Nano-Crystallography and single particle imaging at FELs

Henry Chapman

Center for Free-Electron Laser Science

DESY and University of Hamburg

henry.chapman@desy.de

KEK - DESY meeting

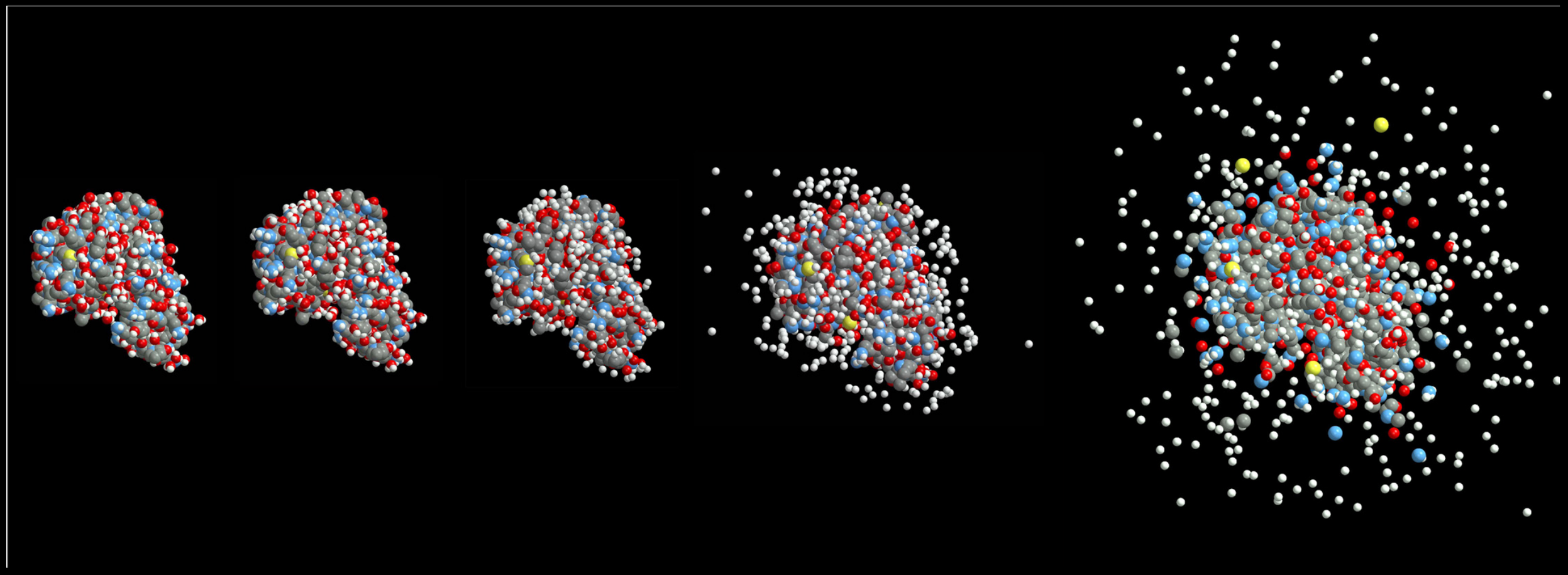
Center for Free-Electron Laser Science (CFEL)

Coherent Imaging & Scattering	***Henry Chapman***	hammeskrause architekten
Condensed Matter Structural Dynamics	***Andrea Cavalleri***	
Atomic Resolution Structural Dynamics	***Dwayne Miller***	
Theory	***Robin Santra***	
Laser Science	***Franz Kärtner***	
Max Planck Advanced Study Group	***Gerard Meijer (Joachim Ulrich)***	
U Hamburg Advanced Study Group	***Wilfried Wurth***	

Experiments and analyses are carried out as a large collaboration

CFEL-DESY	A. Barty, M. Liang, T. White, D. Deponte, S. Stern, A. Martin, C. Caleman, K. Beyerlein, R. Kirian, K. Nass, F. Stellato, F. Wang, H. Fleckenstein, L. Gumprecht, L. Galli, S. Bajt, M. Barthelmess
ASU	J. Spence, P. Fromme, U. Weierstall, B. Doak, R. Kirian, X. Wang, I. Grotjohann, R. Fromme
MPG CFEL ASG	I. Schlichting, R. Shoeman, L. Lomb, S. Kassemeyer, S. Bari, T. Barends, J. Steinbrener, D. Rolles, S. Epp, A. Rudenko, L. Strüder, R. Hartmann, L. Foucar, N. Kimmel, P. Holl, J. Ullrich
SLAC-PULSE	M. Bogan, D. Starodub, R. Sierra, C. Hampton, D. Loh
SLAC-LCLS	S. Boutet, G. Williams, M. Seibert, J. Kryzwinski, C. Bostedt, M. Messerschmidt, J. Bozek, W. White, R. Coffee, C. Kenney, R. Herbst, J. Pines, P. Hart, J. Morse, P. Emma, J. Frisch, J. Galayda *and many others*
Uppsala	J. Hajdu, Nic Timneanu, J. Andreasson, M. Seibert, F. Maia, M. Svenda, T. Ekeberg, J. Andreasson, A. Rocker, O. Jonsson, D. Westphal
Euro XFEL	J. Schulz, N. Coppola, A. Aquila
LLNL	S. Hau-Riege, M. Frank, M. Hunter
LBNL	S. Marchesini, J. Holton
Gotheburg	R. Neutze, L. Johansson, D. Arnlund
U. Hamburg	L. Redecke, C. Betzel
U. Tübingen	M. Duszenko, R.Koopman, K. Cupelli
CAMP Team	*Led by Joachim Ullrich and Ilme Schlichting*

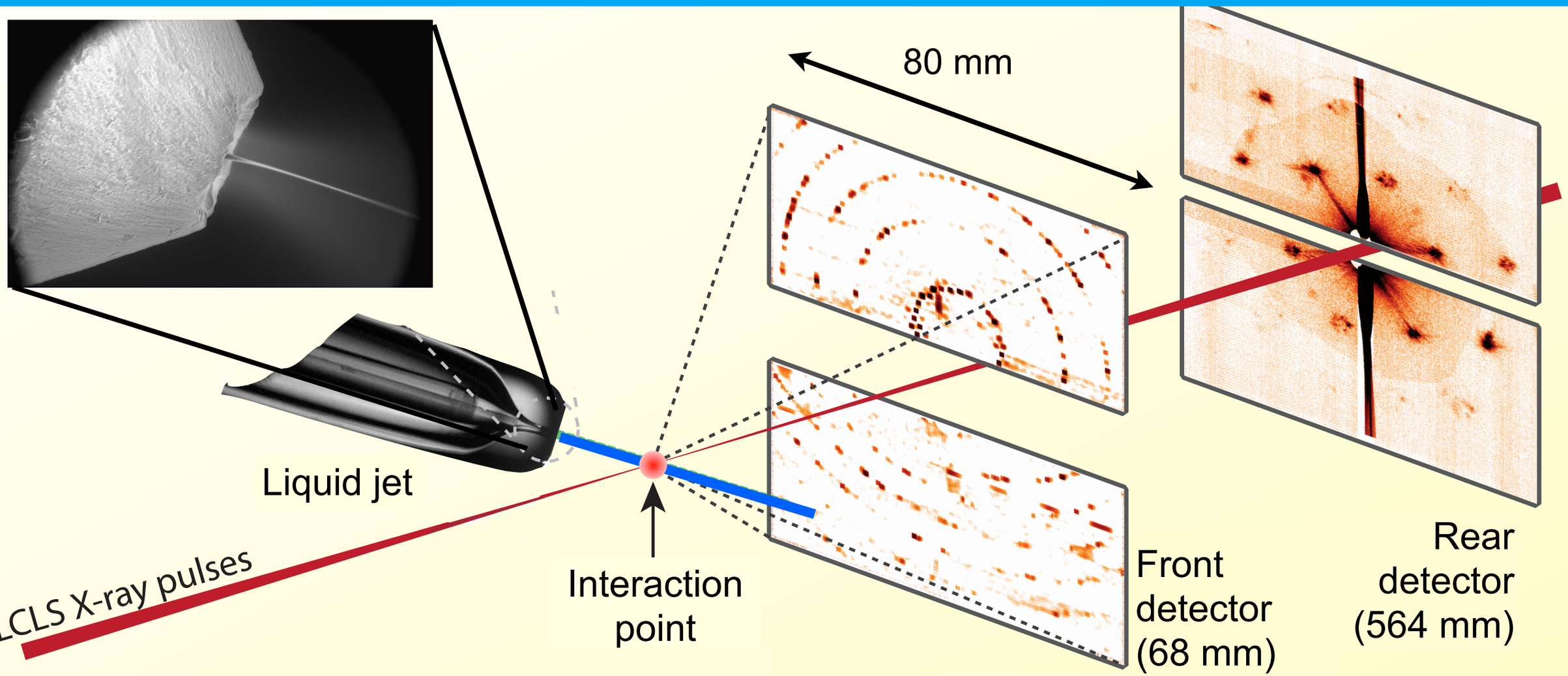
X-ray free-electron lasers may enable atomic-resolution imaging of biological macromolecules

