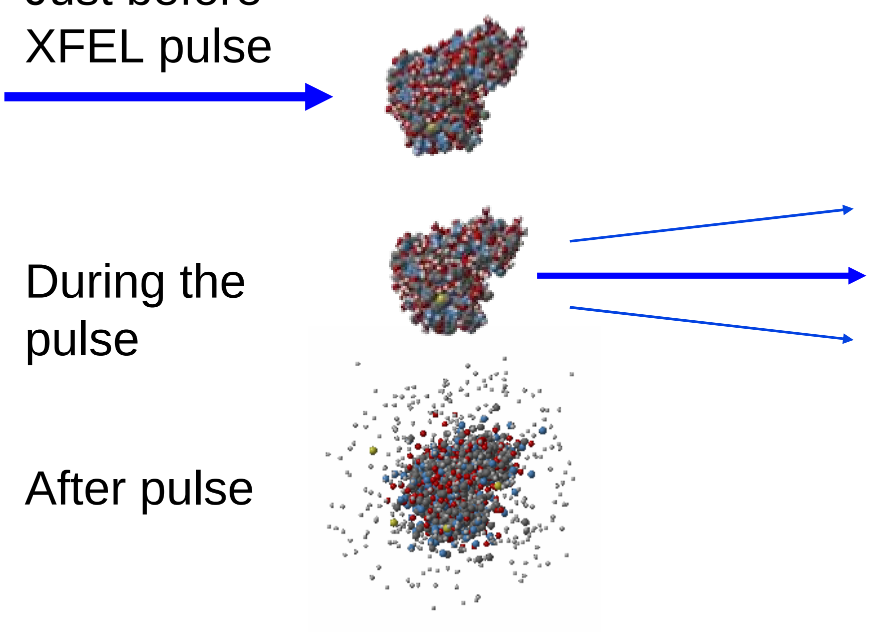
Ultrafast Coherent Diffraction Imaging with a Soft X-Ray Free-Electron Laser

Henry Chapman, LLNL

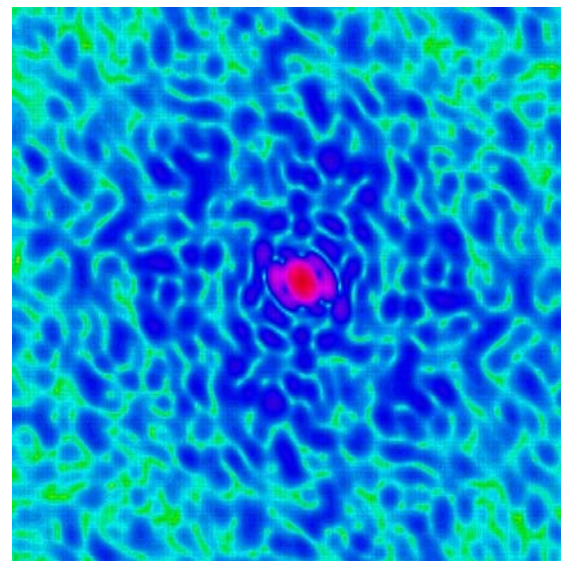
Just before XFEL pulse

During the pulse

After pulse



Diffraction pattern



CBST
CENTER for BIOPHOTONICS SCIENCE and TECHNOLOGY

FEL 2006, 1st September

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Acknowledgements

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Uppsala: Janos Hajdu, Gösta Huldt, Carl Caleman, Magnus Bergh, Nicusor Timeneau, David van der Spoel, Florian Burmeister, Marvin Seibert

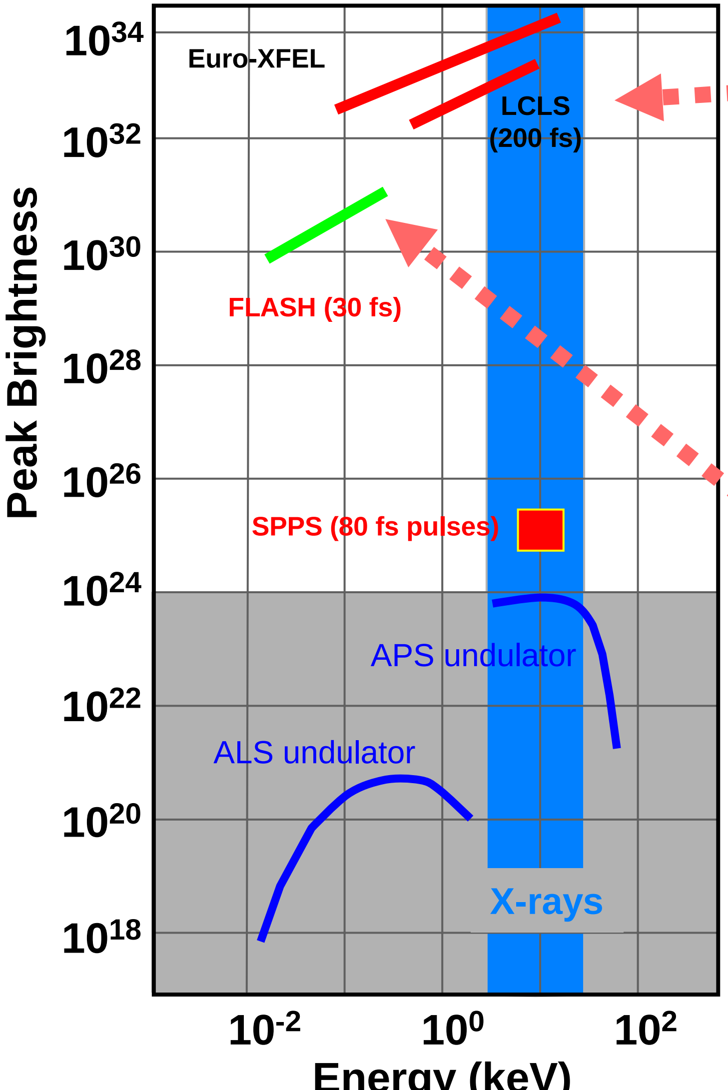
UC Davis: David Shapiro

SLAC: Keith Hodgson, Sebastien Boutet

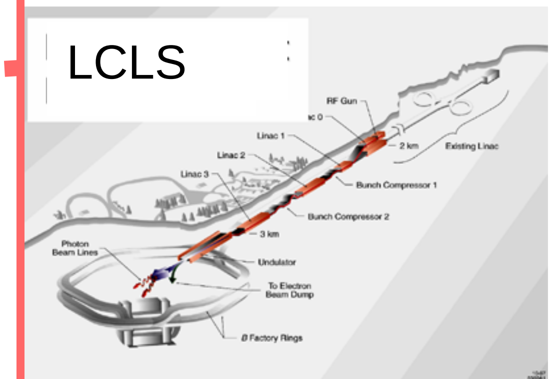
DESY: Thomas Tschentscher, Elke Plönjes, Marion Kulhman, Rolf Treusch, Stefan Dusterer, Jochen Schneider

TU Berlin: Thomas Möller, Christof Bostedt, Matthias Hoener

We are entering a new era in x-ray science



APS=Advanced Photon Source (ANL)
ALS=Advanced Light Source (LBNL)



