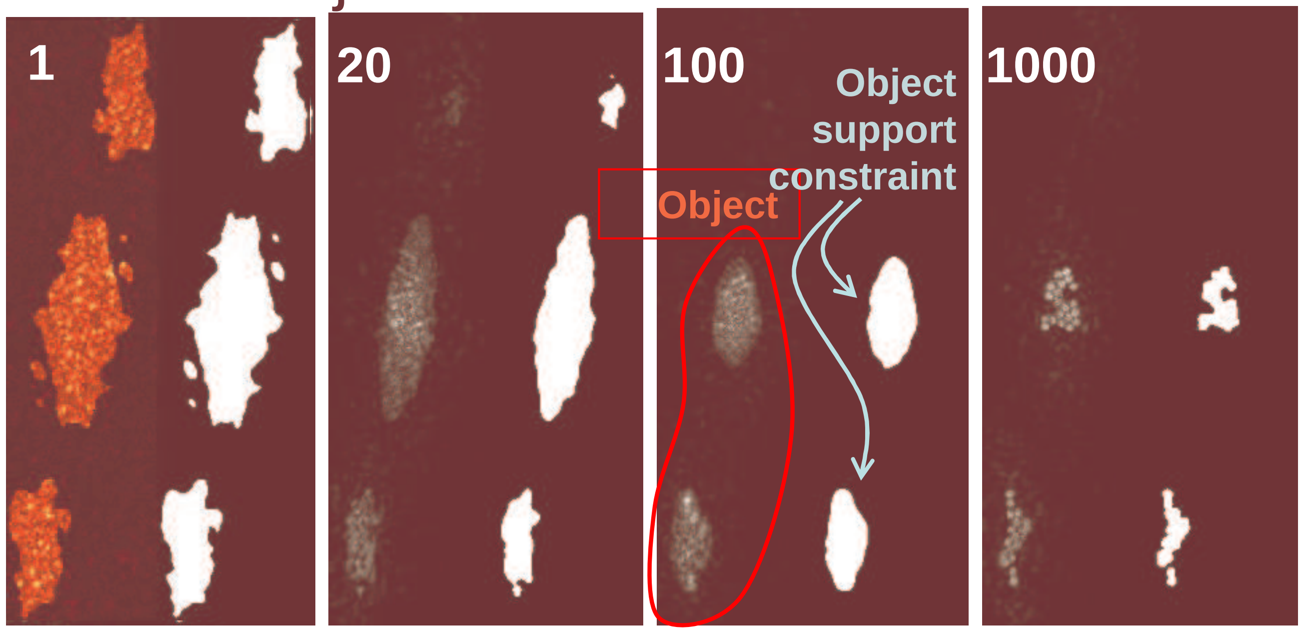
Particle size of 50 nm scatters to 7 degrees at $\lambda = 2$ nm

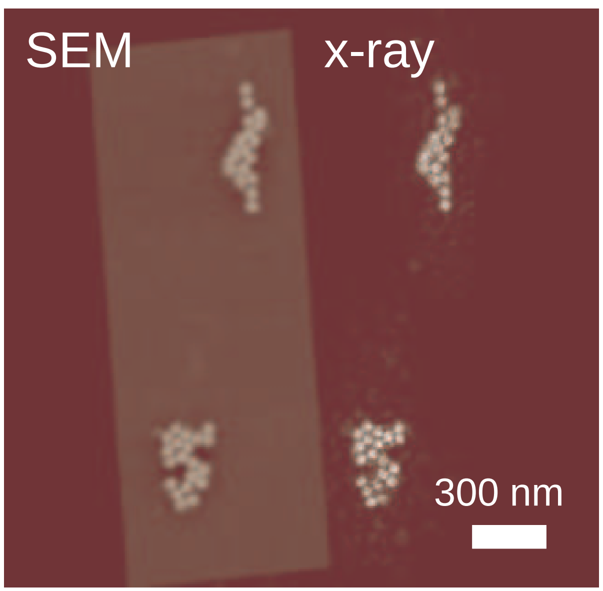


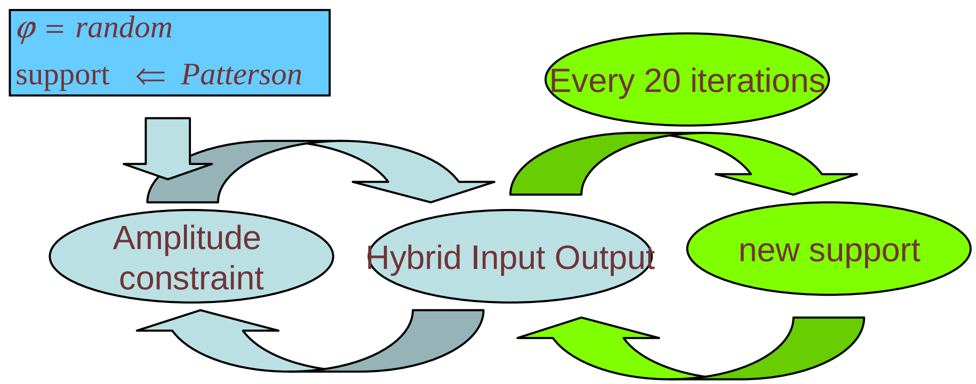
Proc. SPIE **4783**, 65 (2002)

We have eliminated the need of the known shape of the object







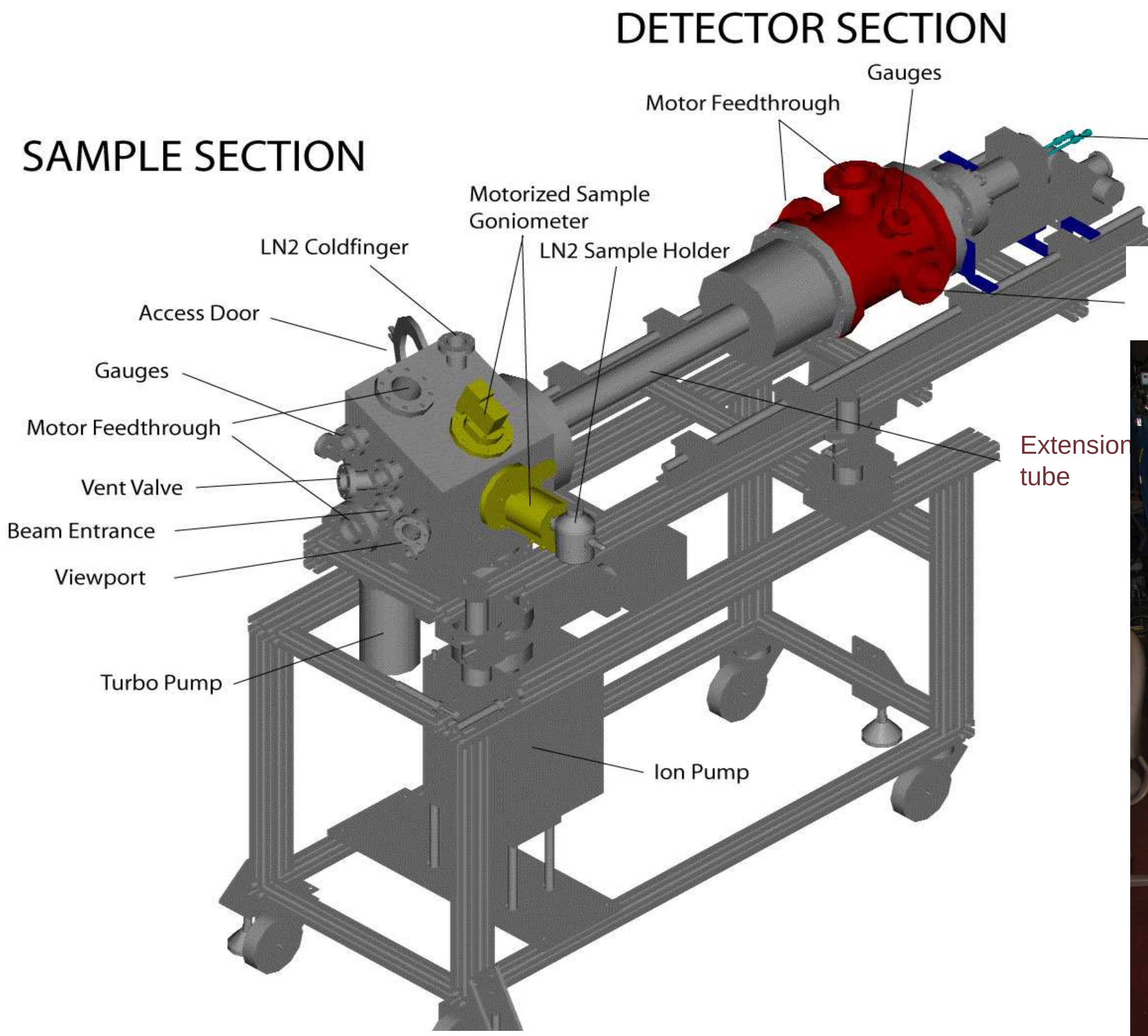


Fienup hybrid input-output

Shrinkwrap extension

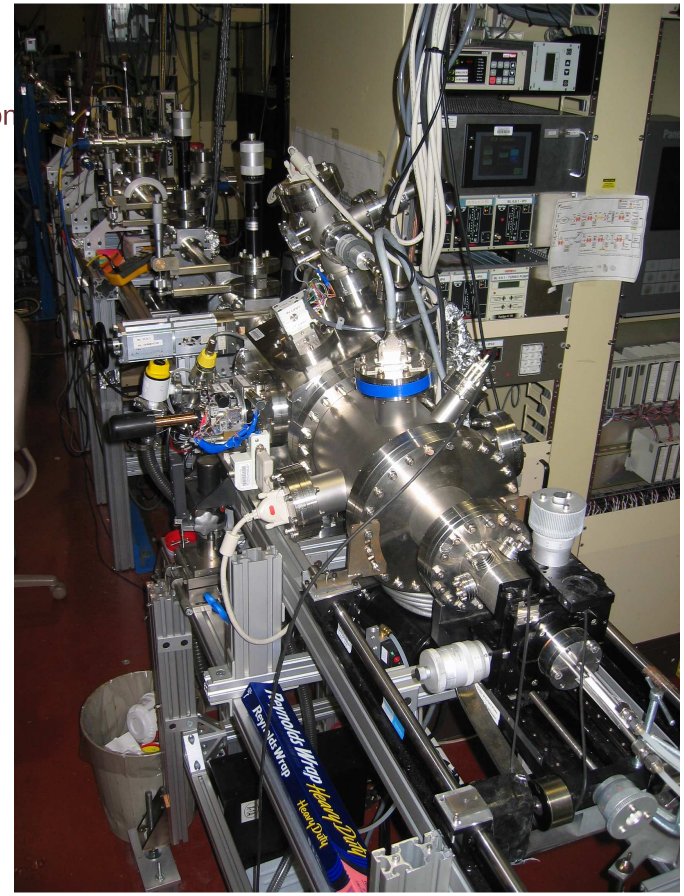
PRB 68, 140101R (2003), [arXiv:physics.optics/0306174]