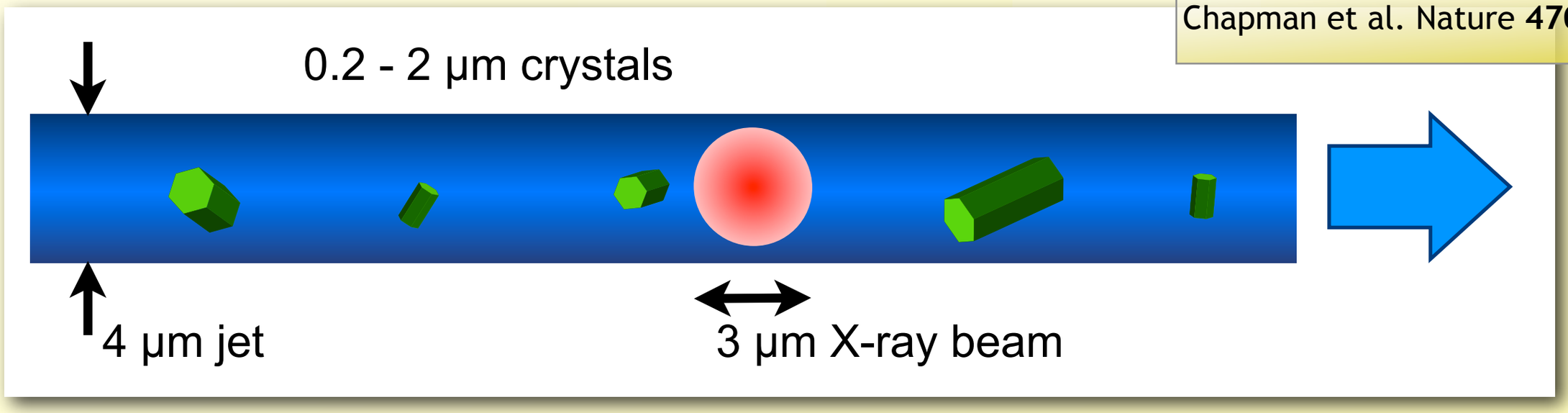


2 fs 5 fs 10 fs 20 fs 50 fs

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

Nanocrystallography is carried out in a flowing water microjet





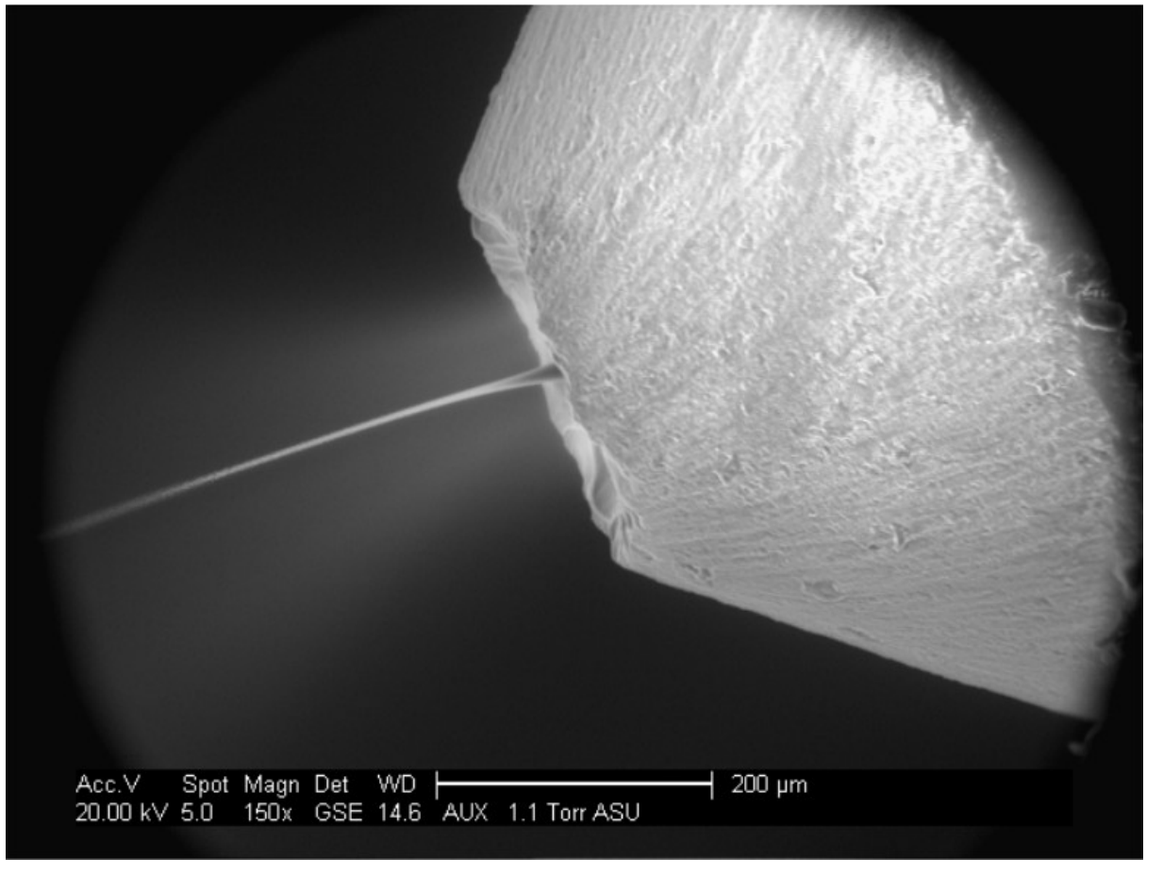
Chapman et al. Nature **470,** 73 (2011)

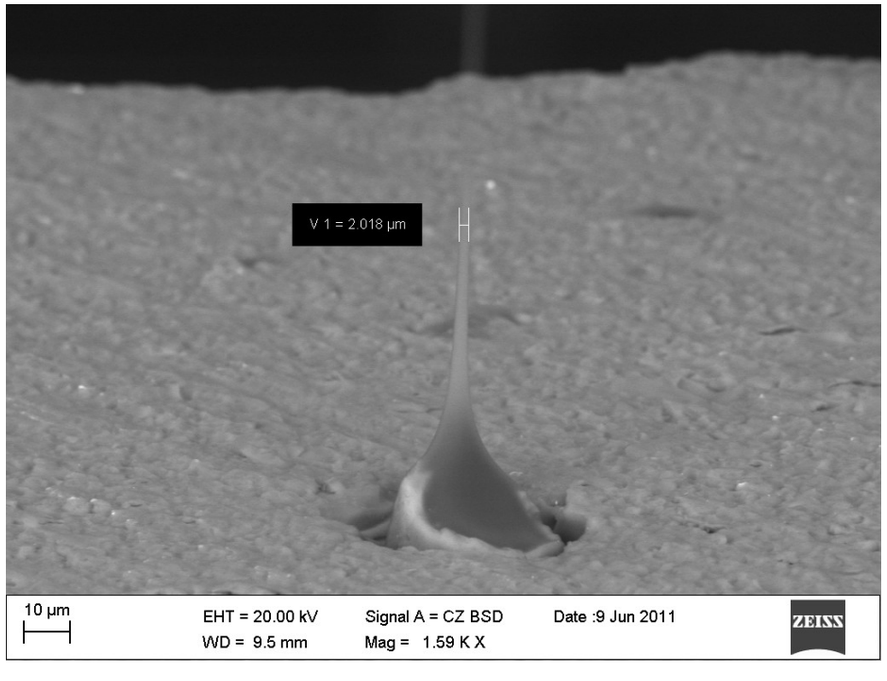
Samples are delivered to the beam in a liquid jet

> Sample delivery (“injection”) technology is **critical** to the success of serial crystallography and many other FEL experiments

Gas dynamic nozzle creates liquid streams with diameters down to 200 nm.