operational 2009

8 keV, 200 fs, 10^{12} photons

Linac Coherent Light Source, SLAC, Stanford

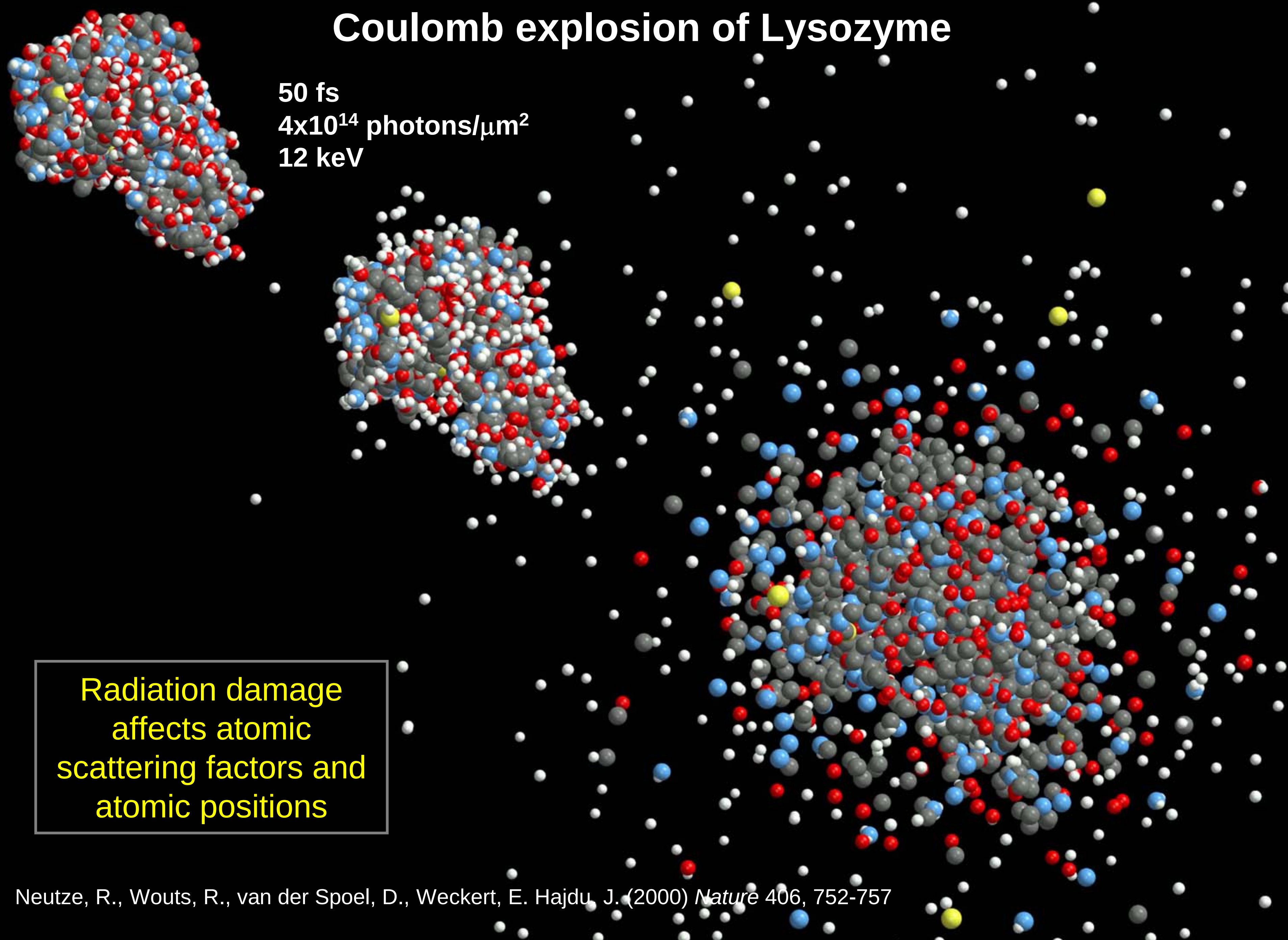
operational now

Current: 38 eV, 30 fs

500 eV, 80 fs, 10^{13} photons

Tesla Test Facility DESY, Hamburg

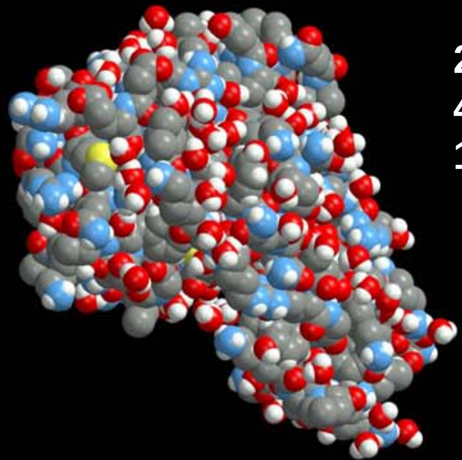
Coulomb explosion of Lysozyme

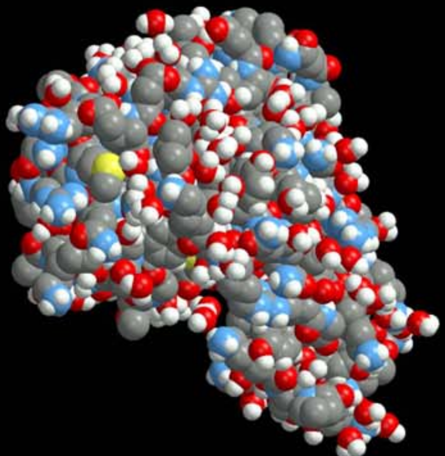


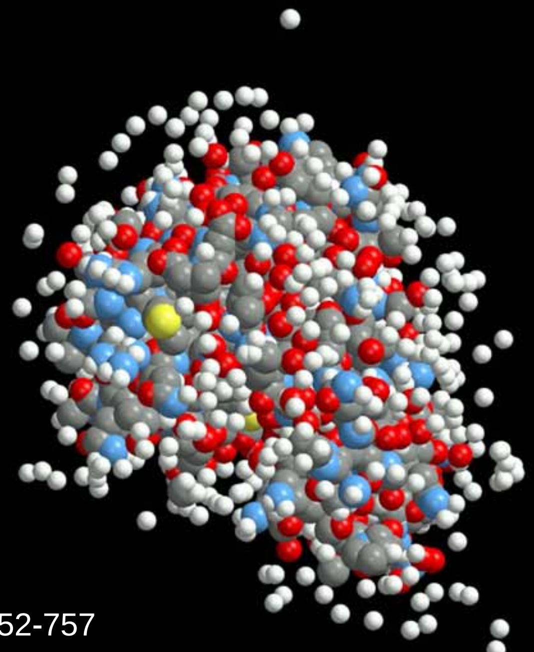
Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. Hajdu, J. (2000) *Nature* 406, 752-757

Coulomb explosion of Lysozyme

20 fs
4×10^{14} photons/μm^2
12 keV





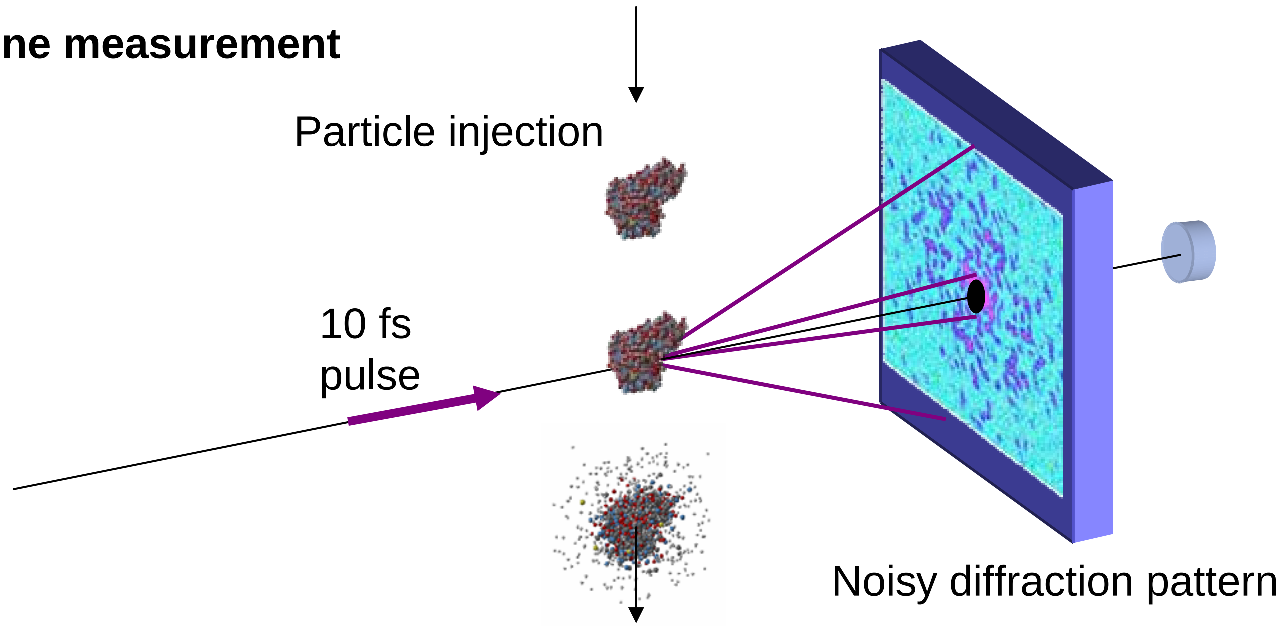


Radiation damage affects atomic positions and atomic scattering factors

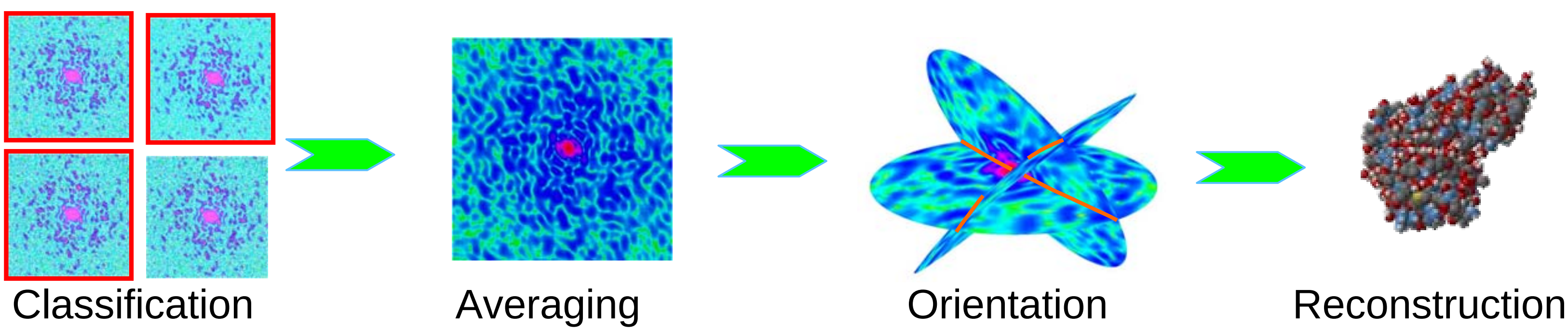
Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. Hajdu, J. (2000) *Nature* 406, 752-757

X-ray free-electron lases may enable atomic-resolution imaging of biological macromolecules