The Stony Brook diffraction chamber allows accurate sample rotation and data acquisition



T. Beetz, et al., J. de Phys. IV 104, 351-359 (2003).

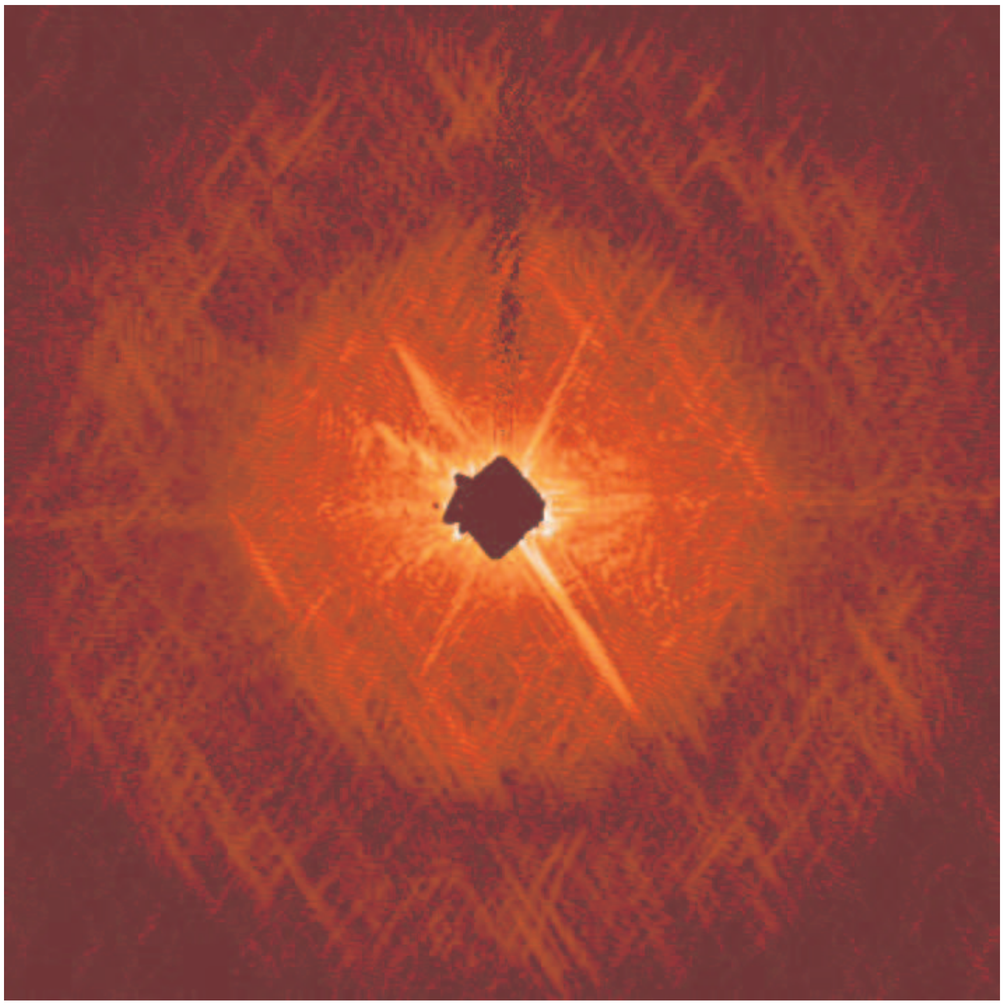
Installed at ALS BL9.0.1



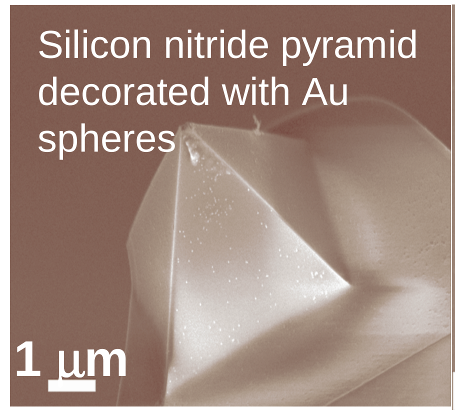
Stony Brook diffraction chamber (Chris Jacobsen and Janos Kirz)

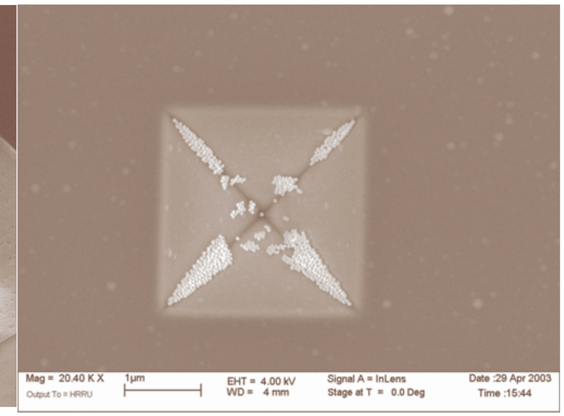
We performed 3D diffraction-imaging experiments

- Complete coverage of reciprocal space by sample rotation
- Use a true 3D object that can be well-characterized by independent means



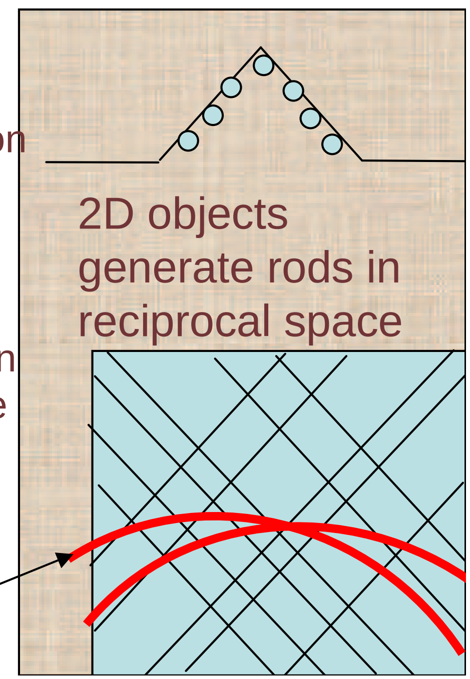
Diffraction pattern





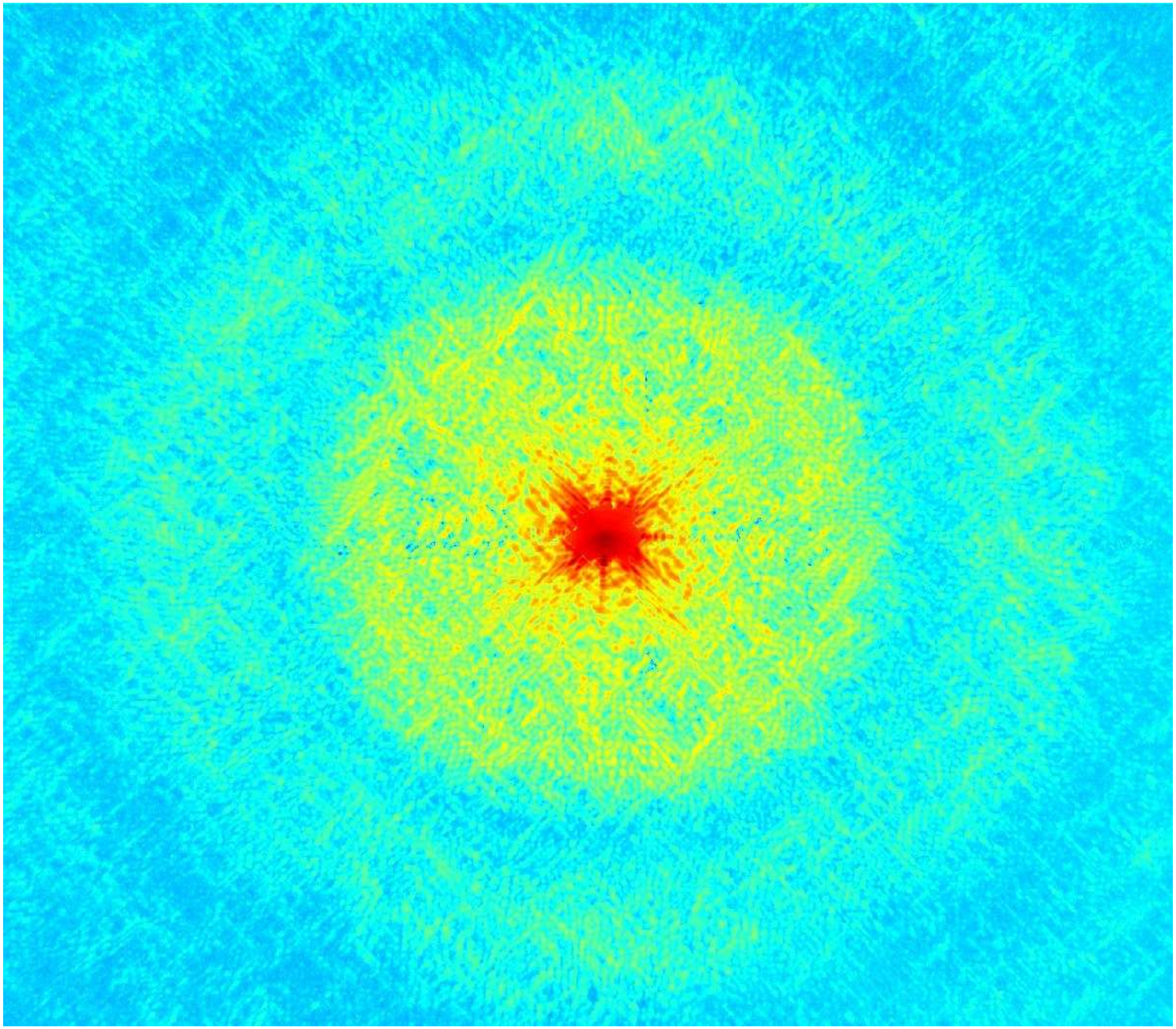
We collected a complete data set with over 140 views with 1° angular spacing.