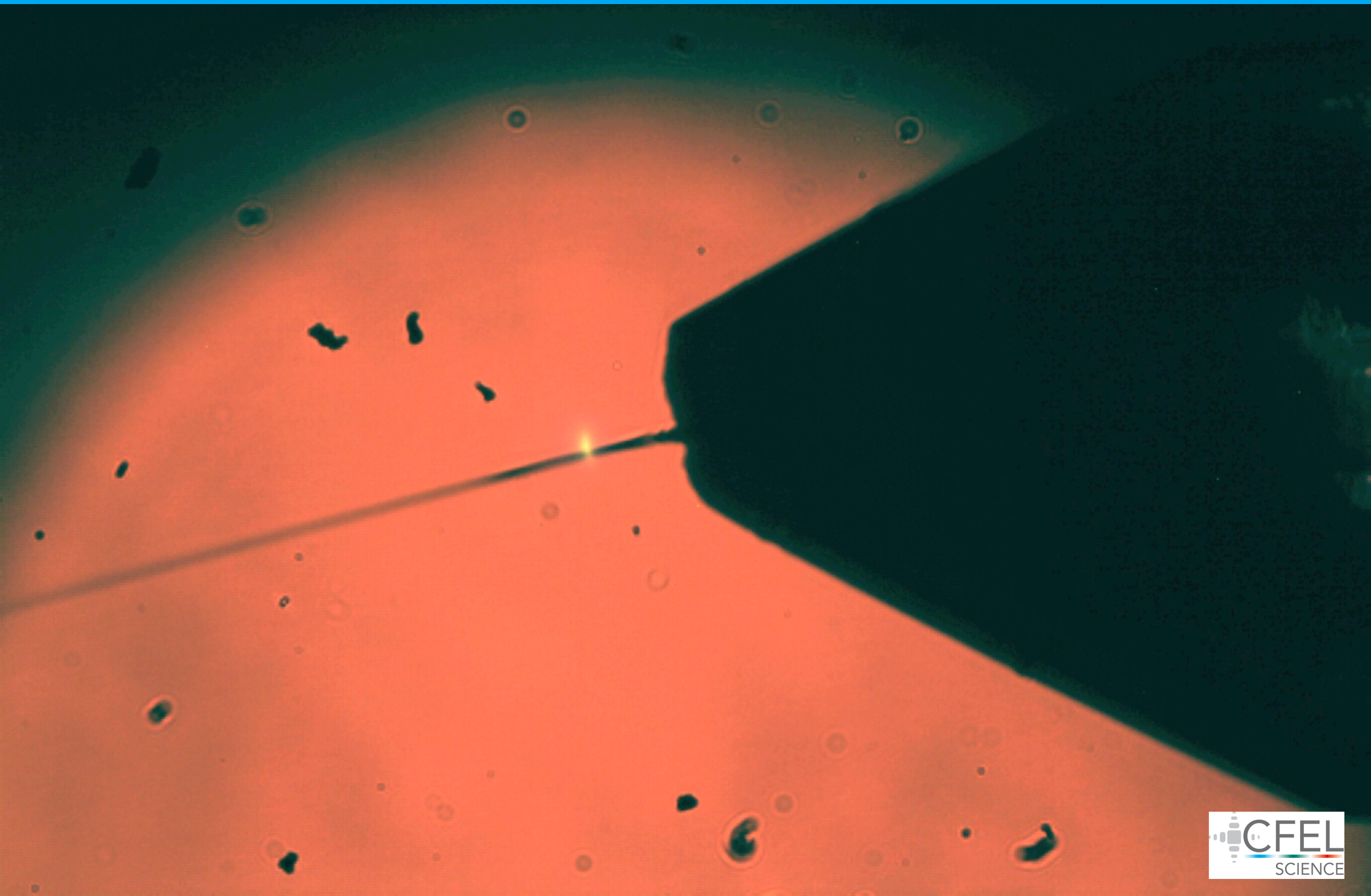
“Droplet on demand” offers potential reductions in sample consumption of an **order of magnitude**.