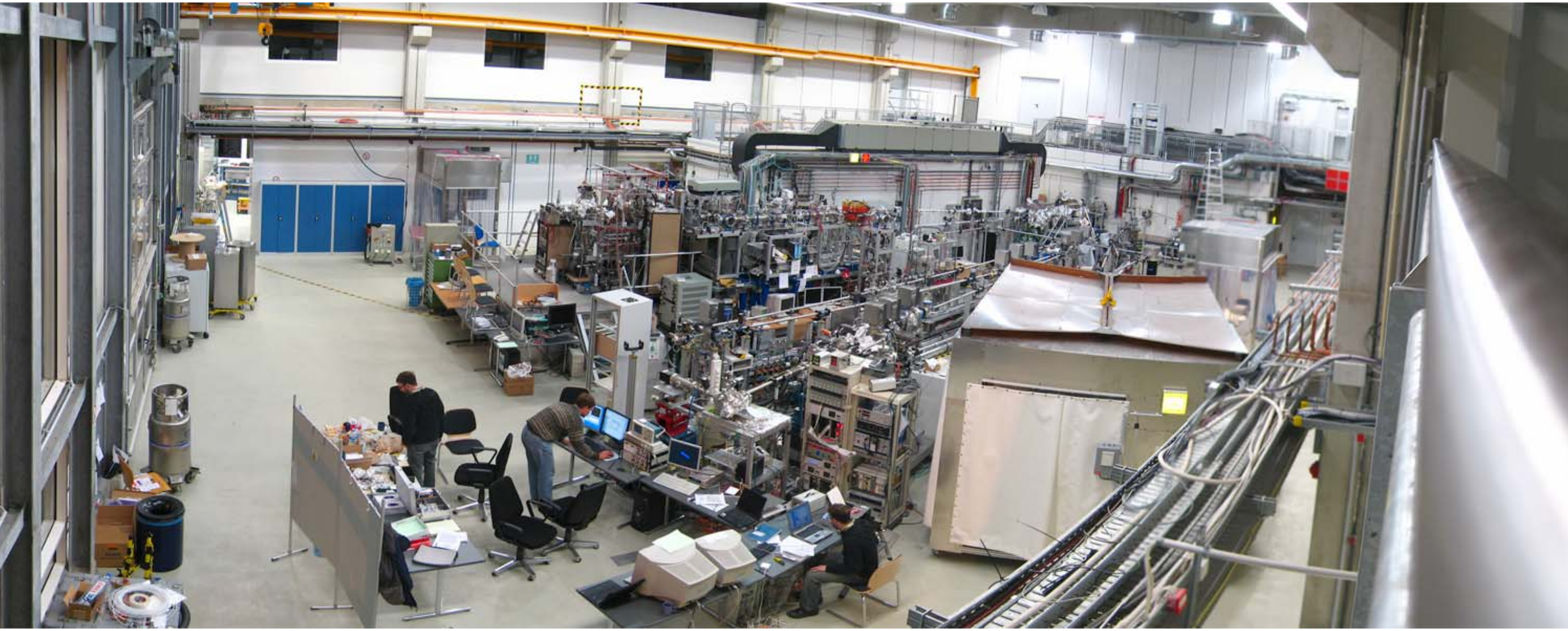
One pulse, one measurement



Combine 10^5-10^7 measurements



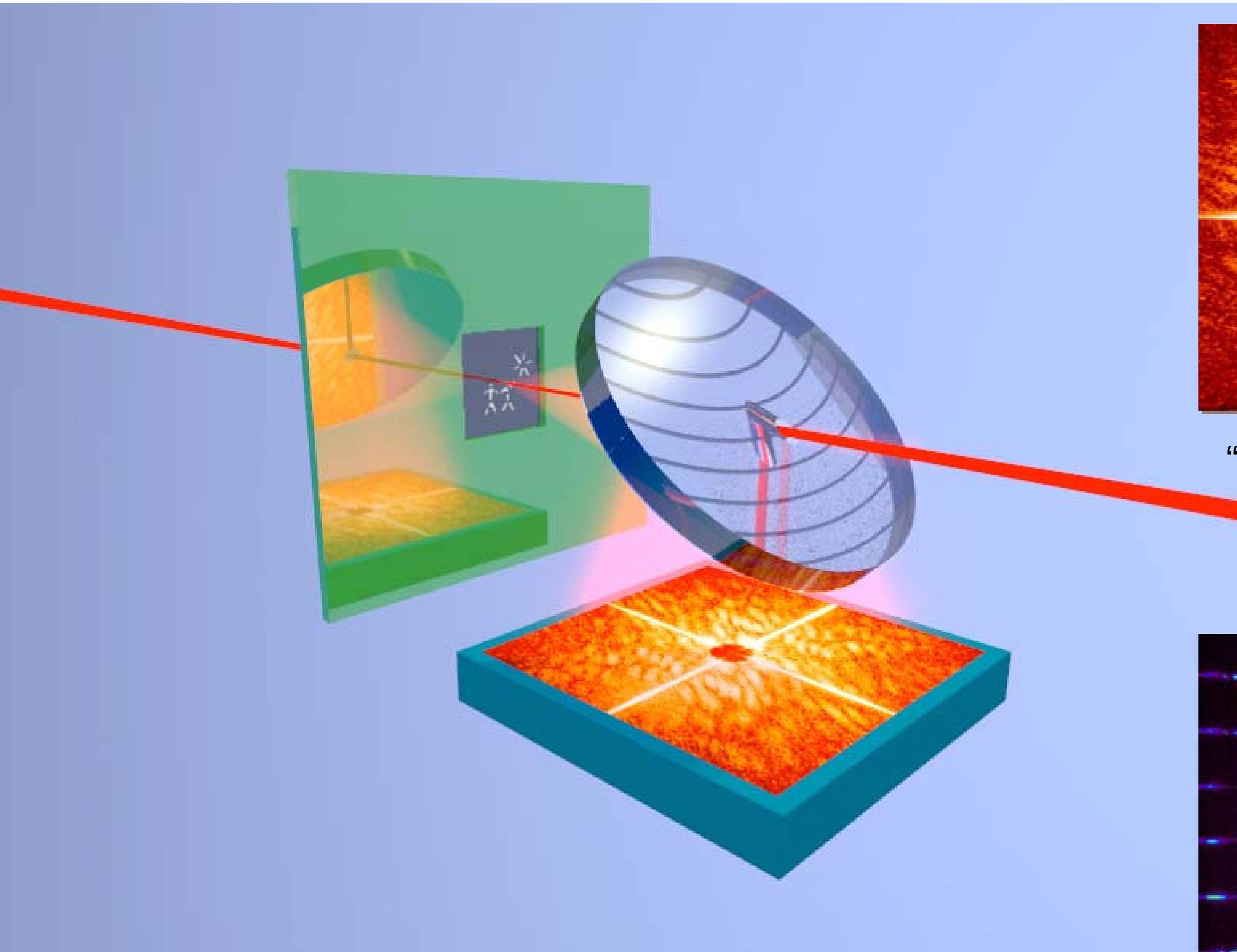
We have carried out experiments at the first soft-X-ray FEL in the world

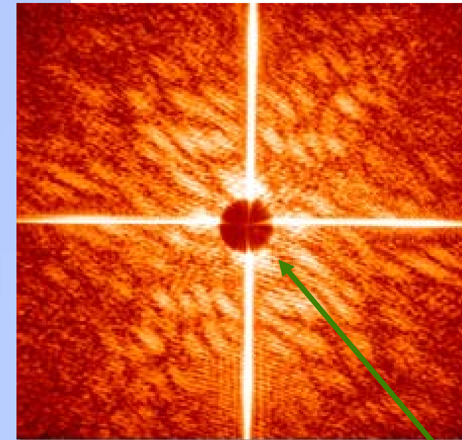


FLASH at HASYLAB, DESY

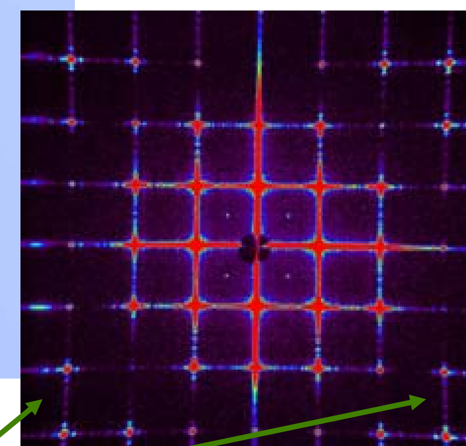
- User facility, FEL radiation to 6 nm wavelength
- Initial FEL Operation August 2005 at 32 nm and <30 fs pulses, 10^{13} photons

Our diffraction camera can measure forward scattering close to the direct soft-X-ray FEL beam





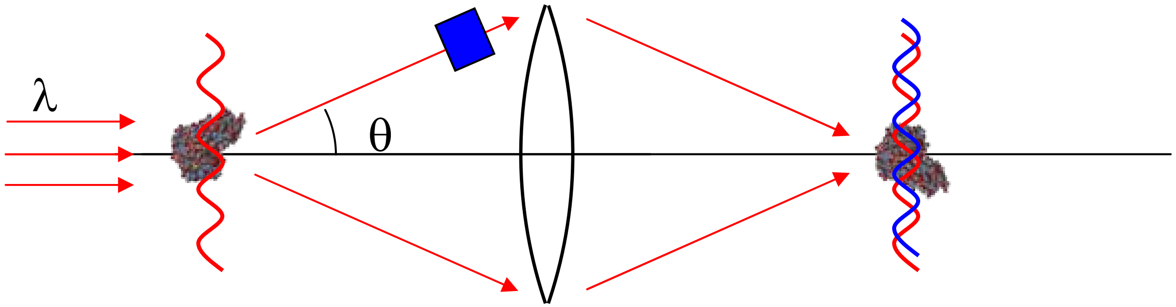
“Soft edge” prevents any scatter from the hole