Cross-section



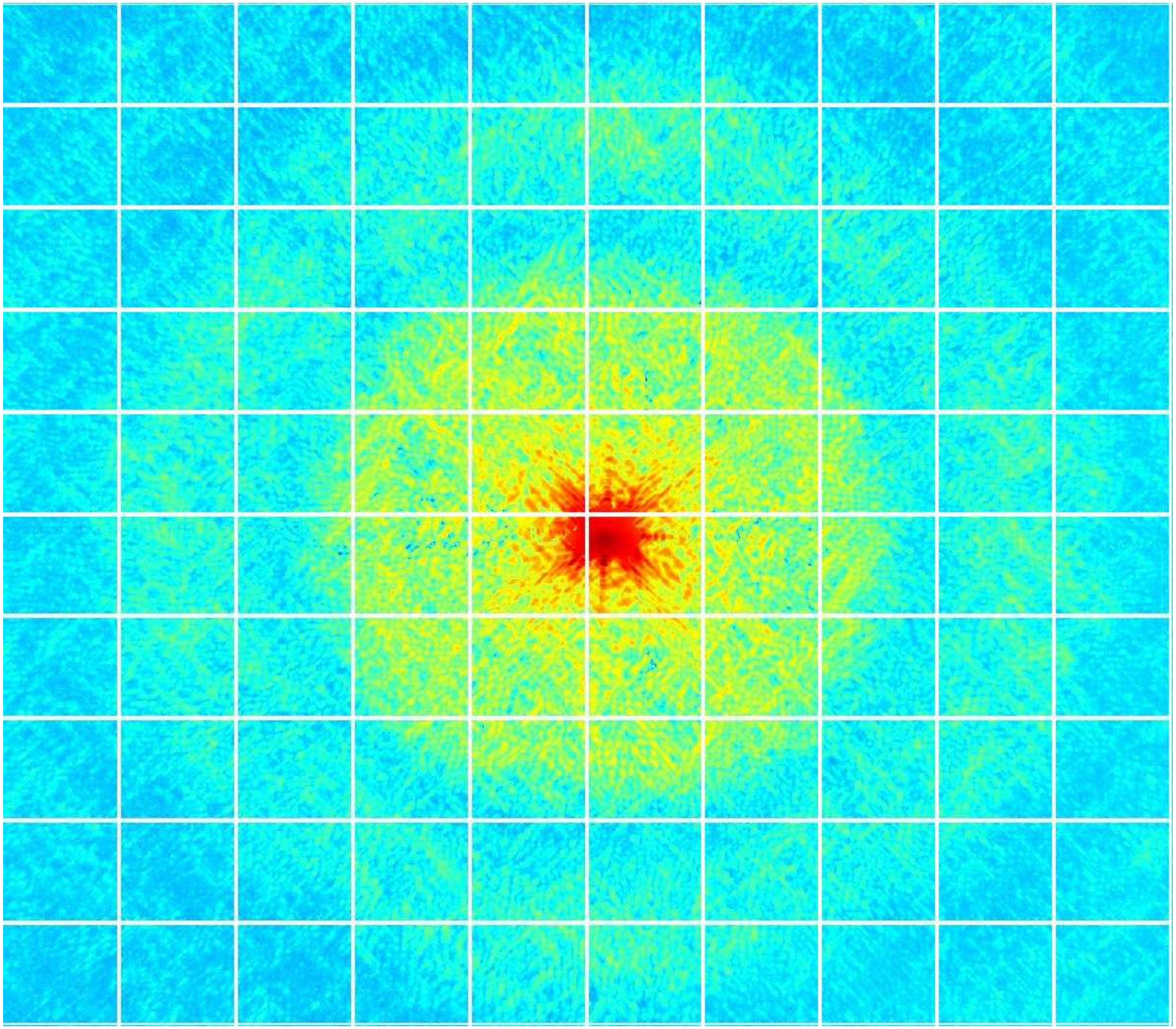
Ewald sphere

Inspection of the data (I)



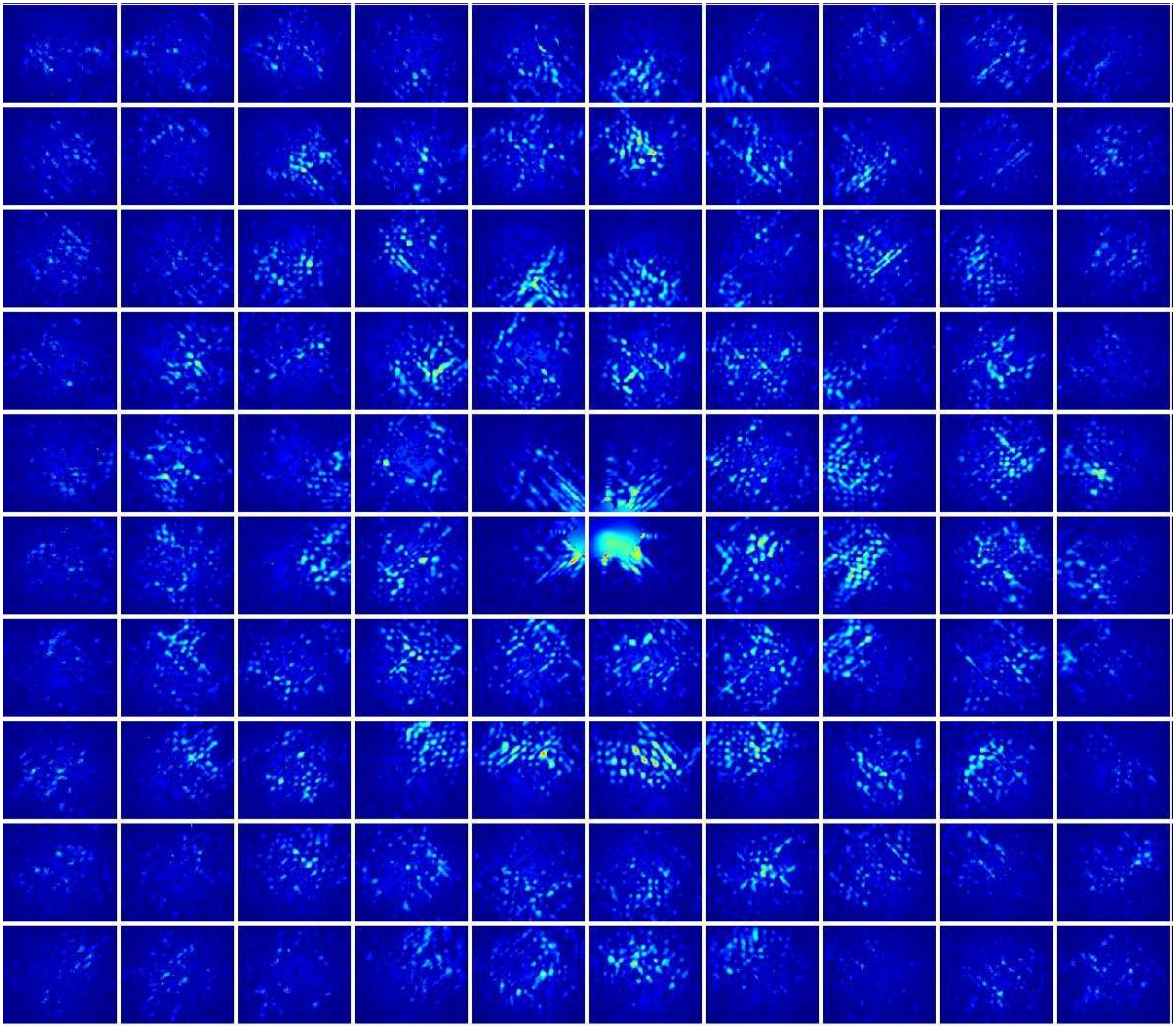
Diffraction Pattern

Inspection of the data (II)



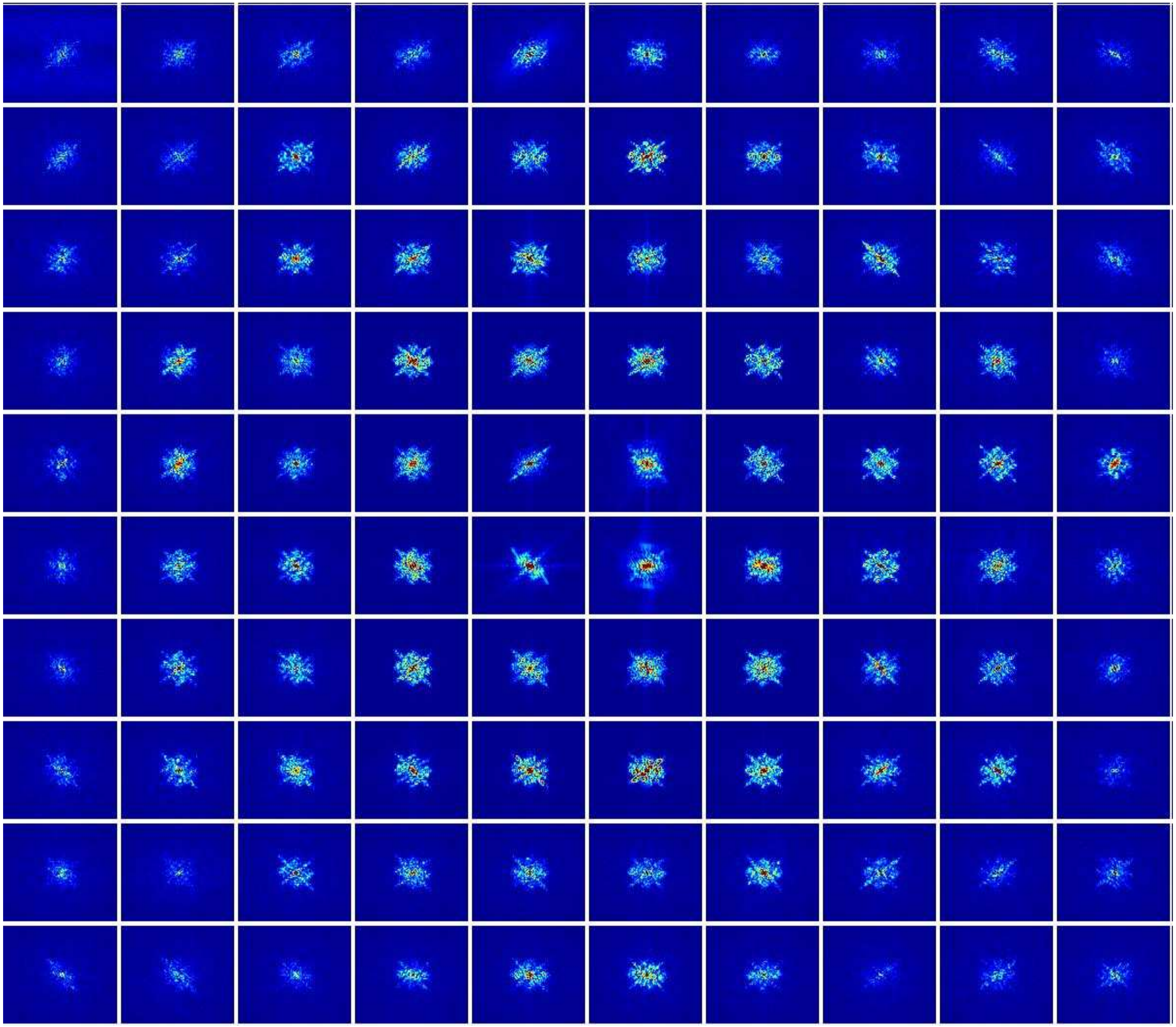
Divide into many pieces

Inspection of the data (III)