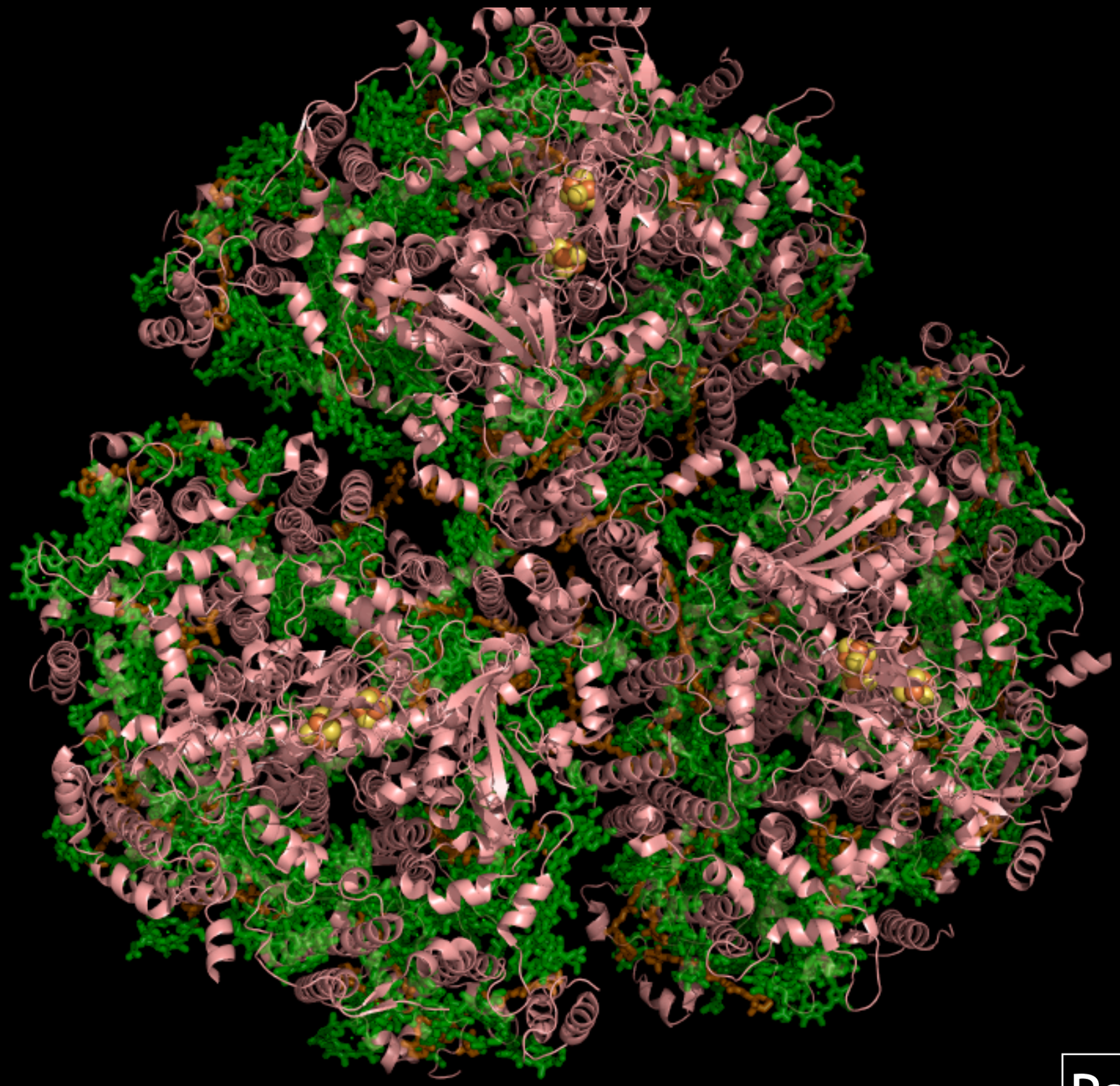


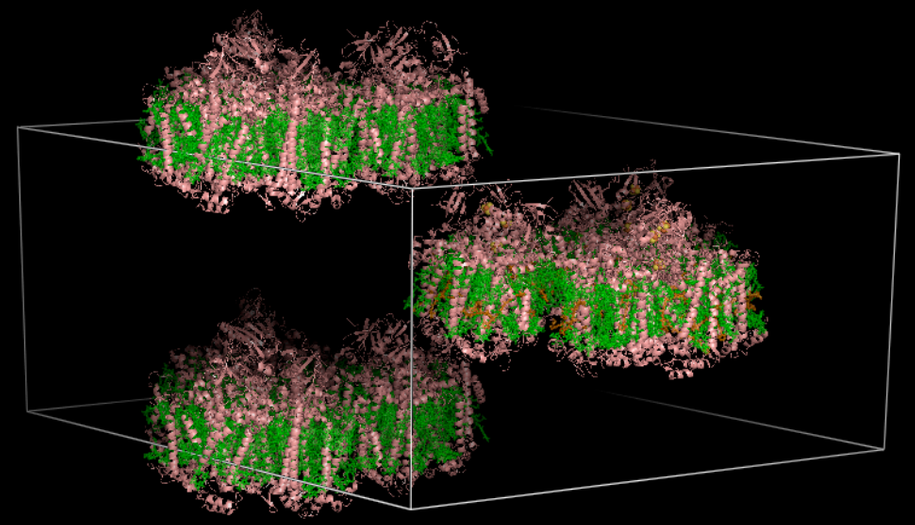
Dan DePonte, CFEL

Optical emission is observed for dose rates above about 20 MGy/fs

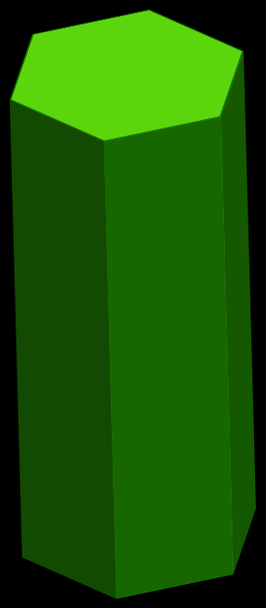


First experiments were carried out on Photosystem I



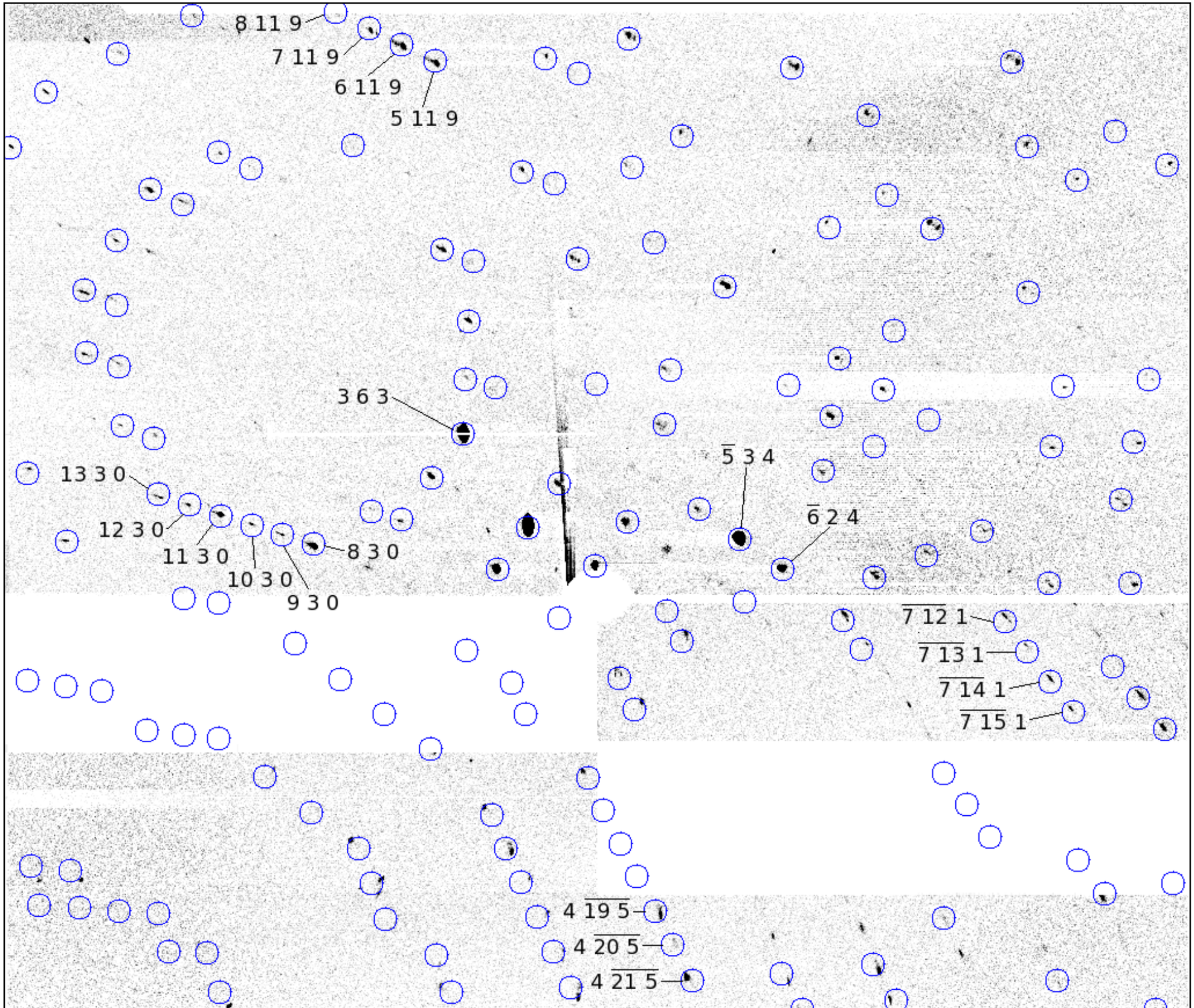


a = *b* = 288 Å
c = 167 Å

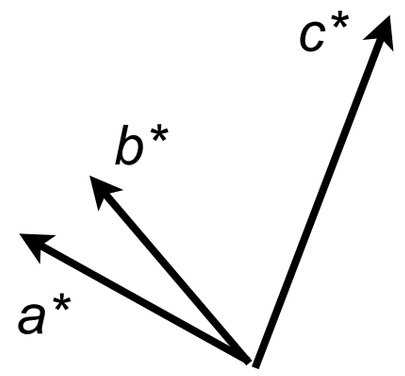


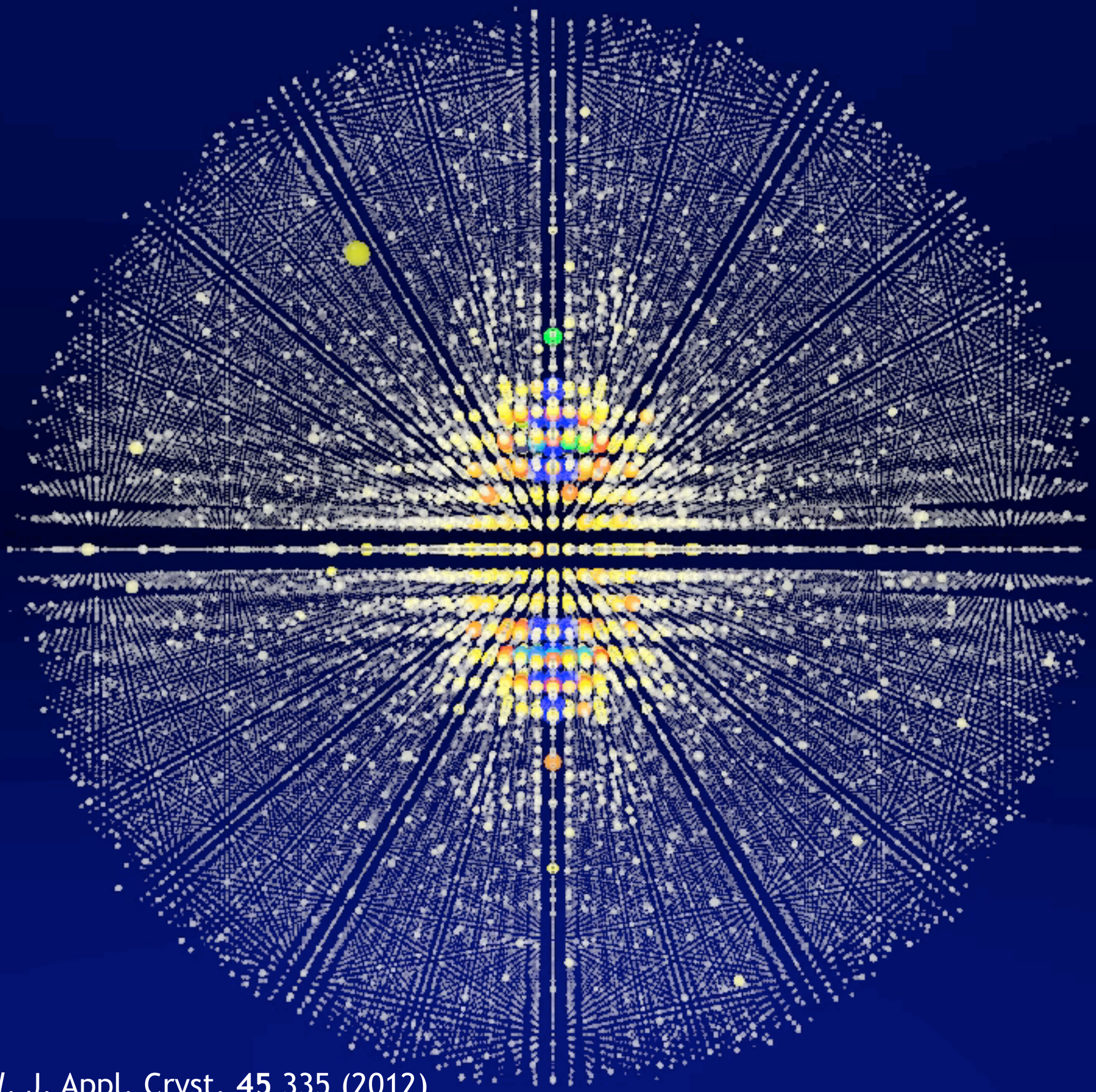
Petra Fromme, ASU

Each pattern is indexed



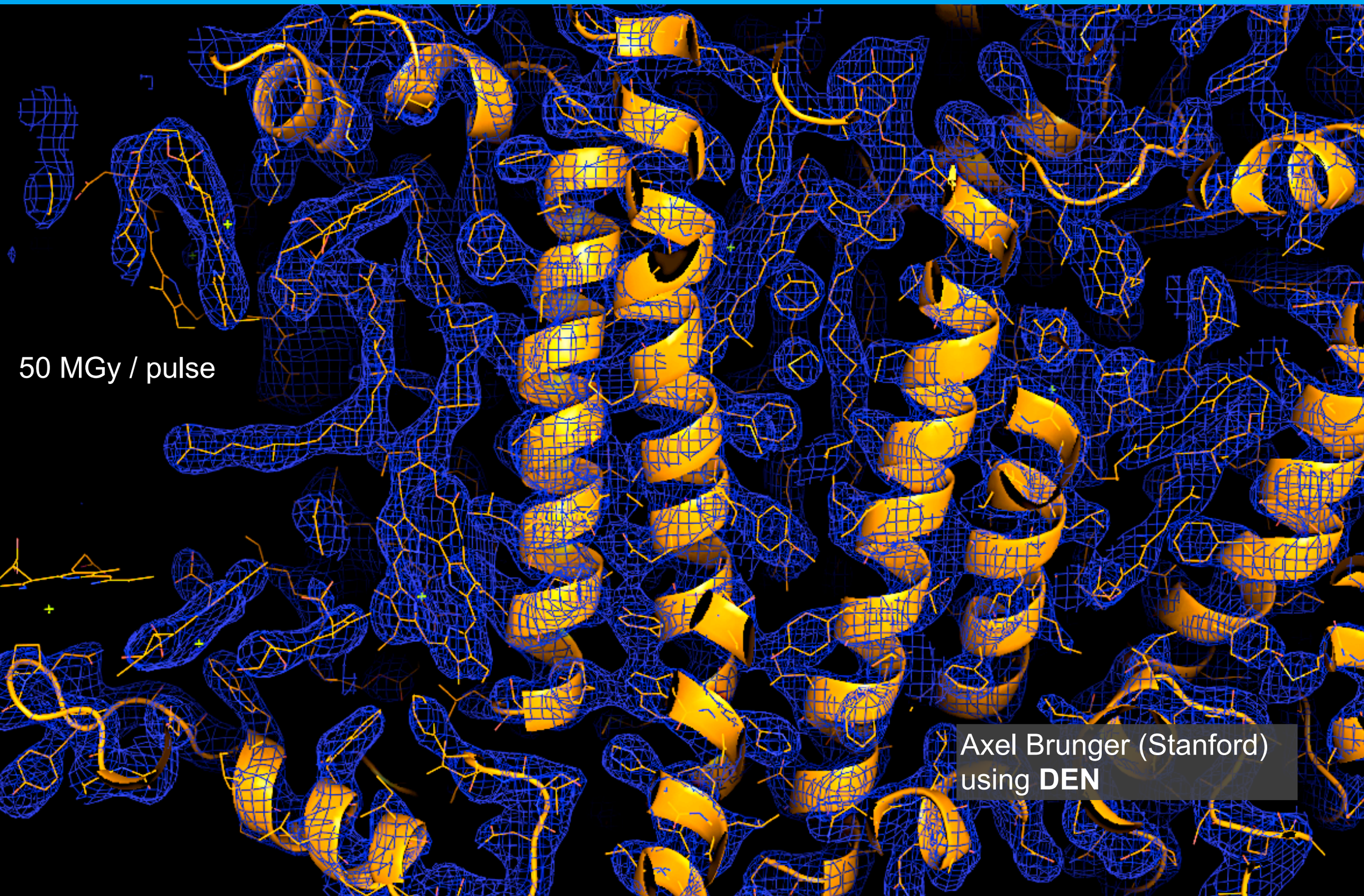
Tom White (CFEL)
Rick Kirian (ASU)



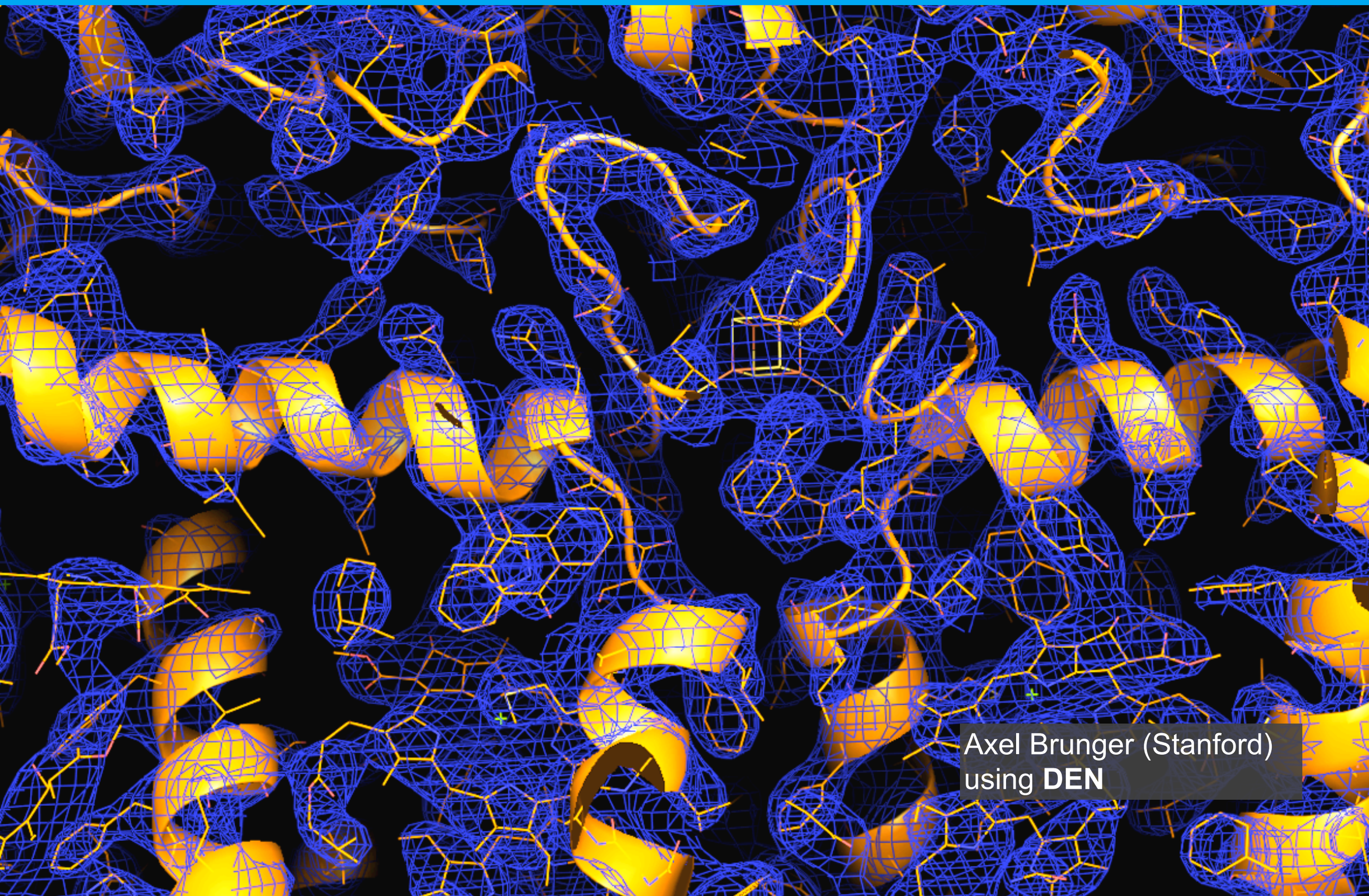