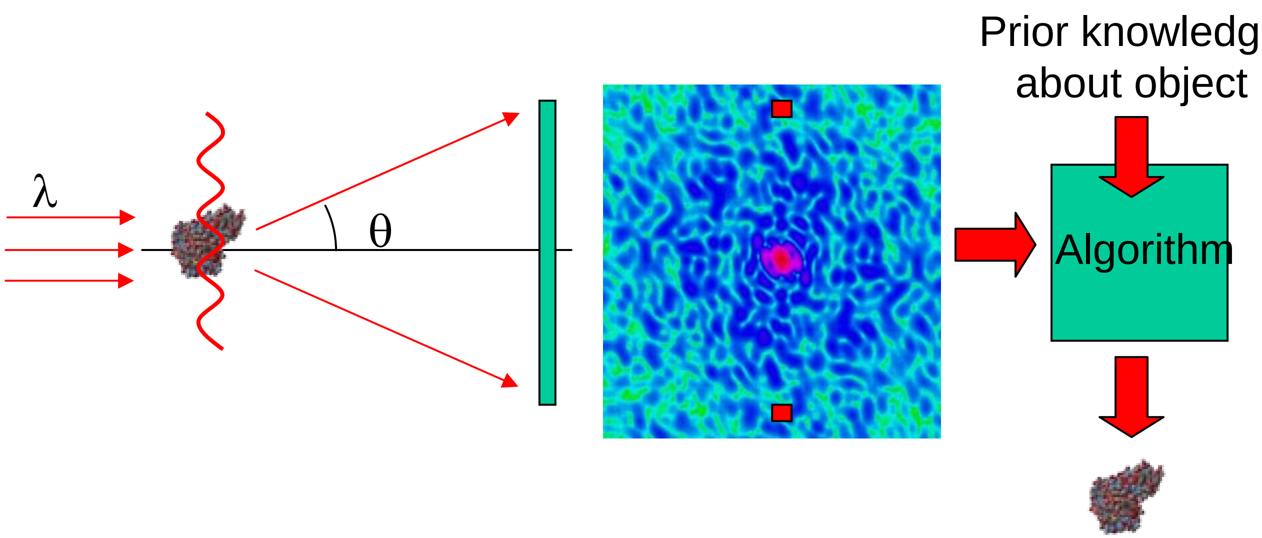
Multilayer reflectivity is uniform across the 30° to 60° gradient

Coherent diffractive imaging is lensless

Use a computer to phase the scattered light, rather than a lens



A lens recombines the scattered rays with correct phases to give the image

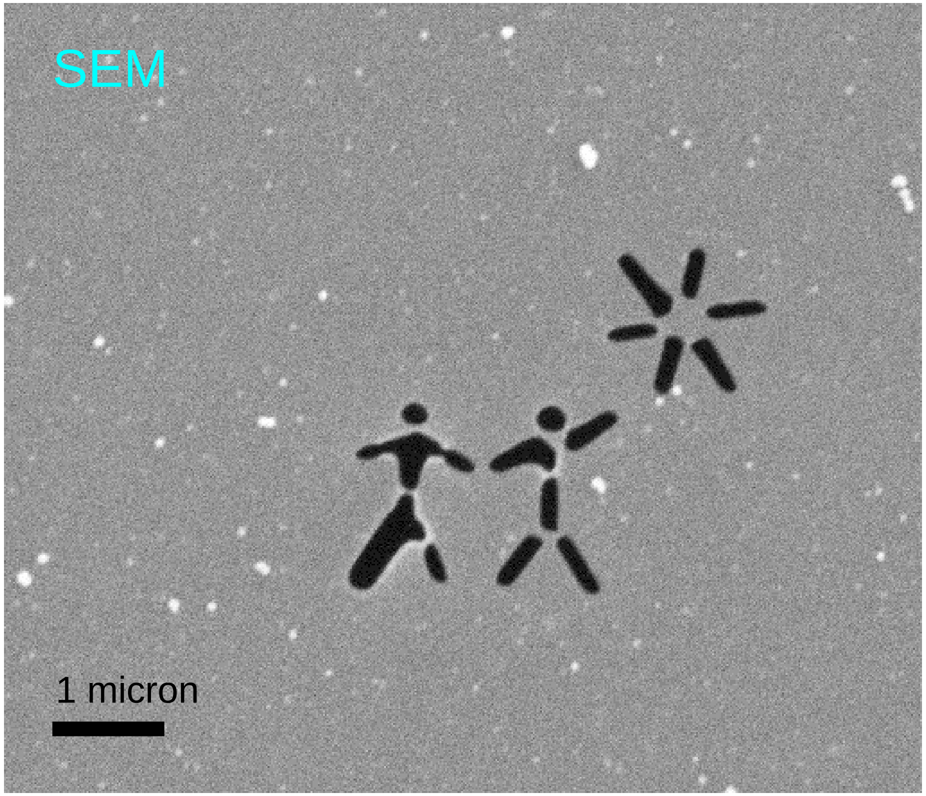


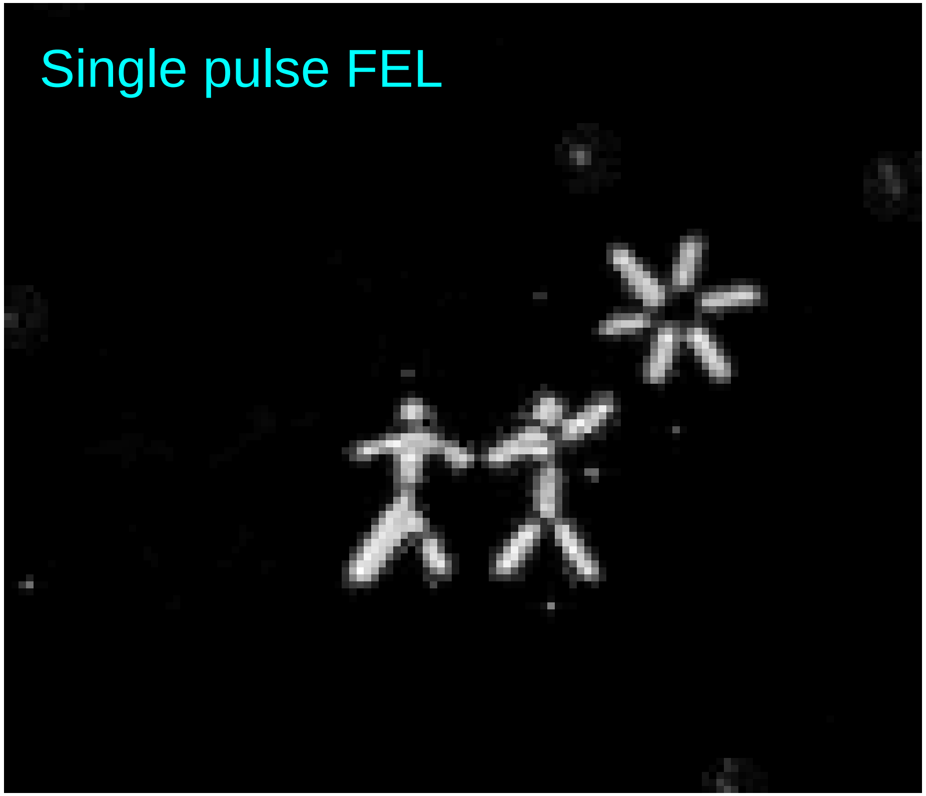
An algorithm finds the phases that are consistent with measurements and prior knowledge

Resolution: $\delta = \lambda / \sin\theta$

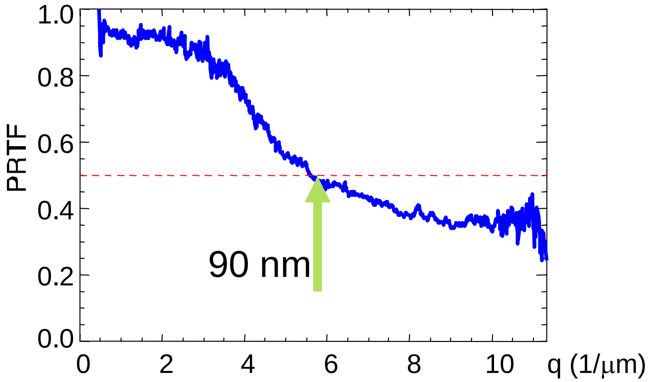
First demonstration with X-rays: John Miao,
P. Charalambous, J. Kirz and D. Sayre, Nature **400** (1999)

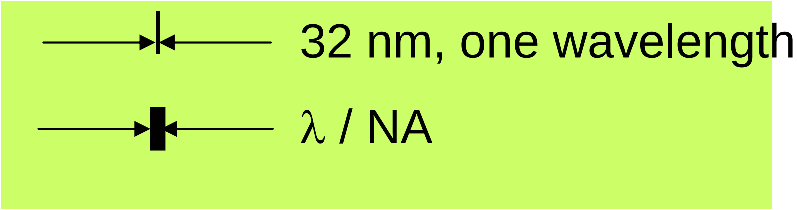
The reconstruction is carried out to the diffraction limit of the 0.26 NA detector