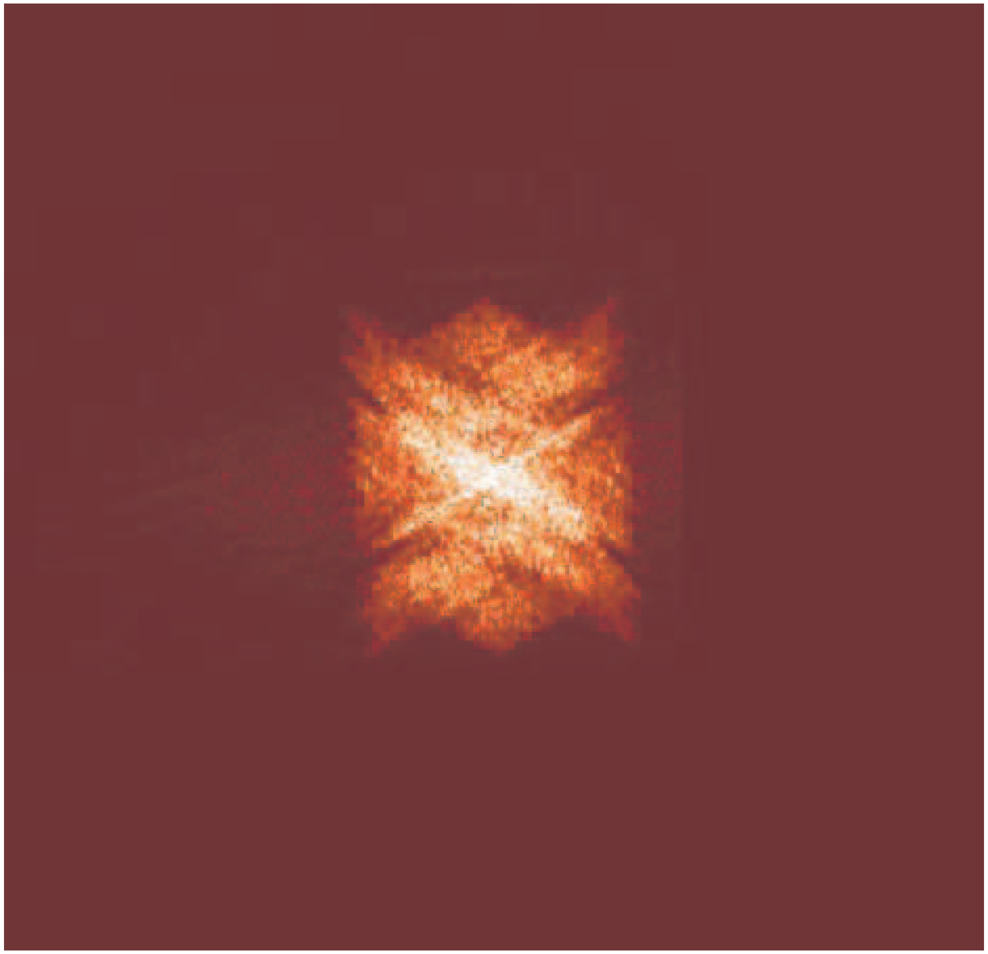
Multiply by gaussians

Inspection of the data (IV)

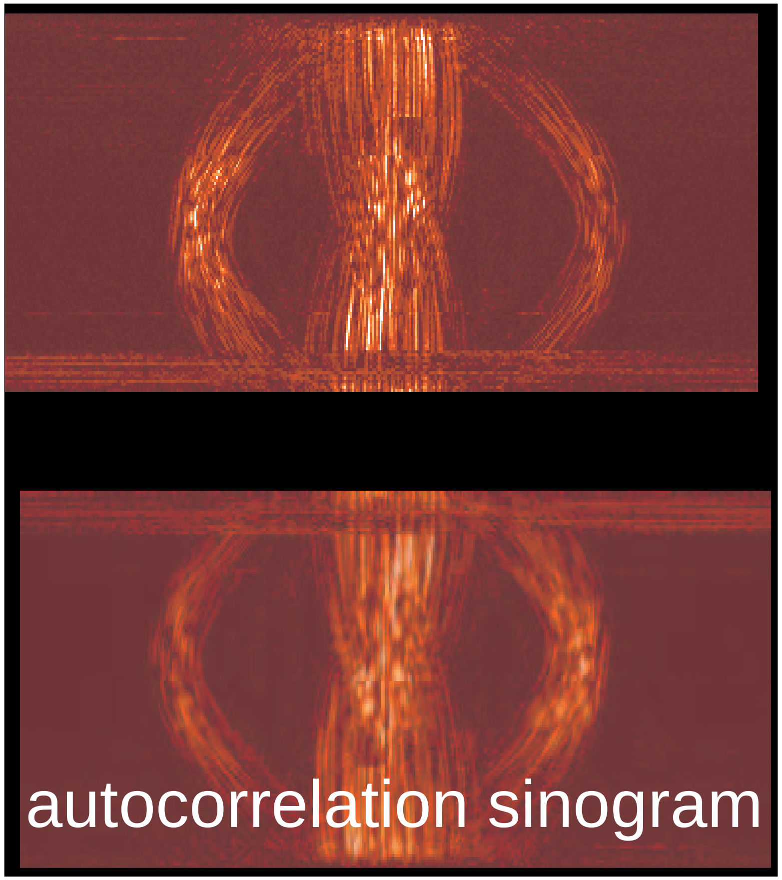


IFFT each patch

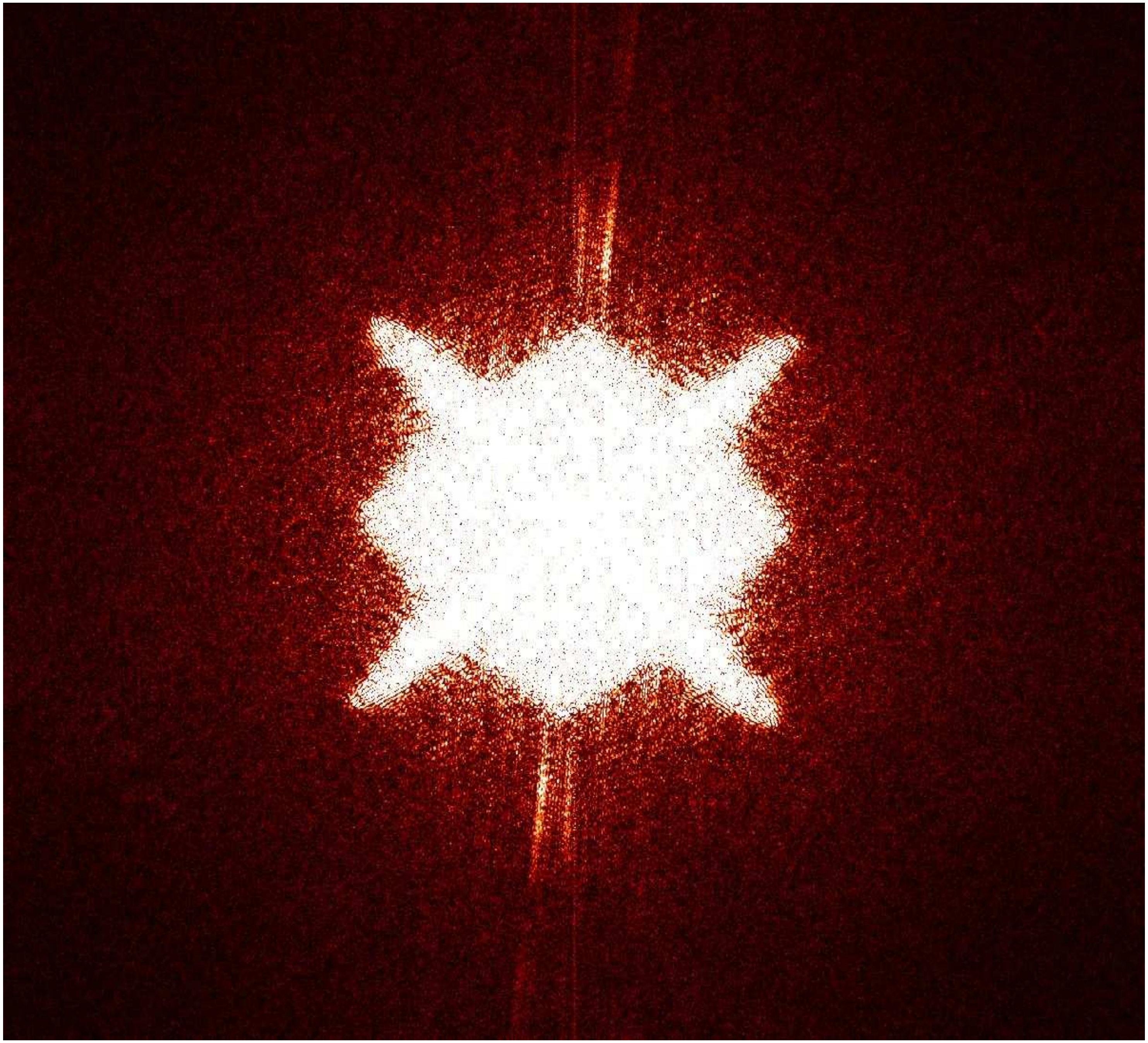
High pass filtered autocorrelation



Autocorrelation
(Fourier transform of diffraction intensity)