Tom White *et al*. J. Appl. Cryst. **45** 335 (2012)

Molecular replacement reconstructs the photosystem I structure



Molecular replacement reconstructs the photosystem I structure



Axel Brunger (Stanford)
using **DEN**

We have a new DESY system for processing and storage

LCLS Data

A typical run at
120 Hz generates
>200 TB of data

~ 1 Petabyte
collected from our
experiments

SGI Altix
72 physical cores
360GB RAM
Shared memory
Direct connected storage

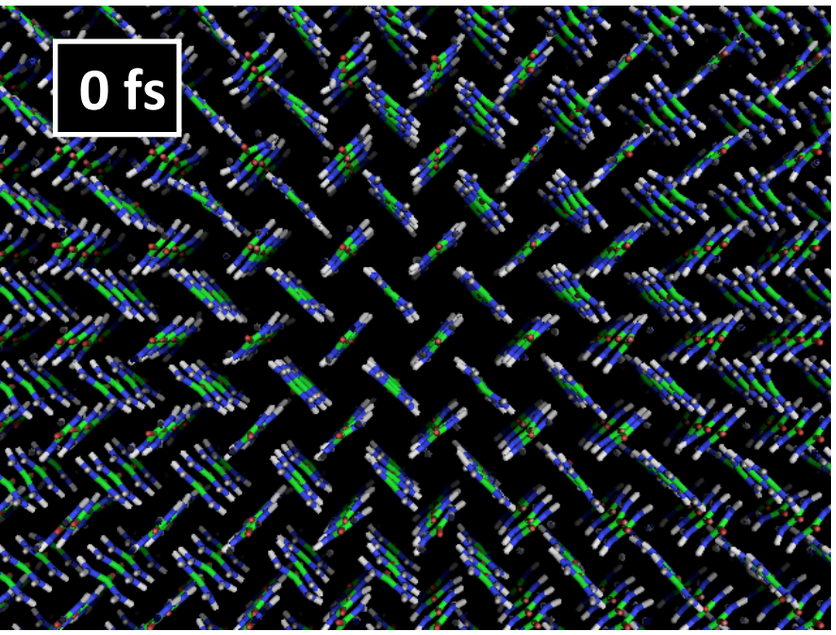
Data Direct Networks SFA10000
60-bay HDD / 4U unit
~1 PB/rack (formatted)
(600 x 2 TB HDDs)