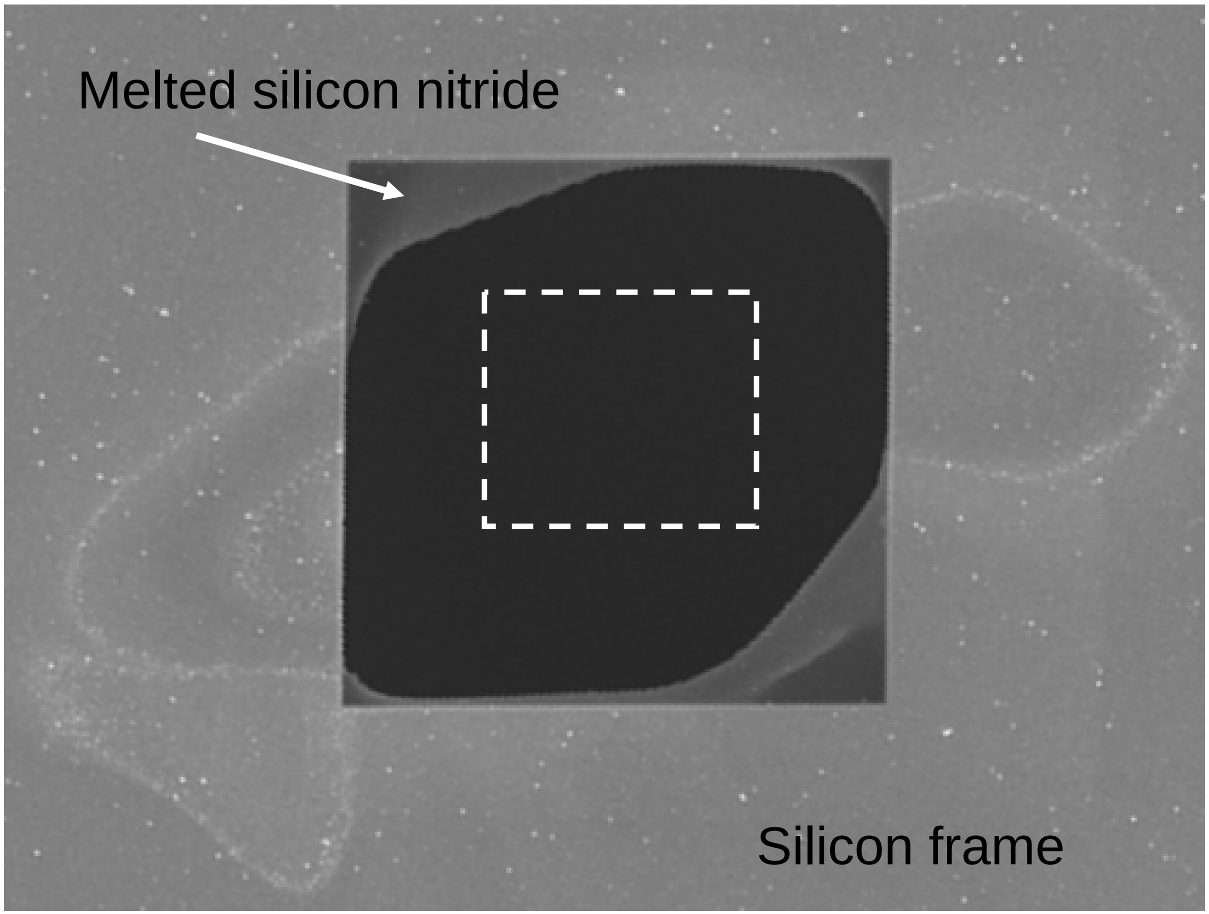
Phase-retrieval transfer function gives an estimate of the resolution of the reconstructed image

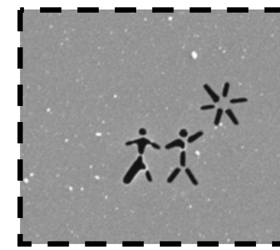




The sample is quite damaged by the FEL pulses

FIB “cowboy” sample after FEL exposure

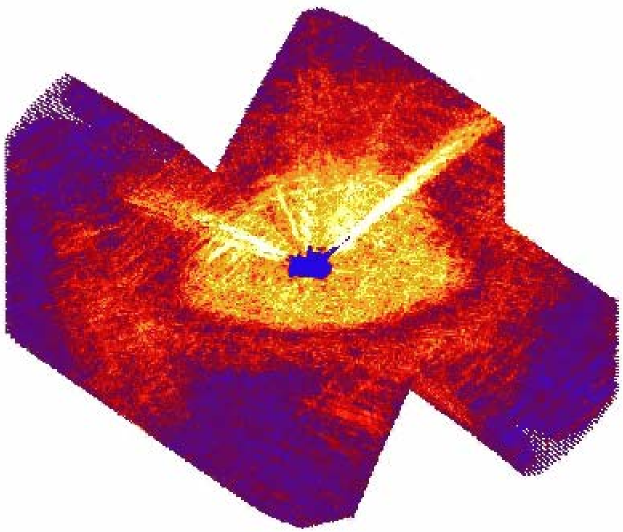




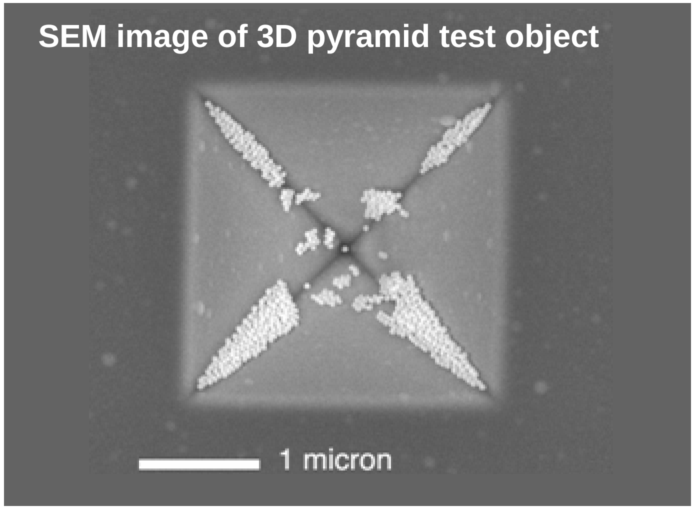
before

10 micron

We have performed full 3D X-ray imaging of non-crystalline material at 10 nm resolution

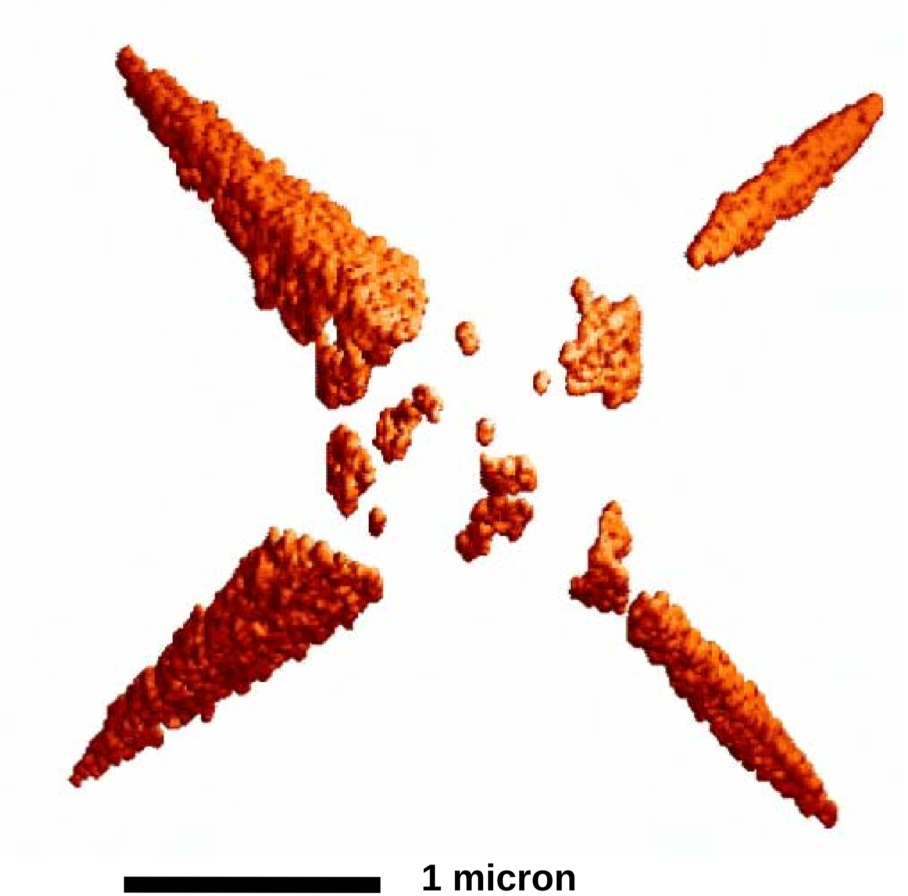


Coherent X-ray diffraction data, rotating the sample -70 to +70 degrees (5×10^8 data points)



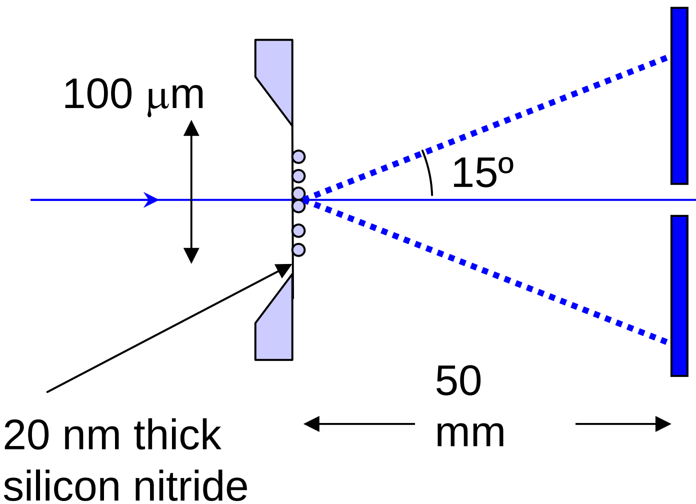
Coherent X-ray diffraction data λ =1.6 nm, from a sample of 50-nm gold spheres arranged on a pyramid

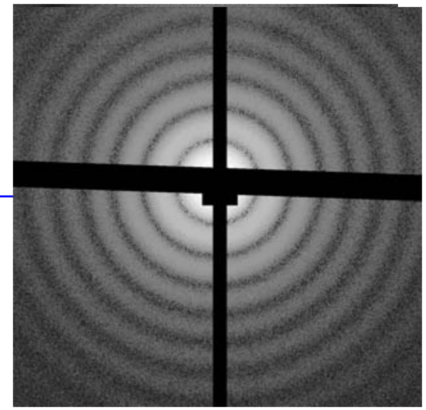
Complete image reconstruction achieved, without any prior knowledge, using our "**shrinkwrap**" algorithm, **parallelized** for 3D on 16-node cluster. Resolution = 10 nm