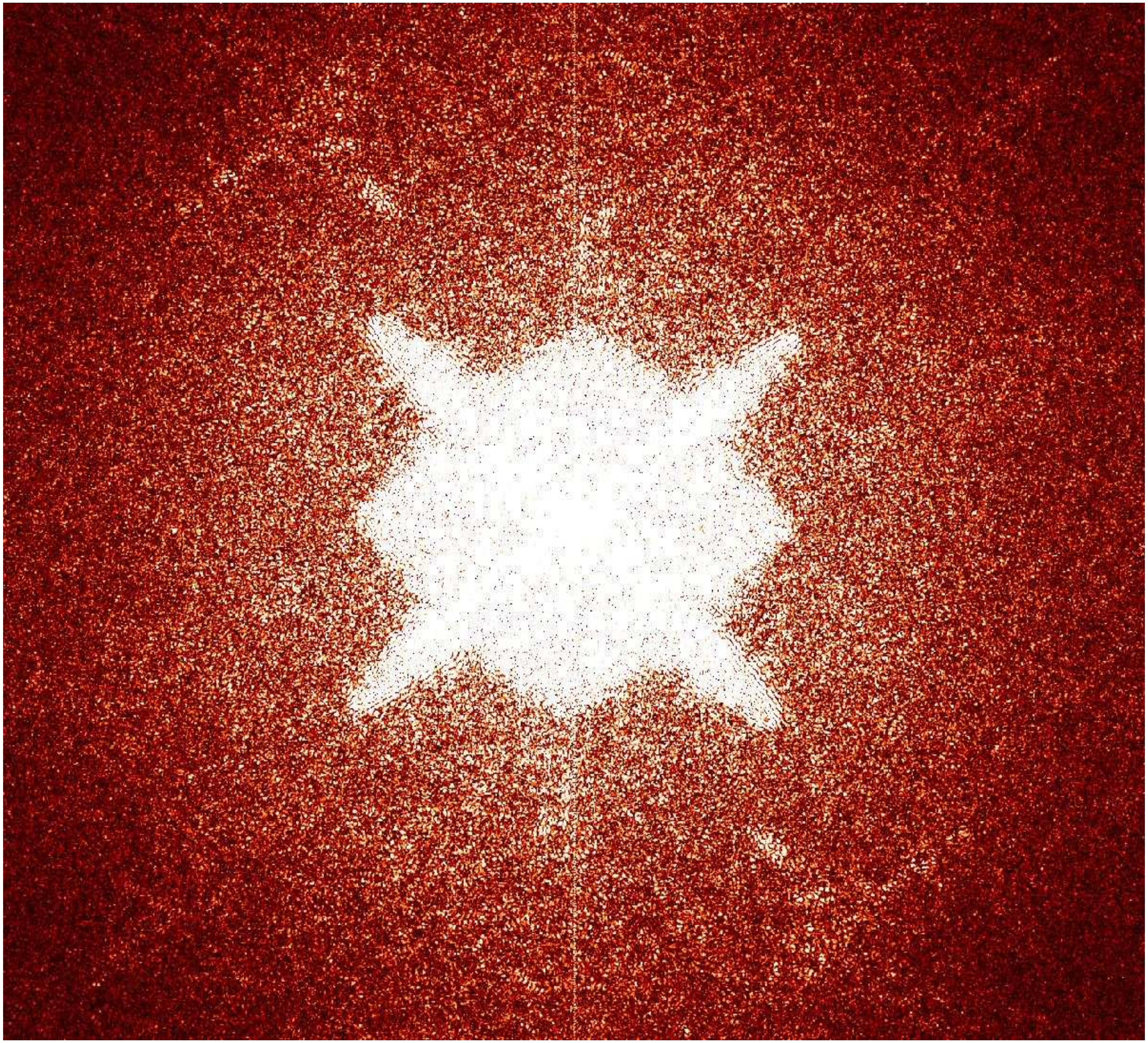


Inspection of the data



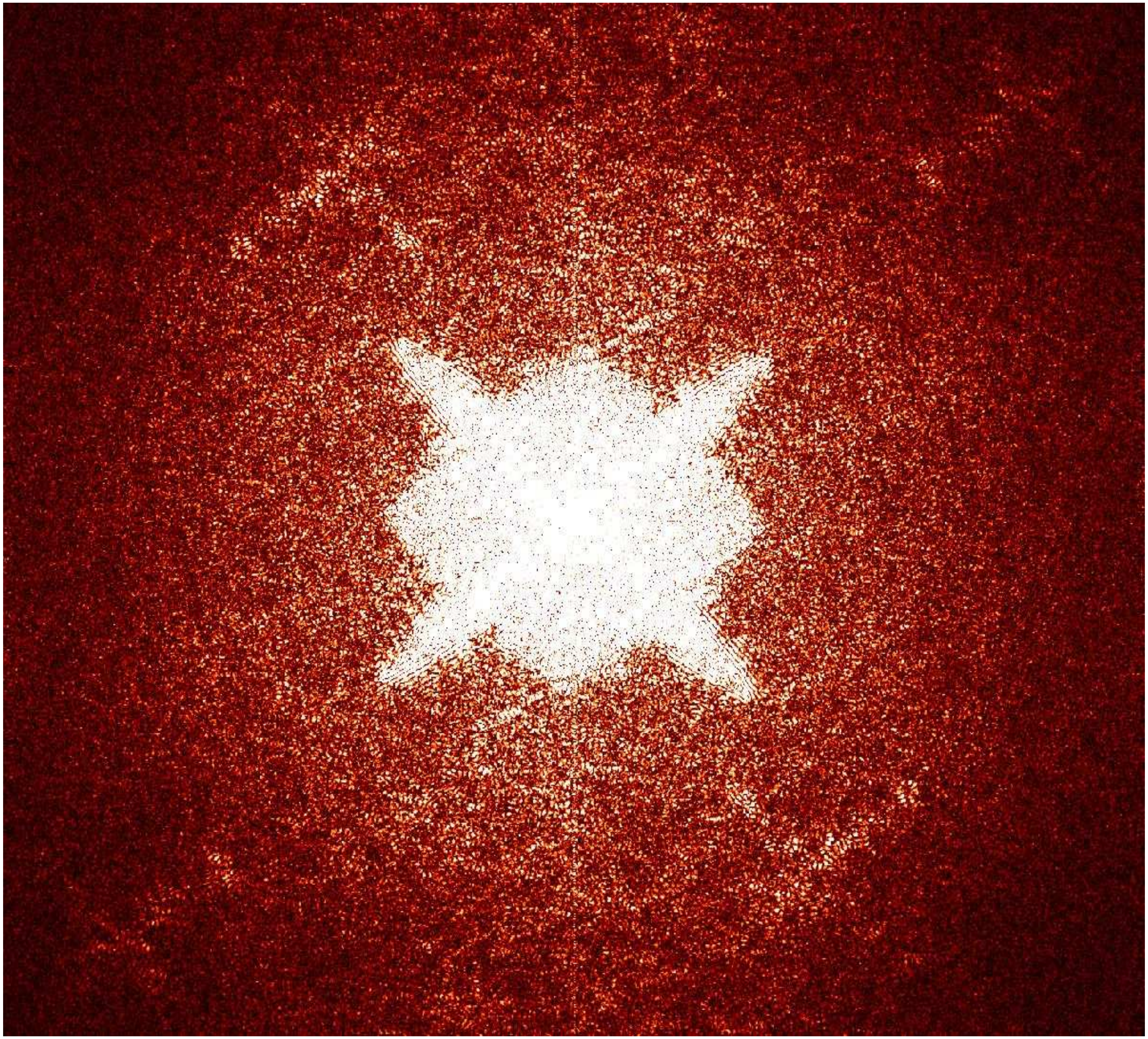
Calculate Autocorrelation function

Hologram



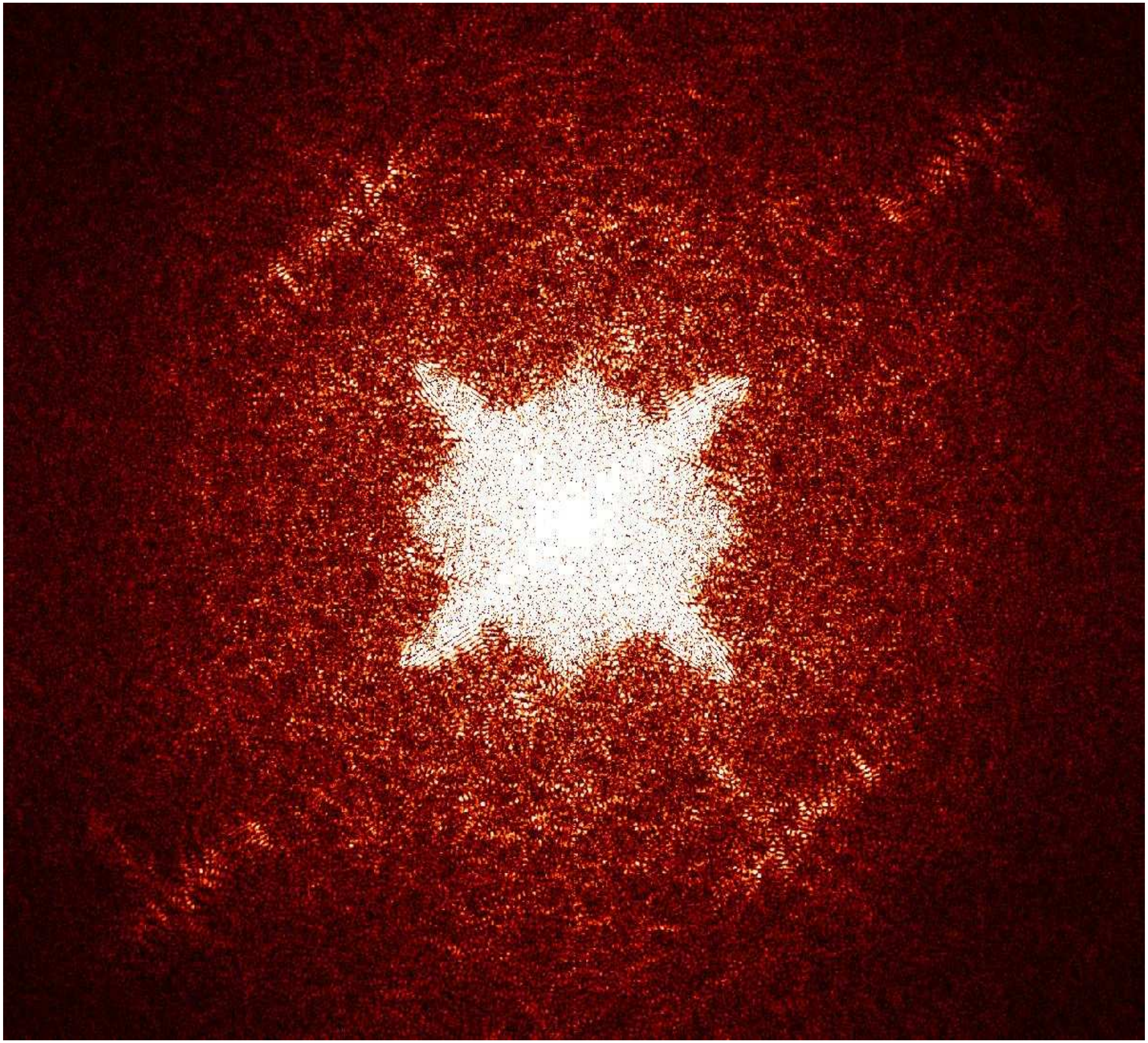
Increase illumination area

Hologram



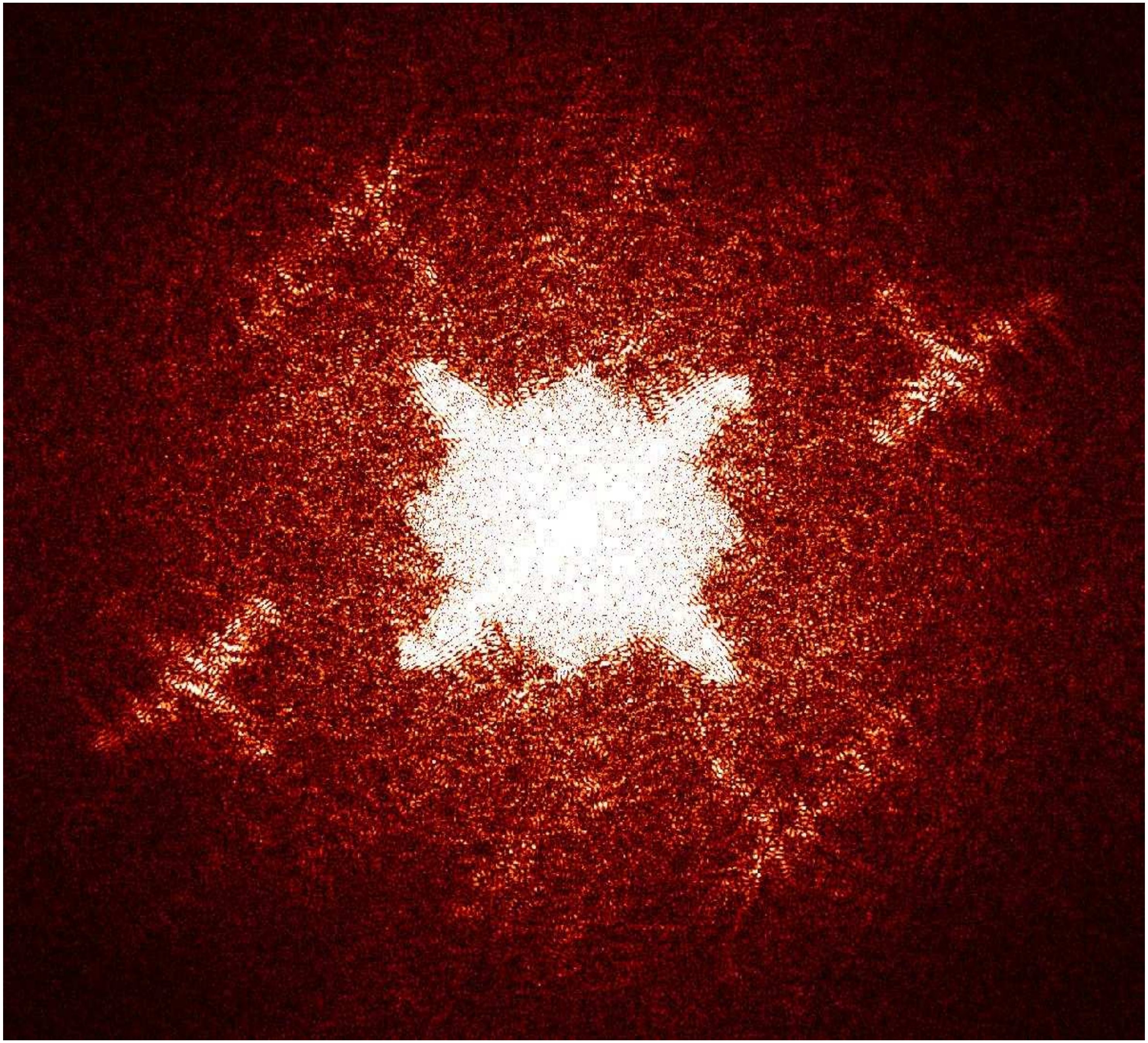
Increase detector distance

Hologram



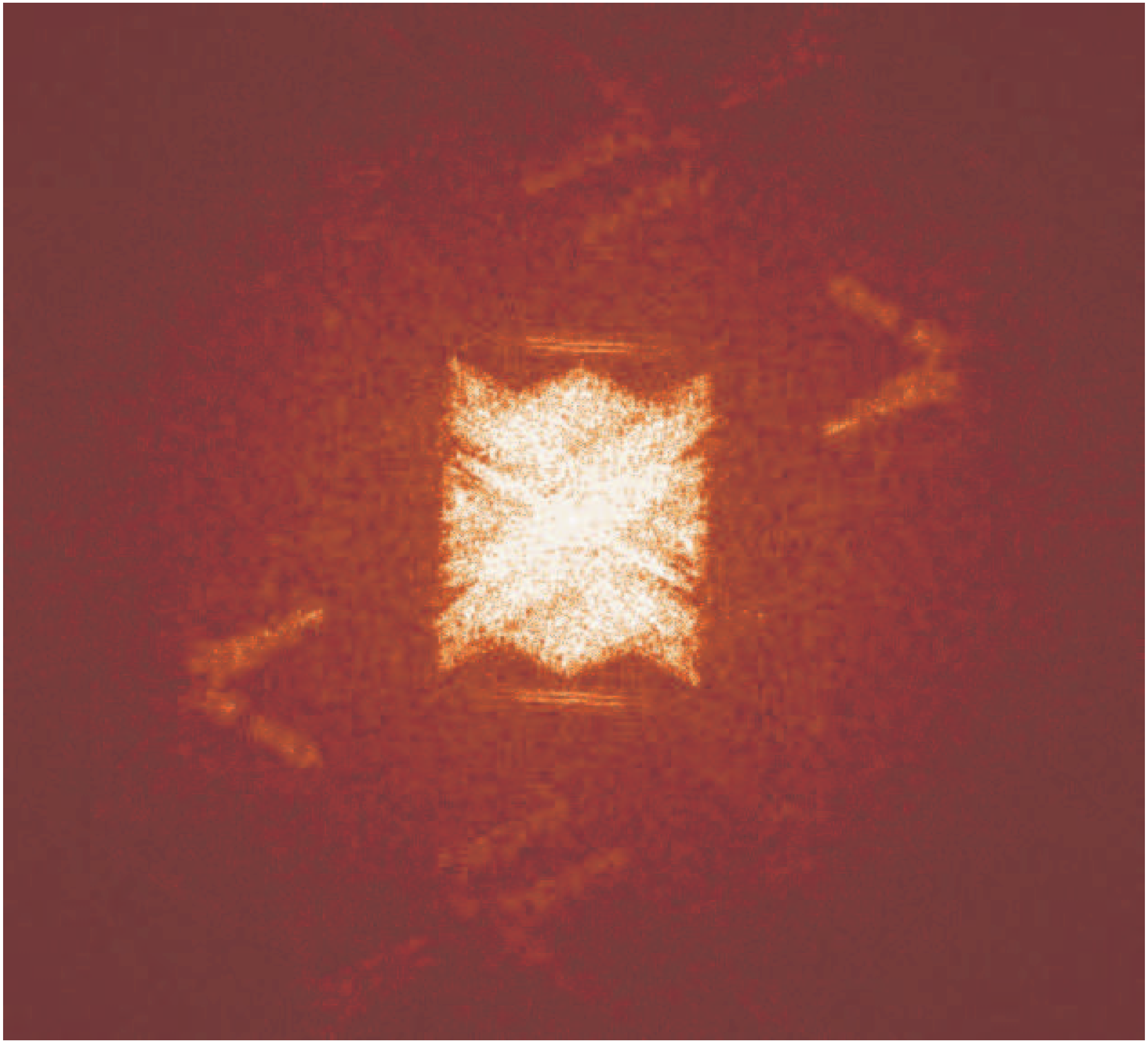
Increase detector distance

Hologram