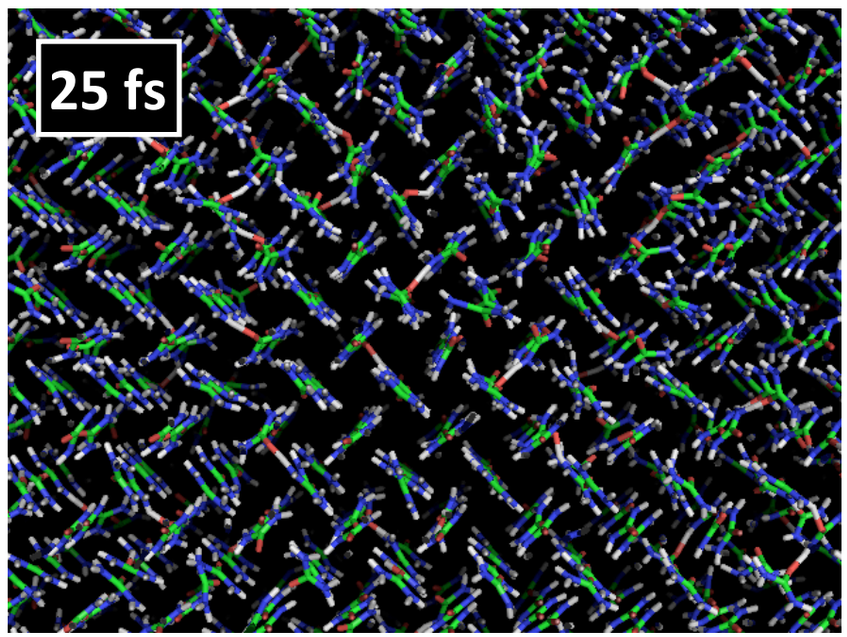
Can process 30 patterns / second

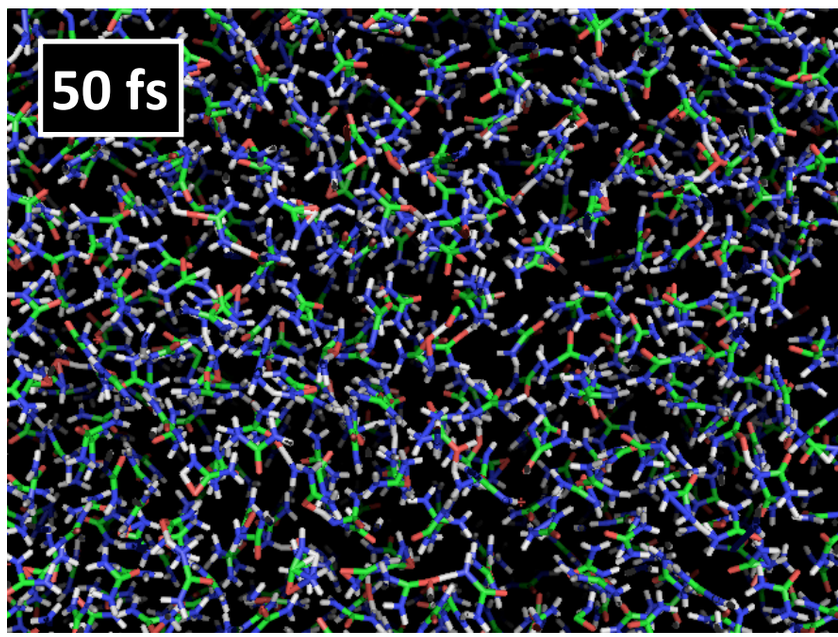
Anton Barty, Tom White, and DESY IT

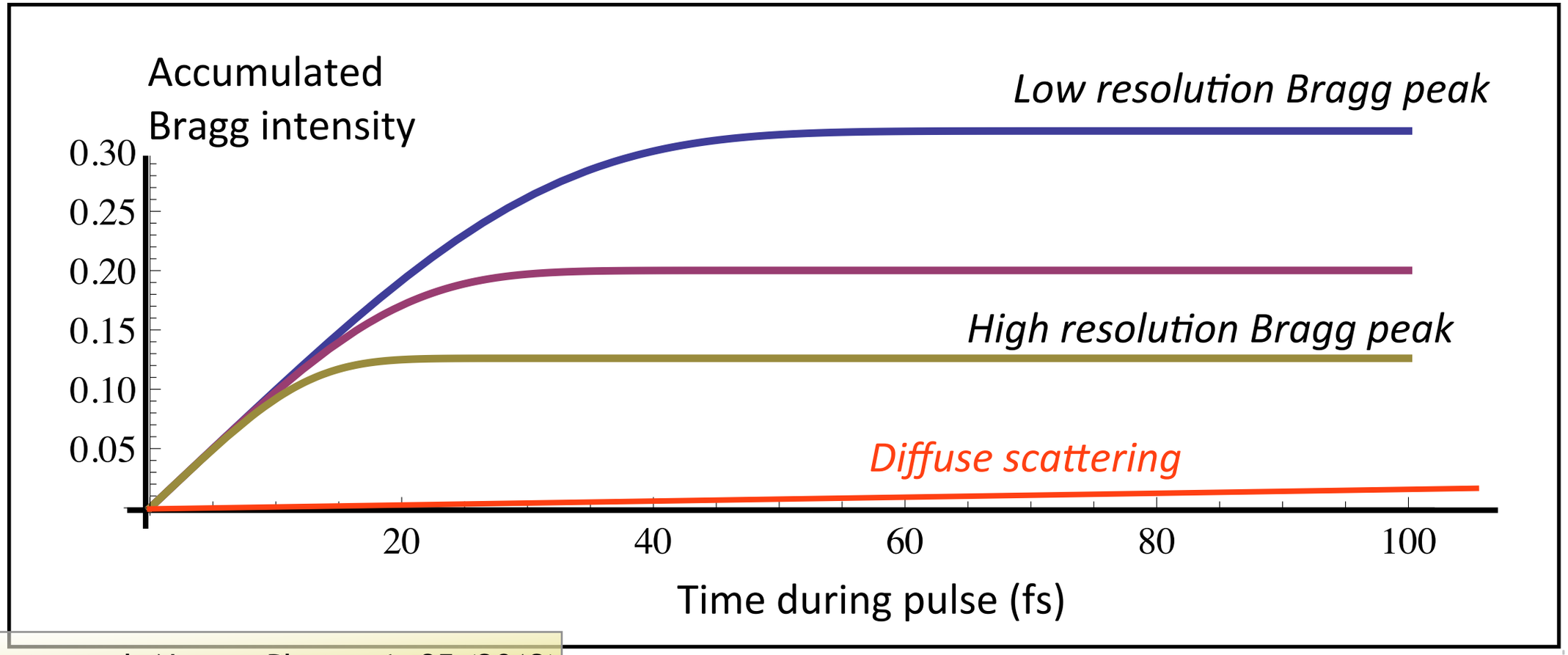
Tom White *et al*. J. Appl. Cryst. **45** 335 (2012)

A crystal only gives Bragg diffraction when it is a crystal!