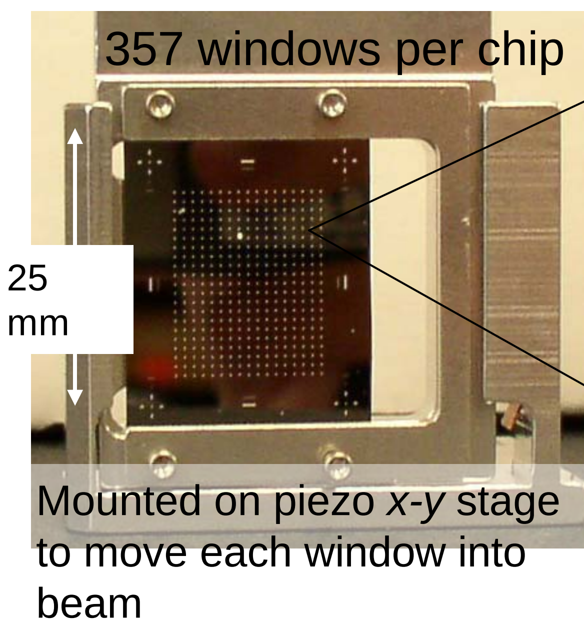
1 micron

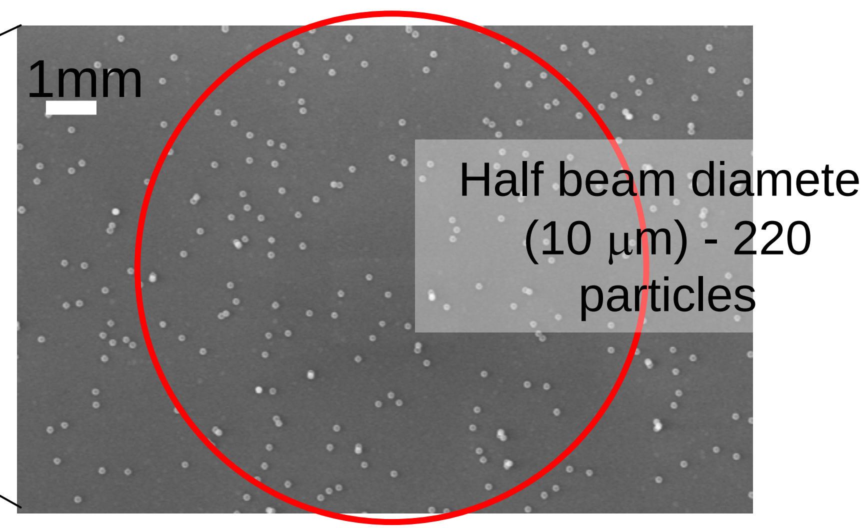
Particle explosion experiments were performed on latex particles on membranes



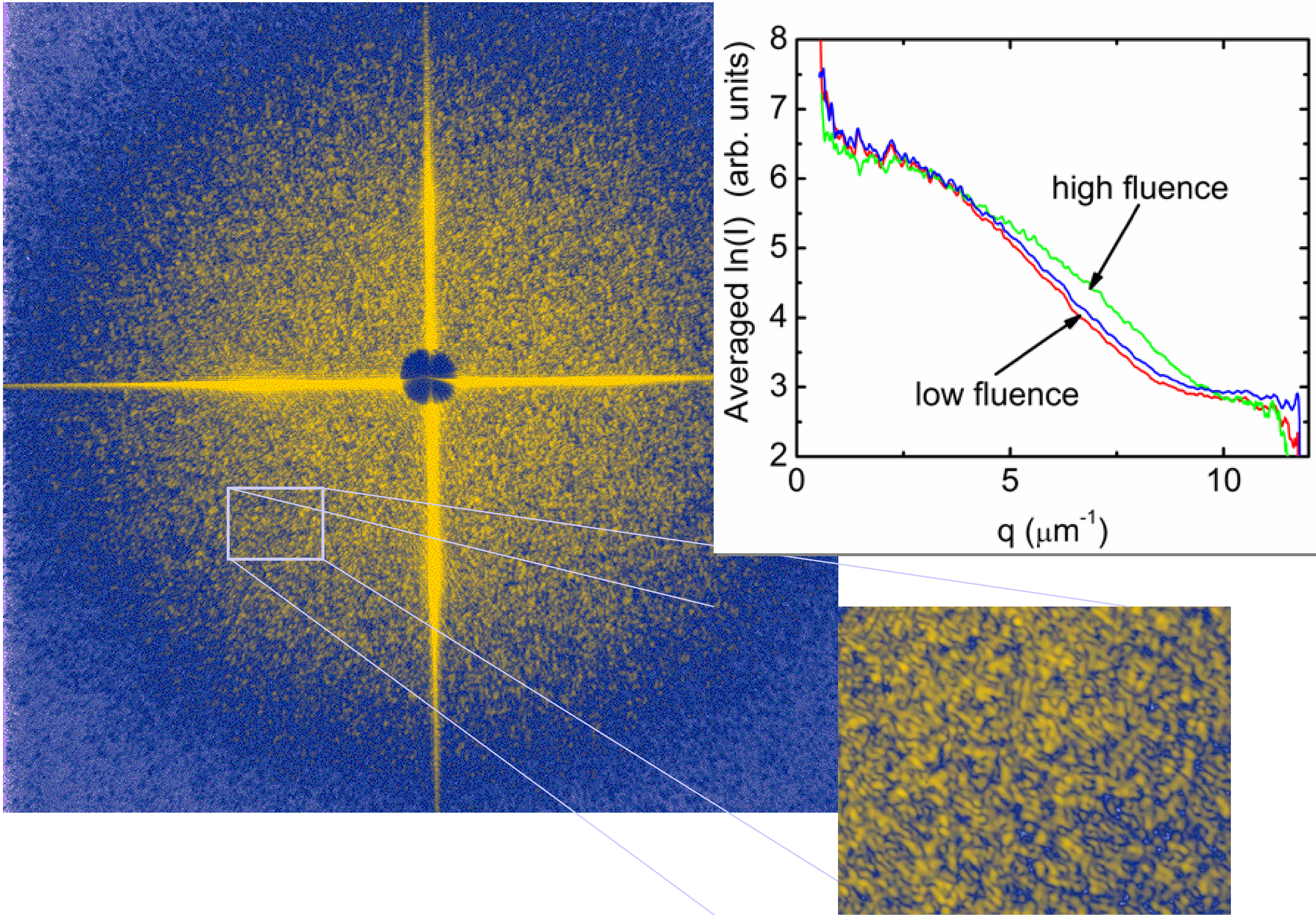


- The particle size is determined by Mie scattering of the VUV-FEL pulse by the particles (FEL pulse is both pump and probe)
- To see a 5% change in radius during pulse, require size distribution of ~1%.



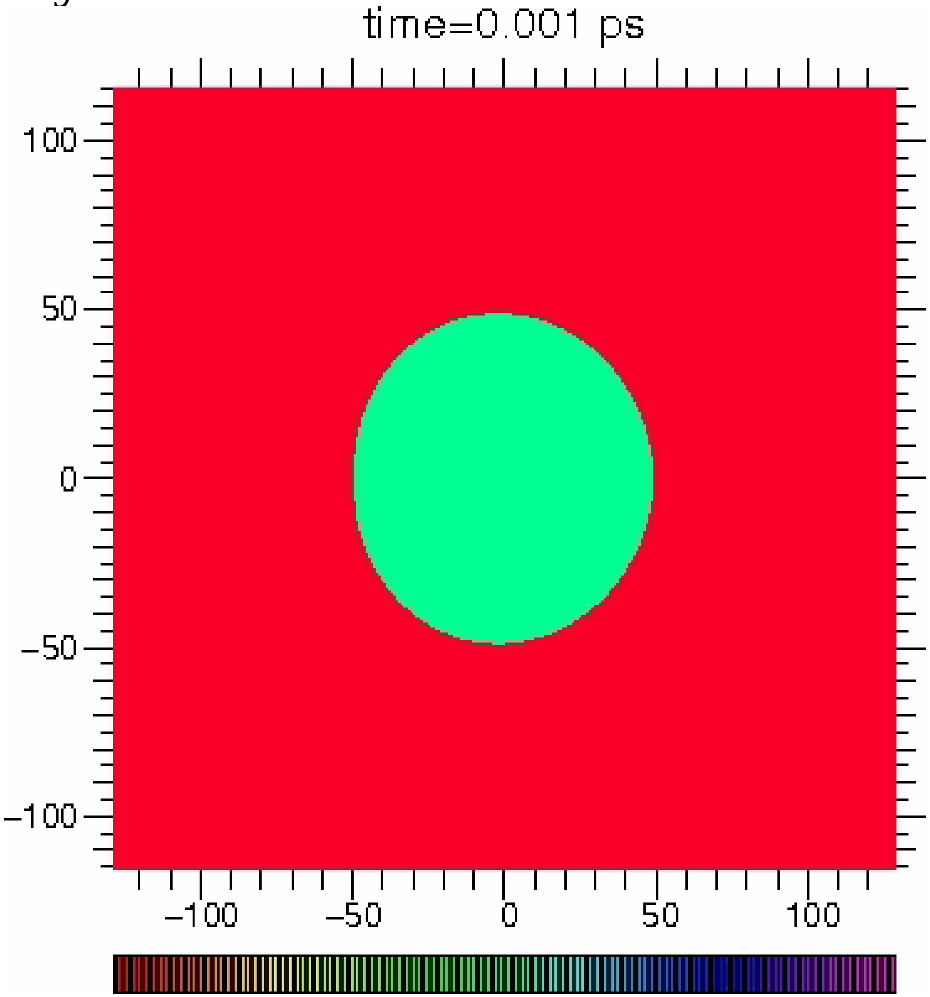


Scattering from balls demonstrates that they retain their shape throughout the duration of the pulse