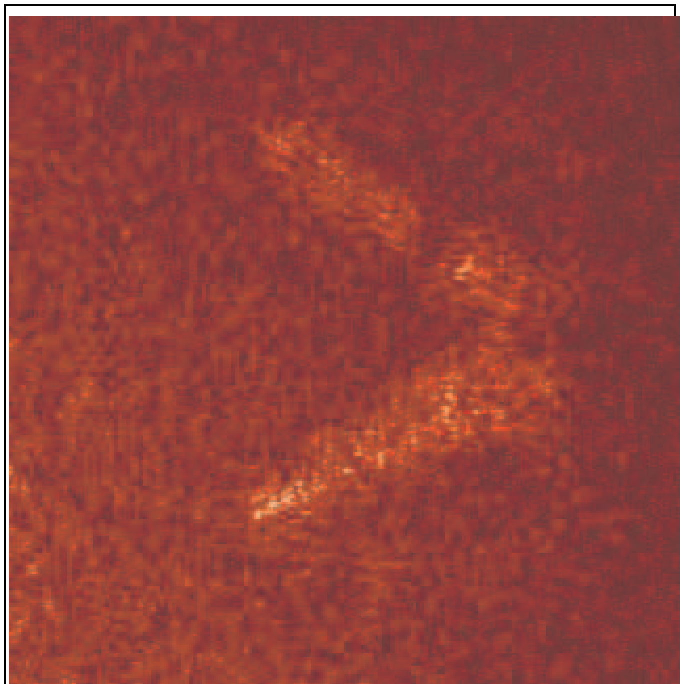
Move beam center to the side

Hologram



Rotate

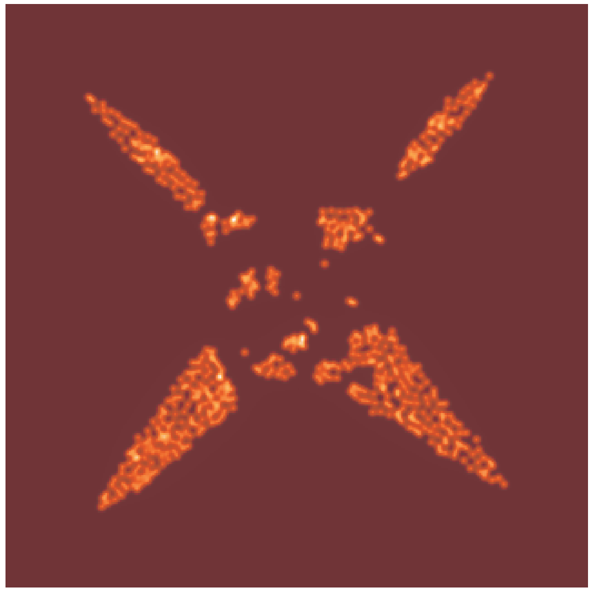
Resolution can be extended by deconvolution



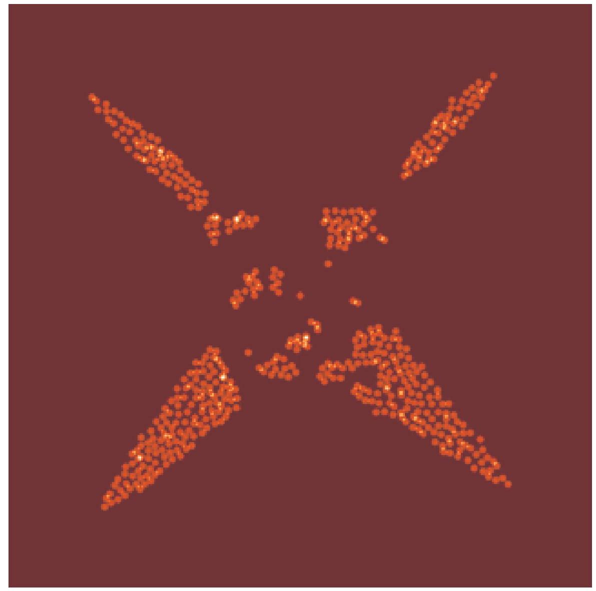
Low-resolution hologram image

The resolution is limited by the information in the diffraction pattern, not the size of the reference object. We can deconvolve if we know the reference object.