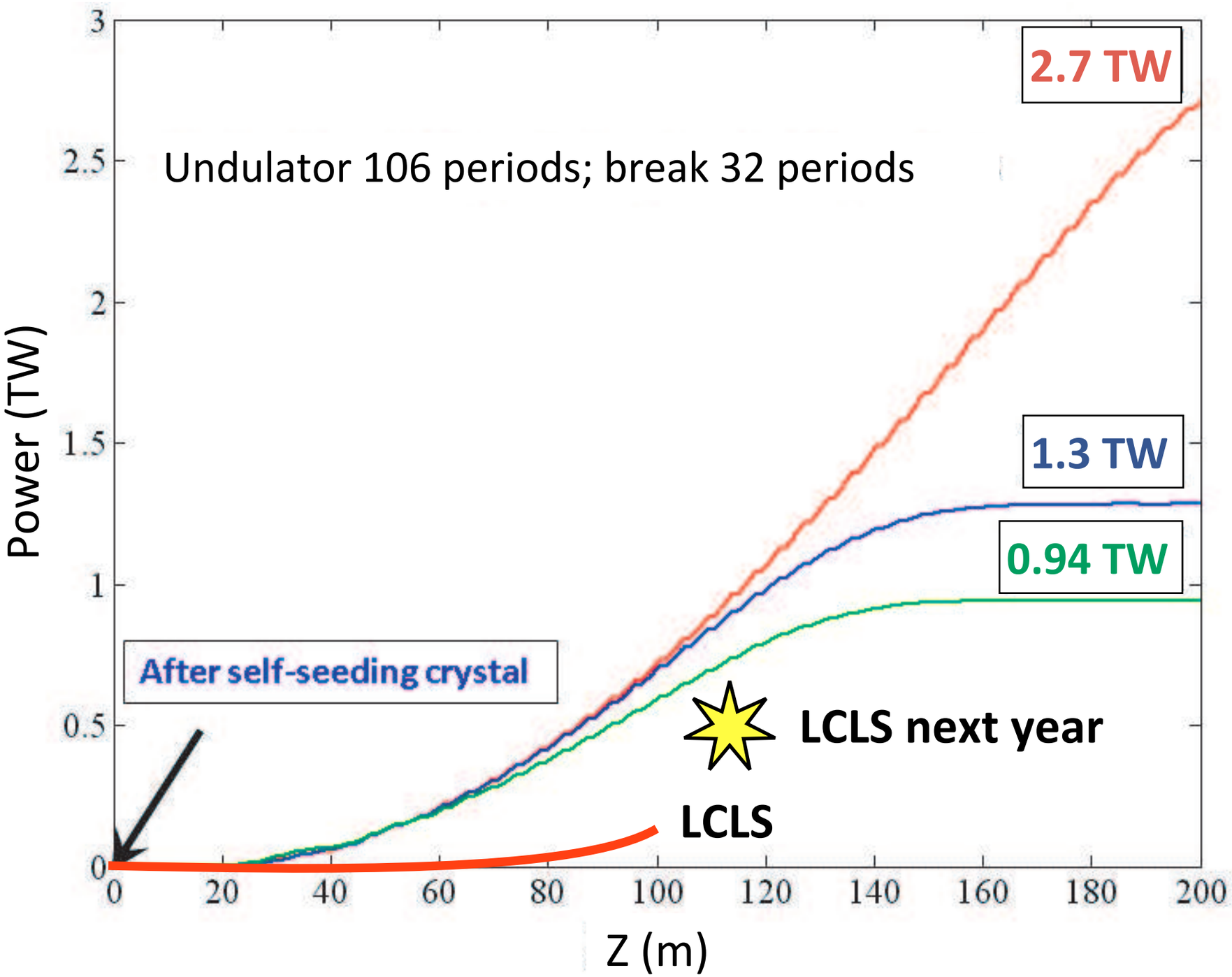






Barty et al. Nature Photon **6,** 35 (2012)

Self-seeding and tapered undulators could increase peak power by a factor of 50



1 TW focused to 1 μm²:
10^{20} W/cm²

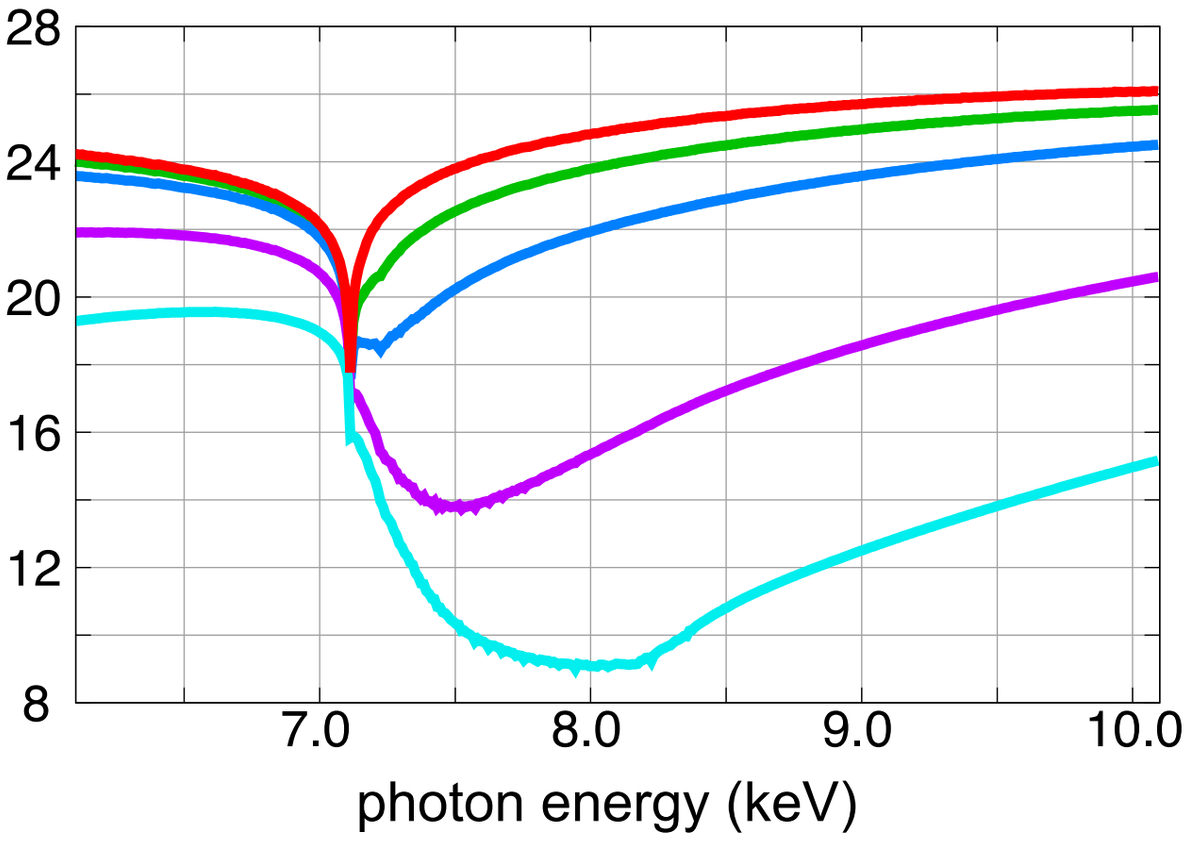
G. Geloni, V. Kocharyan, and E. Saldin.
J. Mod. Opt. **58**, 1391 (2011)

W.M. Fawley *et al*
LCLS Tech note 11-3 (Sept 2011)

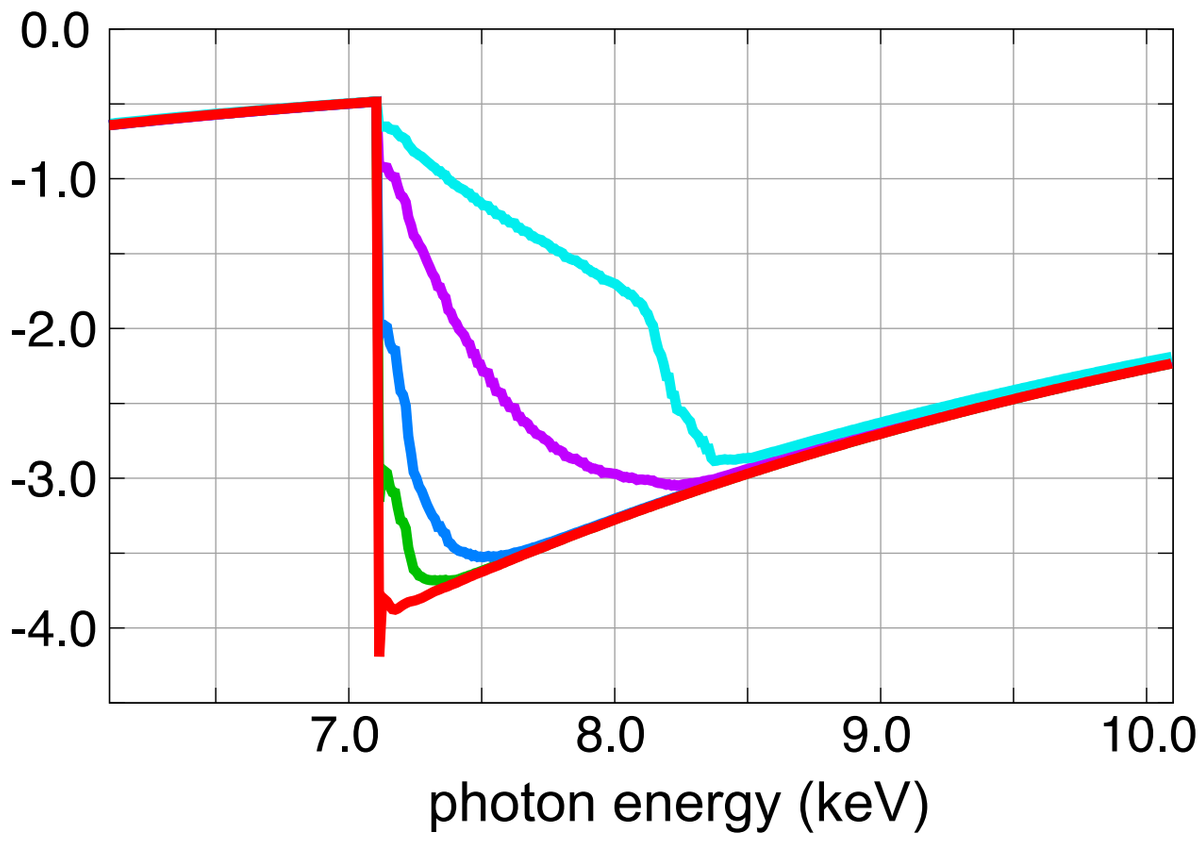
Calculations show that anomalous signals are enhanced by high X-ray intensity