Our VUV hydrodynamic code shows that latex spheres start exploding in ~ 2 ps

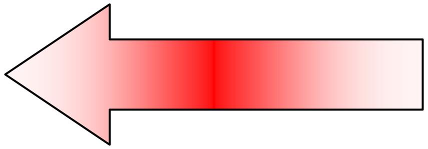
Density



y (nm)

z (nm)

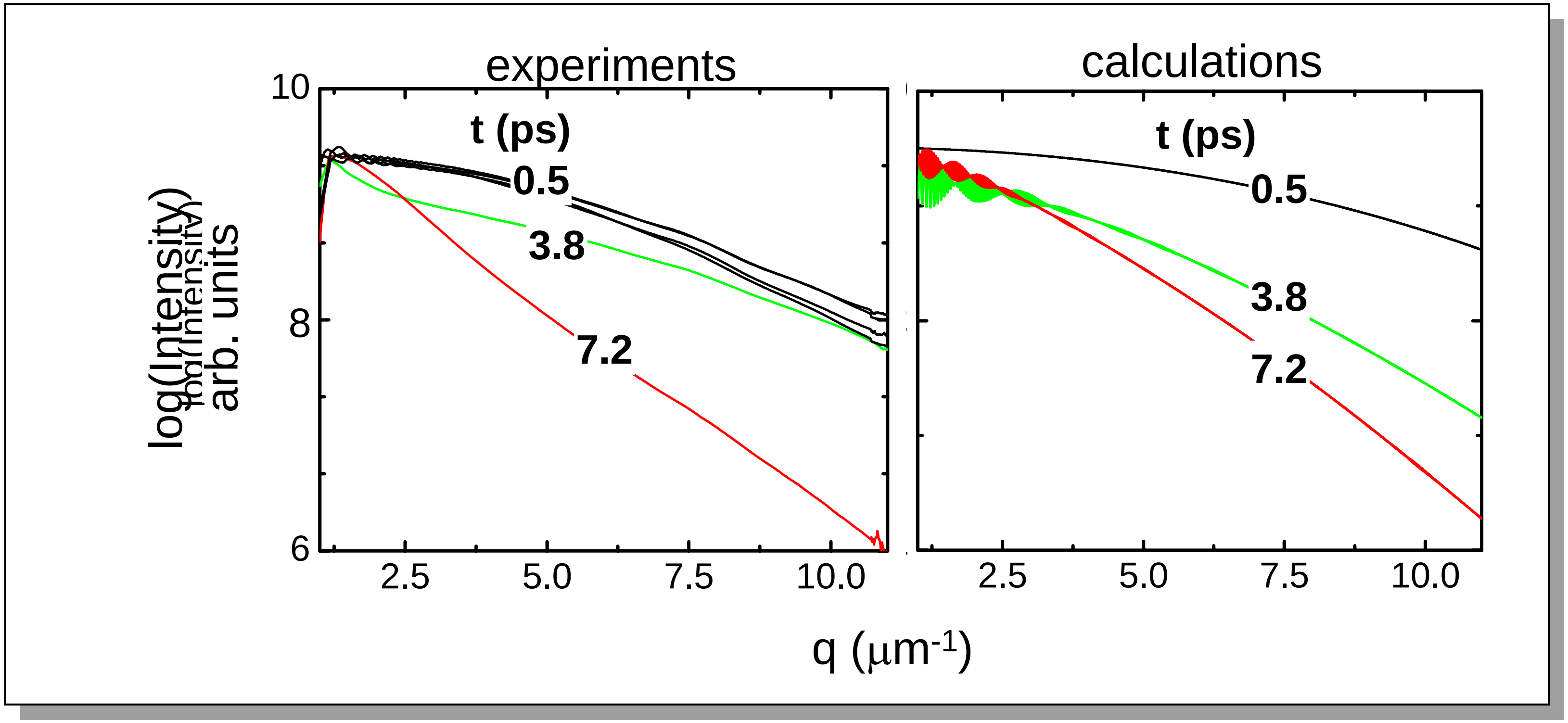
Incident pulse direction



Color scale: 0 g/cm^3 2 g/cm^3

S. Hau-Riege
HYDRA & TABOP

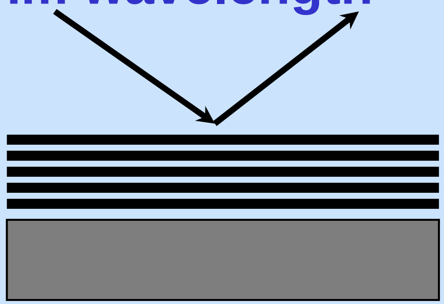
The explosion takes longer than expected from our hydrodynamic model



• Experiments and simulations show a similar trend of the particle exploding
• The onset of explosion occurs later than predicted
• Measurements will be improved with better pulse diagnostics and shorter wavelength

First EUV-FEL experiments show that structural information can be obtained before destruction

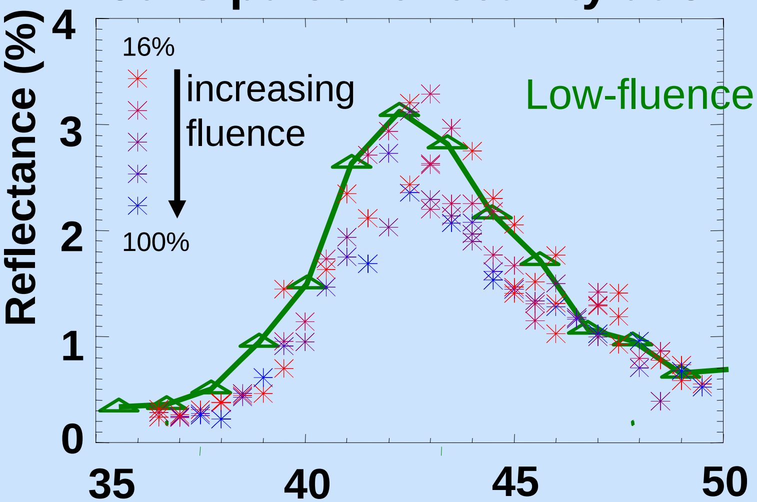
During 30 fs pulse (10^{14} W cm^{-2}) 32 nm wavelength