[arXiv:physics.optics/0405036]

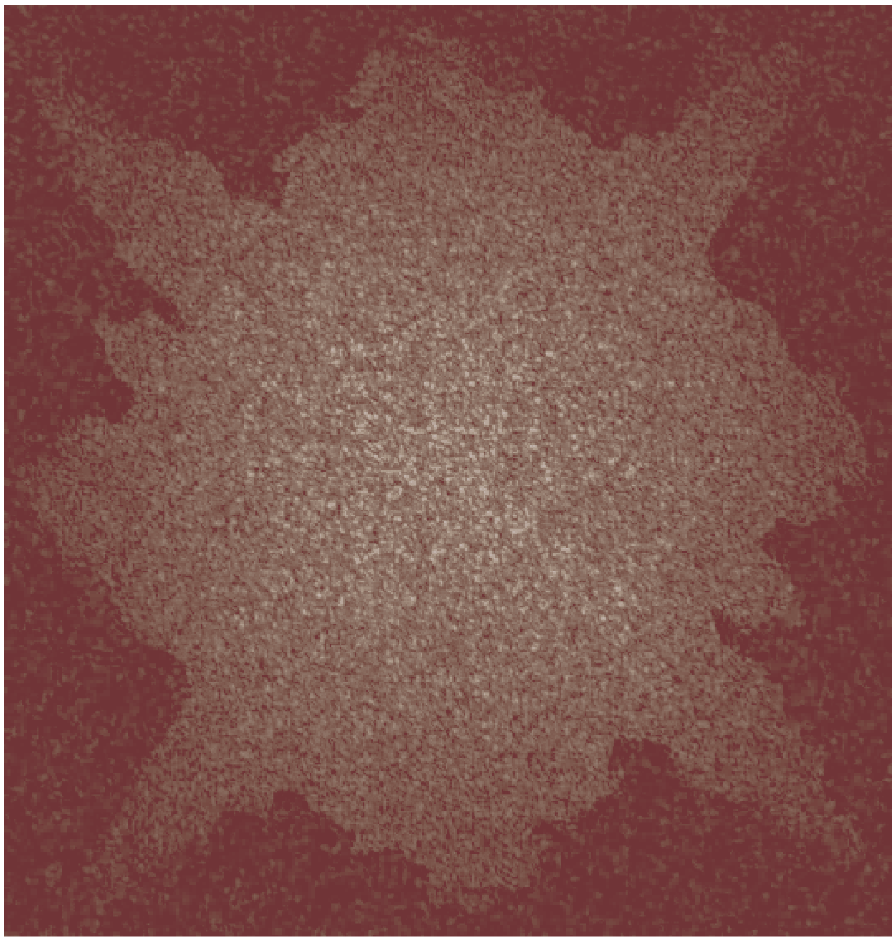


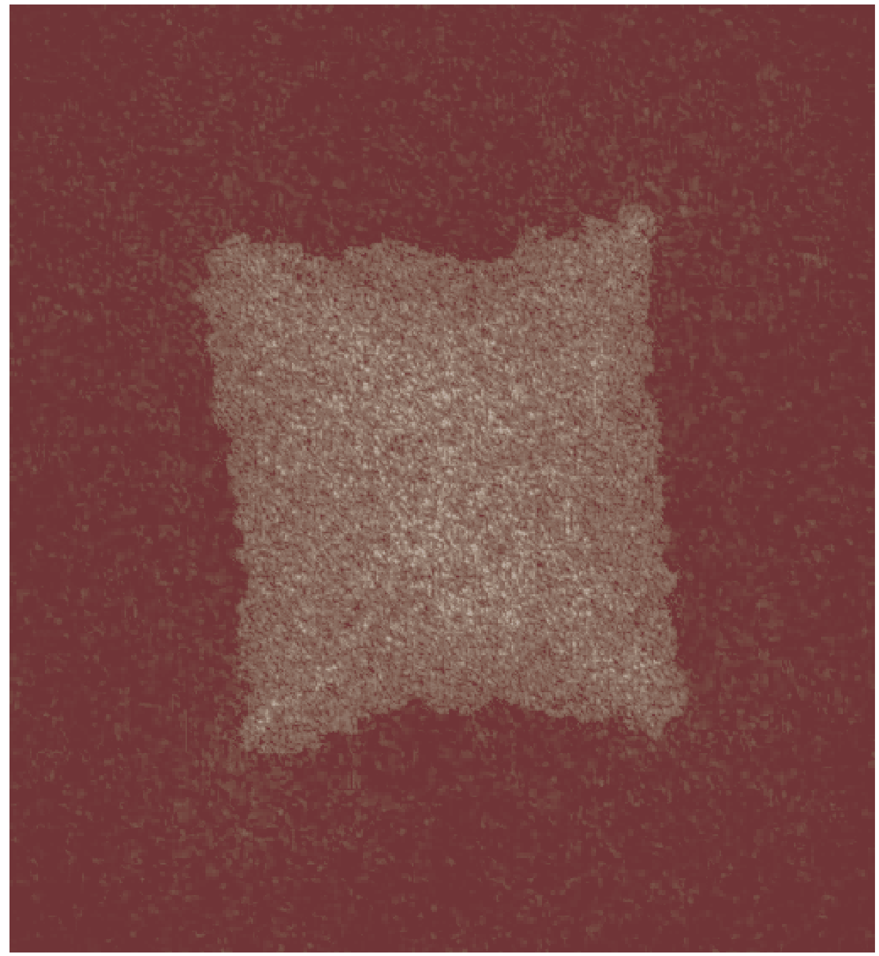
Simulated hologram image (50 nm reference object)



Simulated hologram image (deconvolved)

Shrinkwrap can reconstruct 2D views of 3D objects



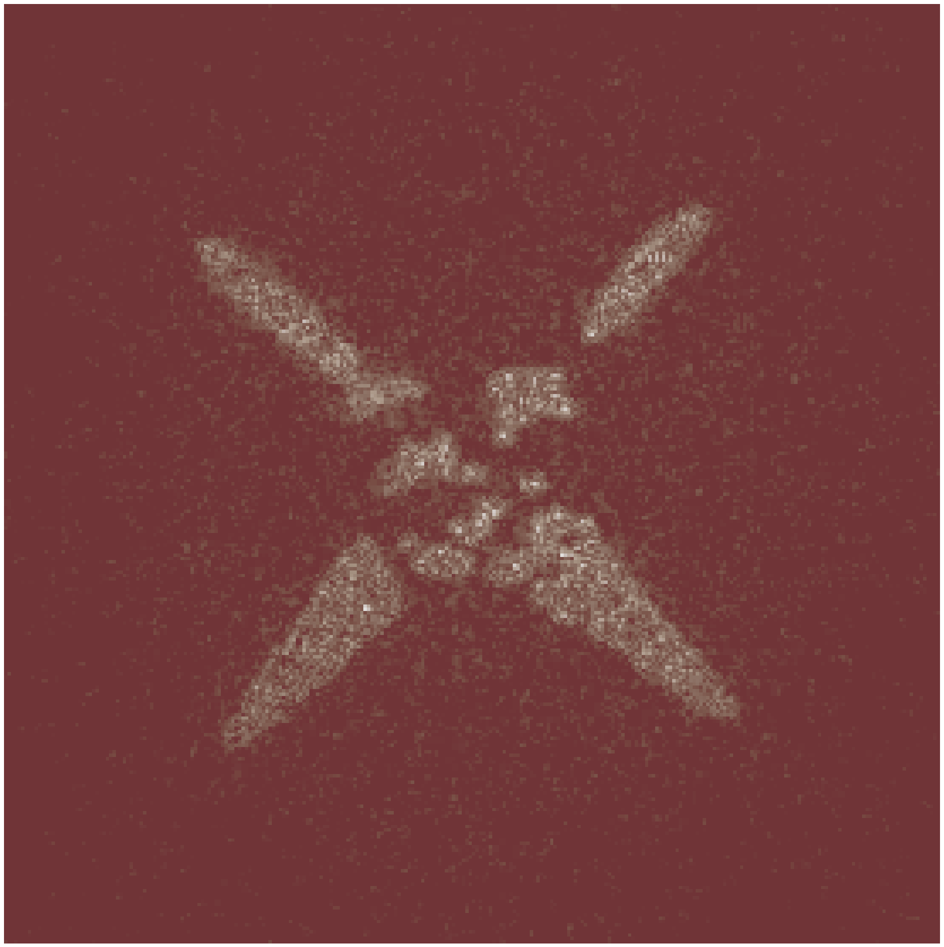


Pyramid orientation:

13 degrees rotation

28 degrees rotation

Multiple view reconstructions



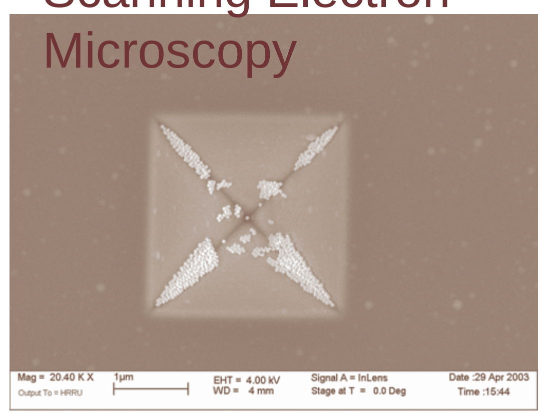
Tomography
(from simulation)

3D-Phase
retrieval

3D- $(1K)^3$ FFT
(109 unknowns)

We need access to the big LLNL computers

Scanning Electron Microscopy



Many error metrics
- real space error (stuff outside support)
- reciprocal space error, (R_{fact})
- difference between reconstructions

Reciprocal space error

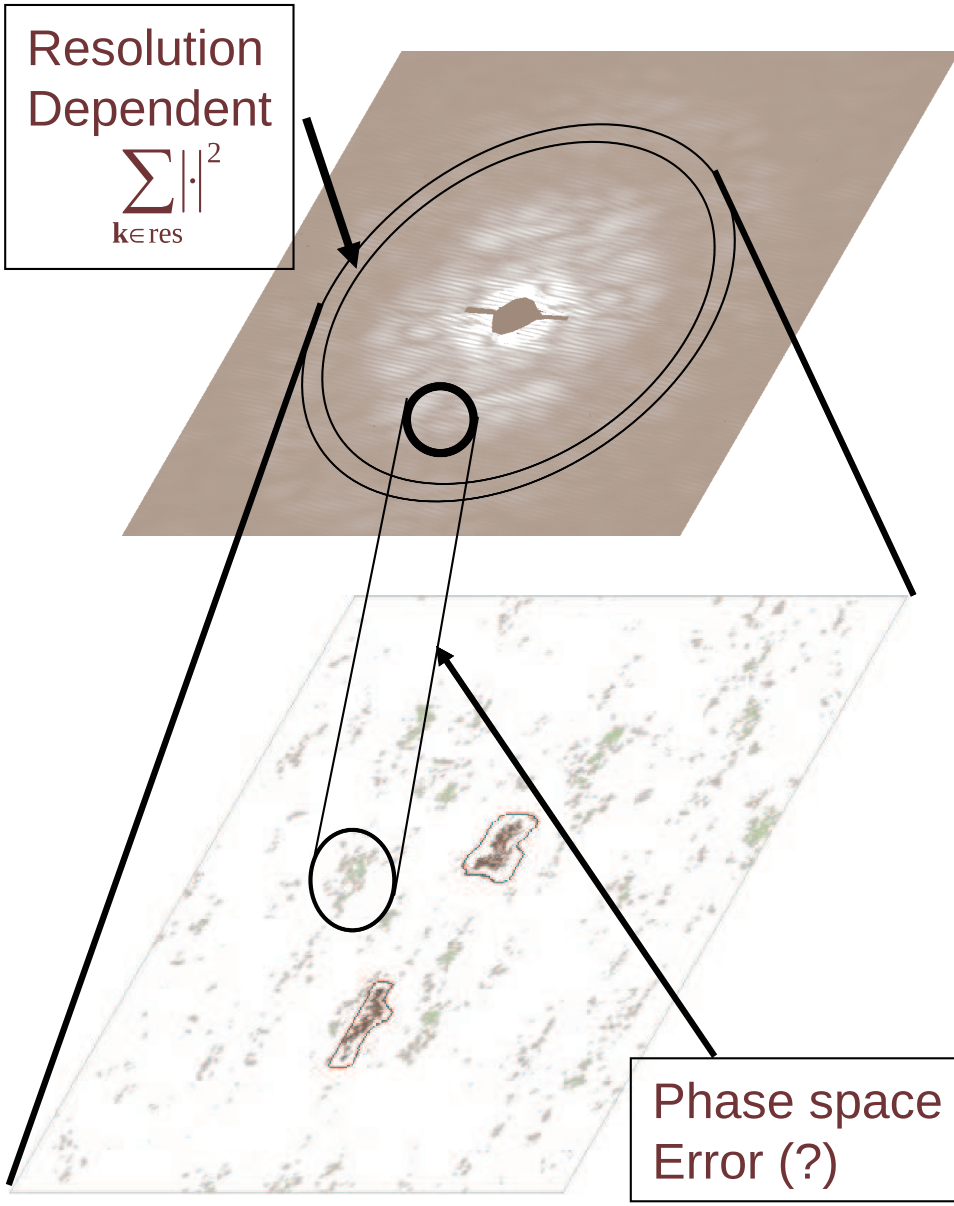
$$R^n = \frac{\sum_{\mathbf{k}} \left| \left|\tilde{\rho}_{obs}(\mathbf{k})\right| - \left|\tilde{\rho}^n(\mathbf{k})\right| \right|^2}{\sum_{\mathbf{k}} \left|\tilde{\rho}_{obs}(\mathbf{k})\right|^2}$$