Effective scattering factors for Fe with 2 mJ pulse
Average ionization by end of pulse is +14 for highest fluence

b(λ) → f^0+f'



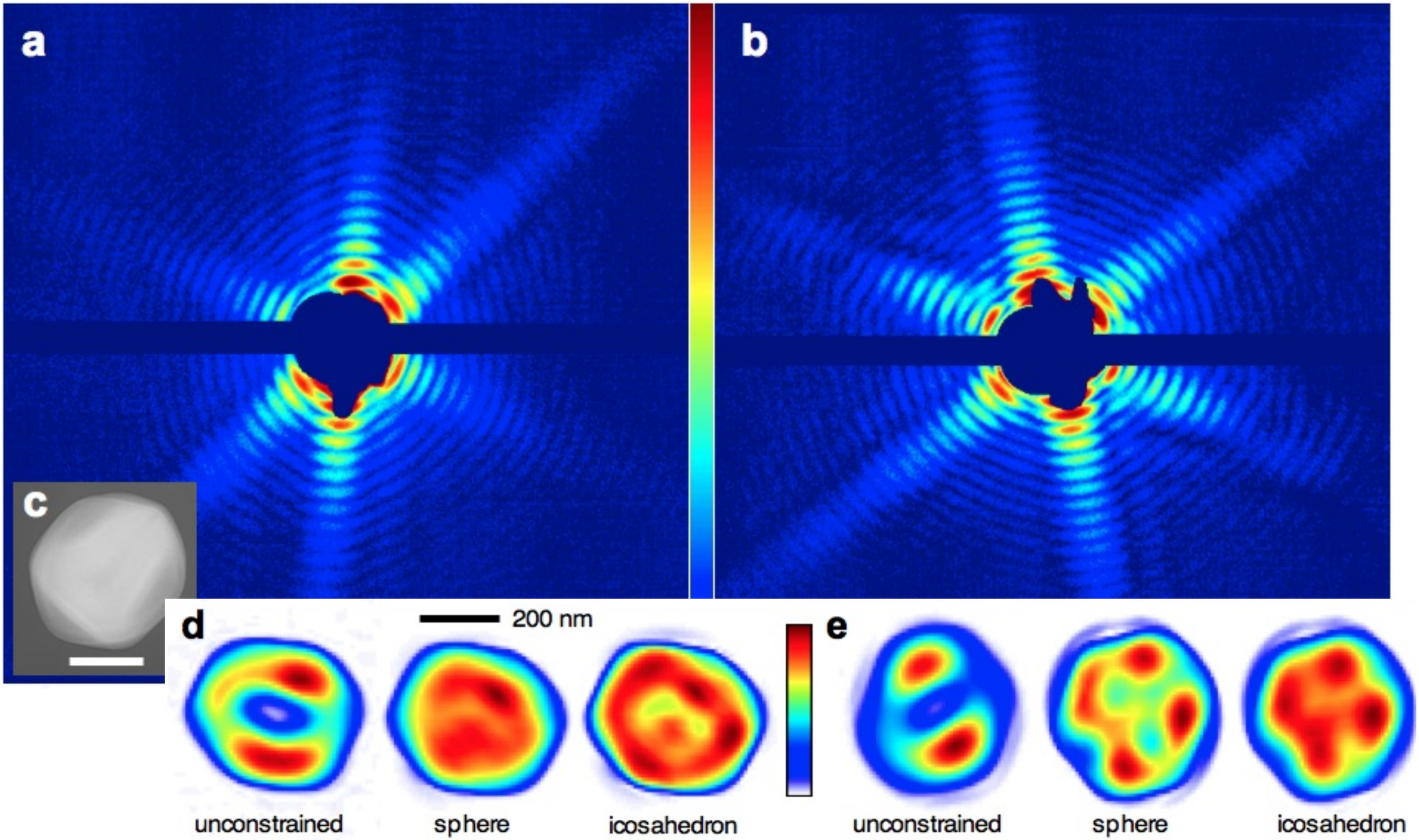
c(λ) → f''



Undamaged		
1.6×10^{17} W/cm^2	1.6 MGy/fs
5×10^{17} W/cm^2	5 MGy/fs
2×10^{18} W/cm^2	20 MGy/fs
2×10^{19} W/cm^2	200 MGy/fs

S.-K. Son, H.N.C., R. Santra, PRL **107**, 218102 (2011).

Single virus particles have been imaged on the fly

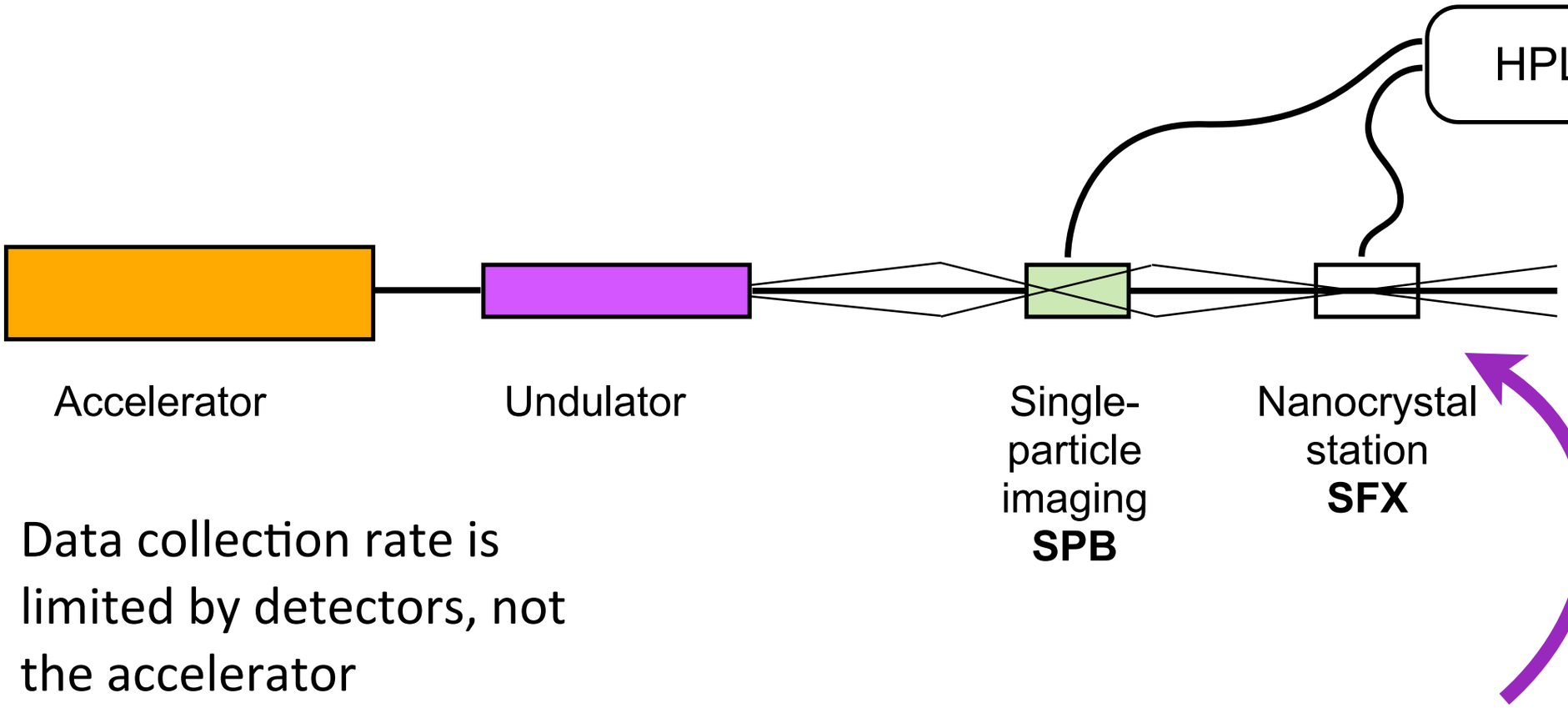


Seibert *et al*. Nature **470**, 78 (2011)

The proposed SFX facility at XFEL will double the output when running

The refocused transmitted beam from the XFEL SPB instrument will be more than sufficient for most crystalline samples. Collect data in parallel (at wavelength chosen by SPB), doubling the output of the facility

Poorly diffracting samples could be redirected to the higher-intensity SPB station



- Crystals
- Nano/micro-crystals
- Solution scattering

Data collection rate is limited by detectors, not the accelerator

Consortium: DESY, Uppsala, Gotheburg, ASU, EMBL, U. Hamburg, PSI, XFEL, Slovak Acad. Sci.

Summary

- “Diffraction before destruction” holds to 1.8 Å resolution
- No effect of radiation damage is observed in refined protein structures
- Structures are determined at room temperature (or other desired temperatures)
- Isotropic atomic displacements terminate the diffraction
- Ionization enhances anomalous signals, giving a route to phasing
- The key metric for this mode of imaging is X-ray *intensity* (photons per unit area per unit time). The optimal X-ray FEL source is that of highest pulse power