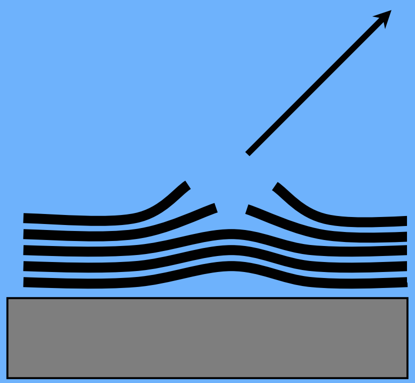
Reflectivity unchanged

Multilayer *d* spacing not changed by more than 0.3 nm

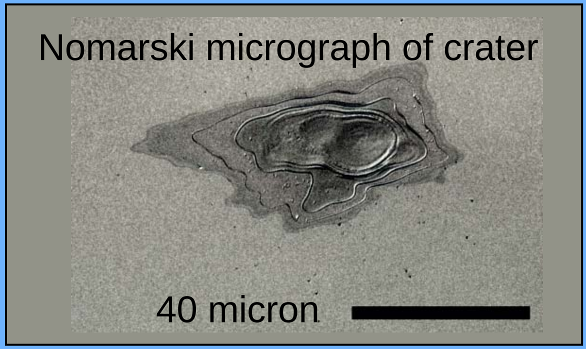
30 fs pulse reflectivity at 32nm

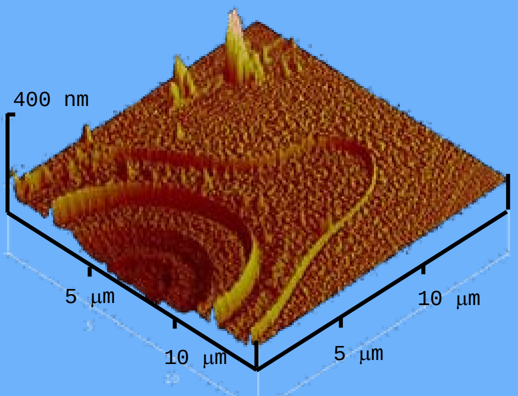


After pulse



Plasma forms, layers ablate

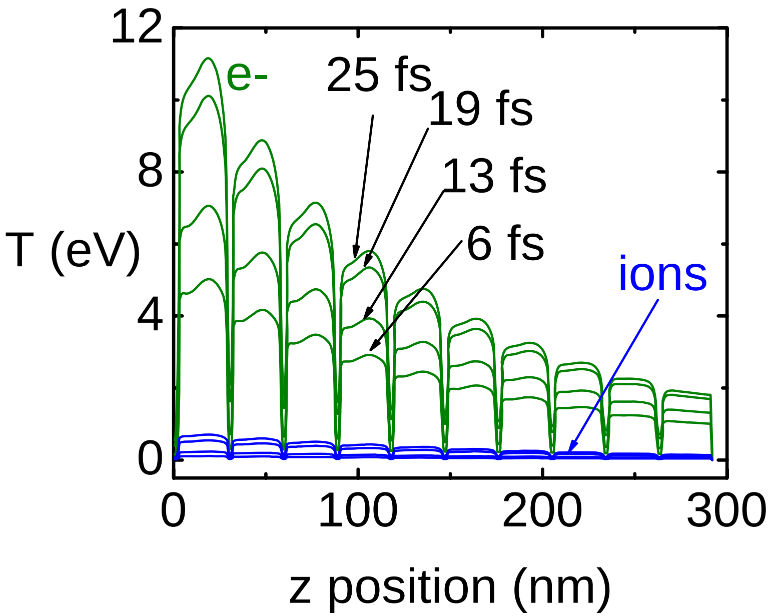


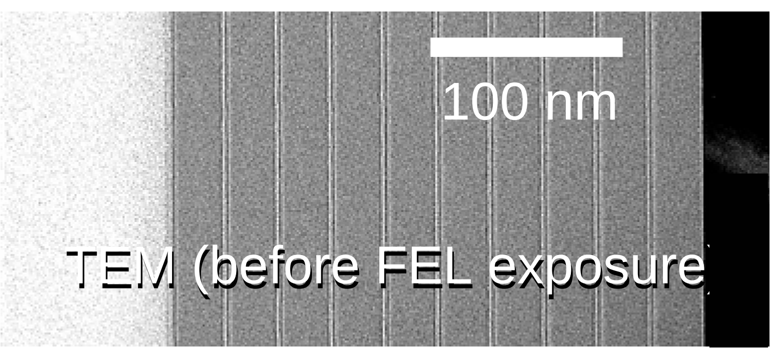


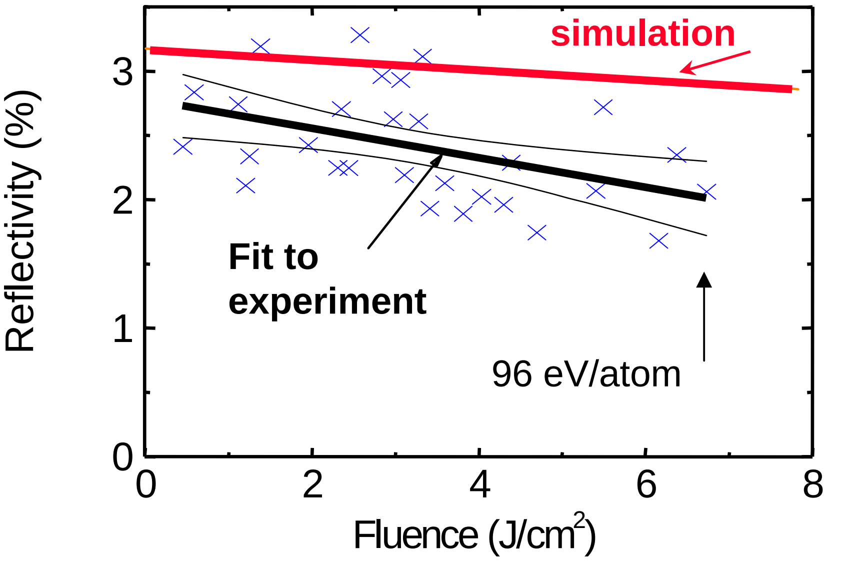
With J. Kryzwinski, R. Sobierajski, L. Juha et al

There is no motion at 3Å during the pulse, but the change in optical constants is larger than expected

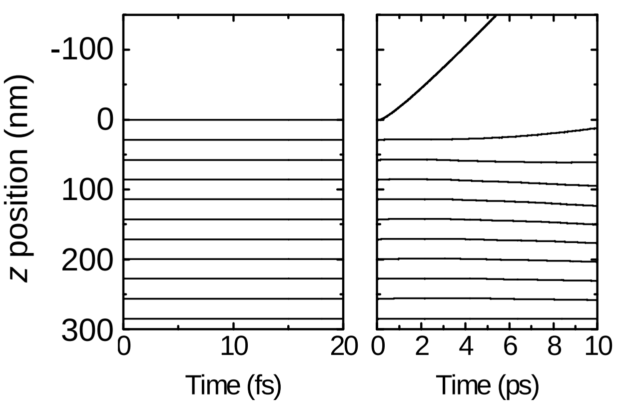
Temperature profile in the multilayer



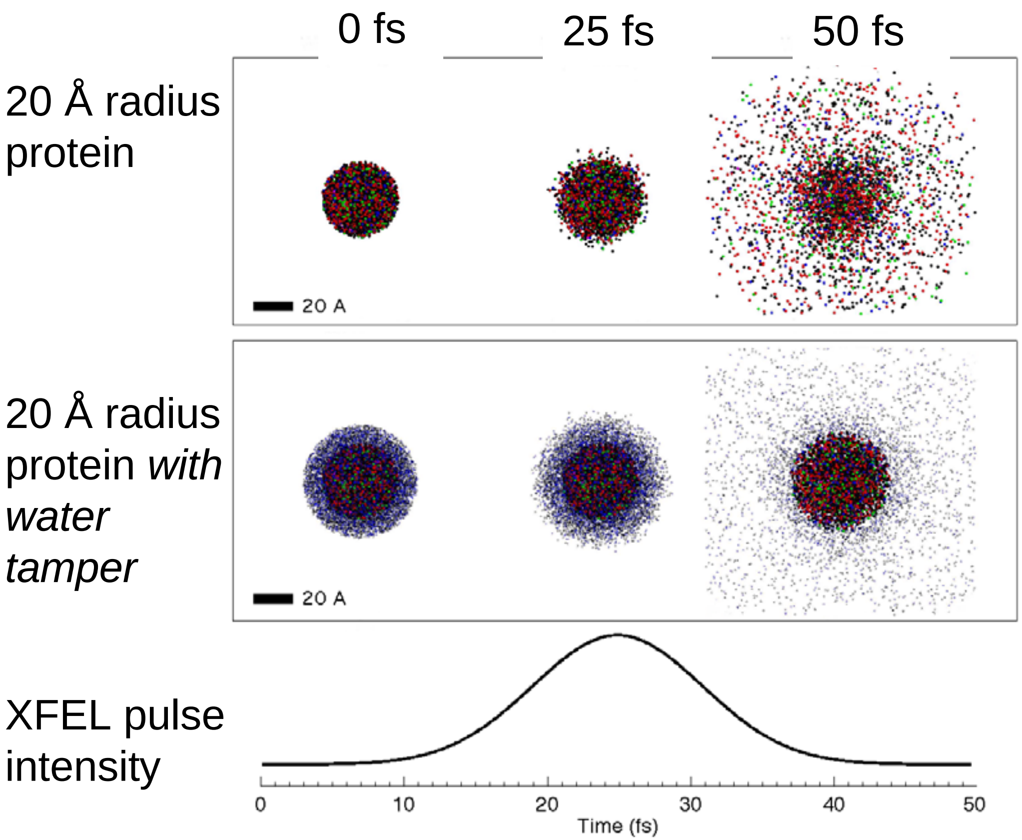


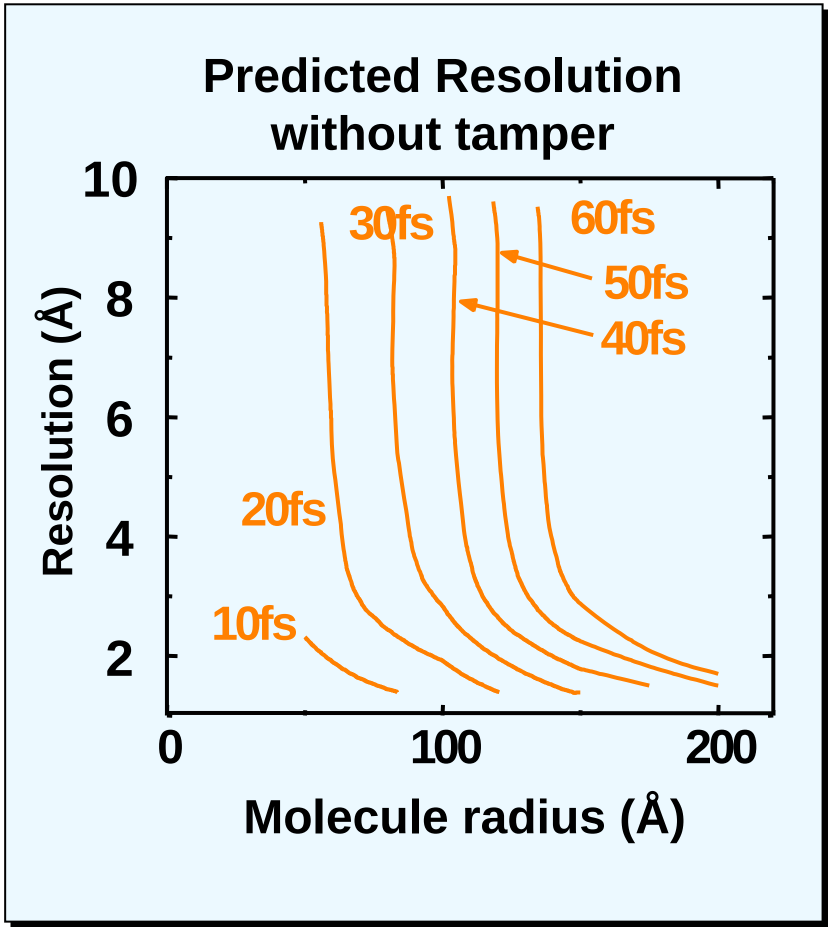


Motion occurs after the pulse



Our model predicts atomic resolution imaging is feasible





S. Hau-Riege, R. London, A. Szoke, G. Huldt
Phys. Rev E **69** 051906 (2004); Phys. Rev E **71** 061919

Acknowledgements

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