Real space error

$$\varepsilon_{\mathrm{s}}^n = \frac{\sum_{\mathbf{x}} \left|\mathbf{P}_{\mathrm{s}}\rho^n(\mathbf{x}) - \rho^n(\mathbf{x})\right|^2}{\sum_{\mathbf{x}} \left|\mathbf{P}_{\mathrm{s}}\rho^n(\mathbf{x})\right|^2}$$

Error between reconstructions

$$\varepsilon^{1,2} = \frac{\left\|\rho^1 - \rho^2\right\|^2}{\left\|\frac{1}{2}\left(\rho^1 + \rho^2\right)\right\|^2}$$



In the language of projectors and sets

Parseval

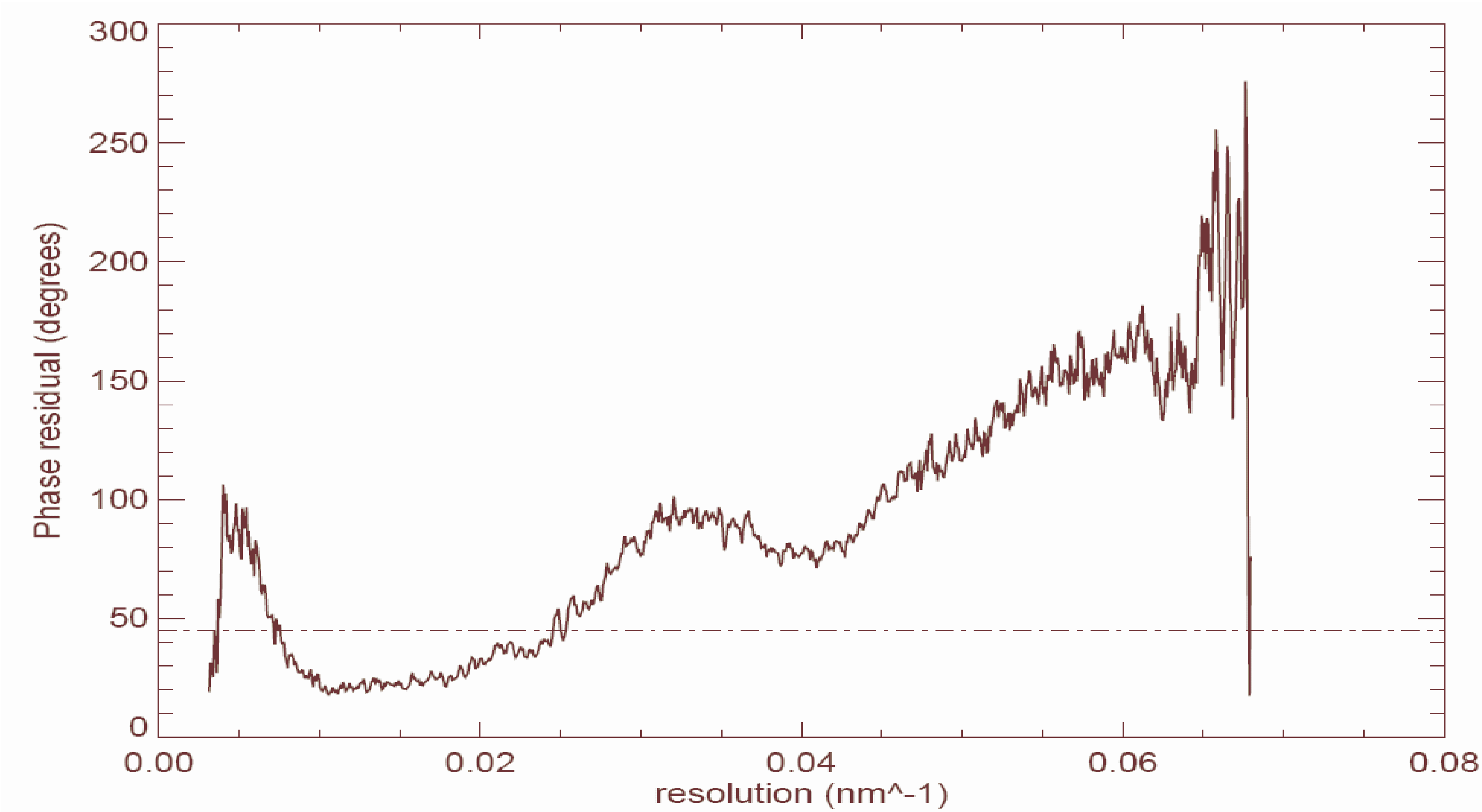
$$\|\cdot\|^2 = \sum_{\mathbf{x}} |\cdot|^2 = \frac{1}{N}\sum_{\mathbf{k}} |\tilde{\cdot}|^2$$

Constraints errors

$$\varepsilon_{\mathbf{m}}^{\mathrm{n}} = \frac{\left\|\mathbf{P}_{\mathbf{m}}\rho^n - \rho^n\right\|^2}{\left\|\mathbf{P}_{\mathbf{m}}\rho^n\right\|^2}$$

$$\varepsilon_{\mathrm{s}}^{\mathrm{n}} = \frac{\left\|\mathbf{P}_{\mathrm{s}}\rho^n - \rho^n\right\|^2}{\left\|\mathbf{P}_{\mathrm{s}}\rho^n\right\|^2}$$

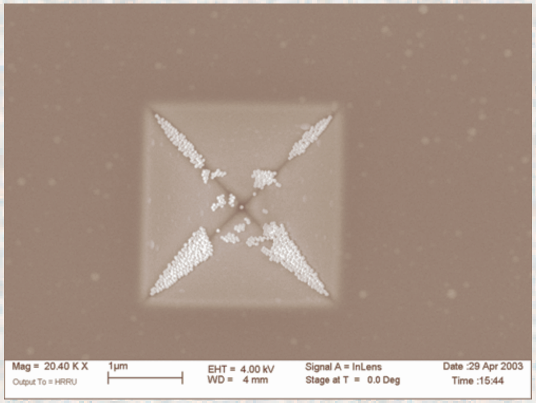
Pyramid data



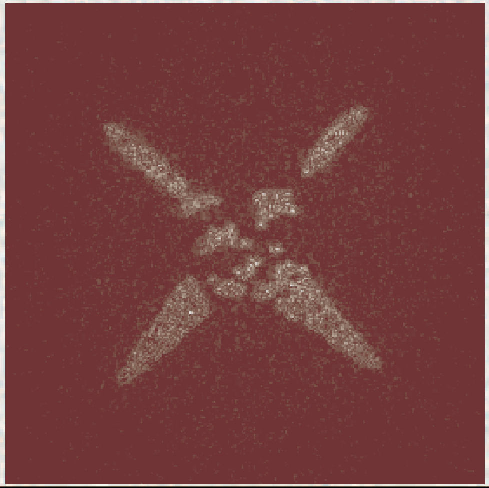
30 seconds exposure

Summary

Scanning Electron Microscopy



2D-Phase retrieval With Shrink-wrap



Tomography (from simulation)

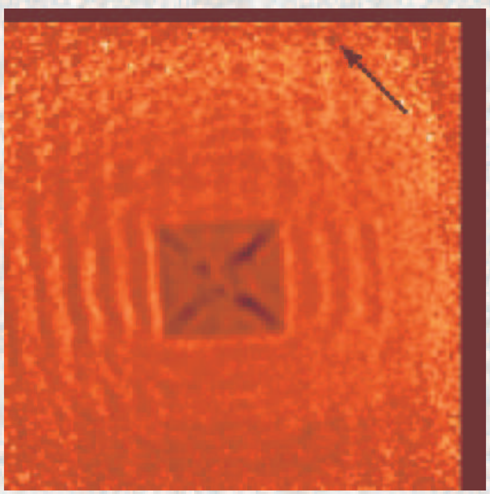
3D-Phase retrieval

3D- (1K)^3 FFT (109 unknowns)

We need access to the big (LLNL) computers

X-ray microscope

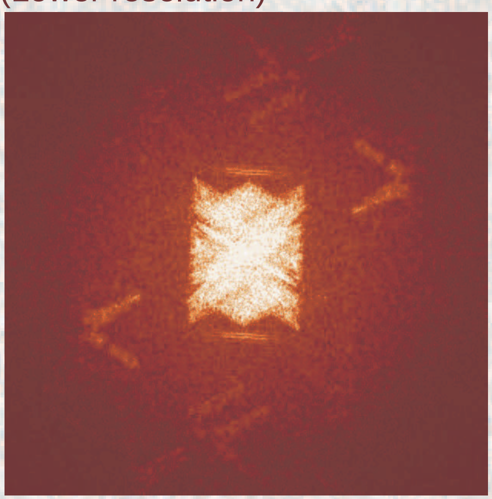
The isolated ball acts as a reference for a **Hologram**



Hologram

•Larger illuminatioan area (Weaker intensity)

•Larger camera distance (Lower resolution)



Algorithms being tested:

•Conjugate-gradient based SPEDEN:

Reconstructing single particles from their diffraction patterns, Stefan P. Hau-Riege, Hanna Szöke, Henry N. Chapman, Abraham Szöke, Stefano Marchesini, Alexander Noy, et al. [arXiv:physics.optics/0403091]

•"Direct Methods"

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