X-ray FELs

Status and Applications

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Workshop on Evolution and Control of Complexity

Argonne, October 11-13, 2010

HELMHOLTZ | GEMEINSCHAFT

DESY

FLASH: VUV and soft X-ray FEL

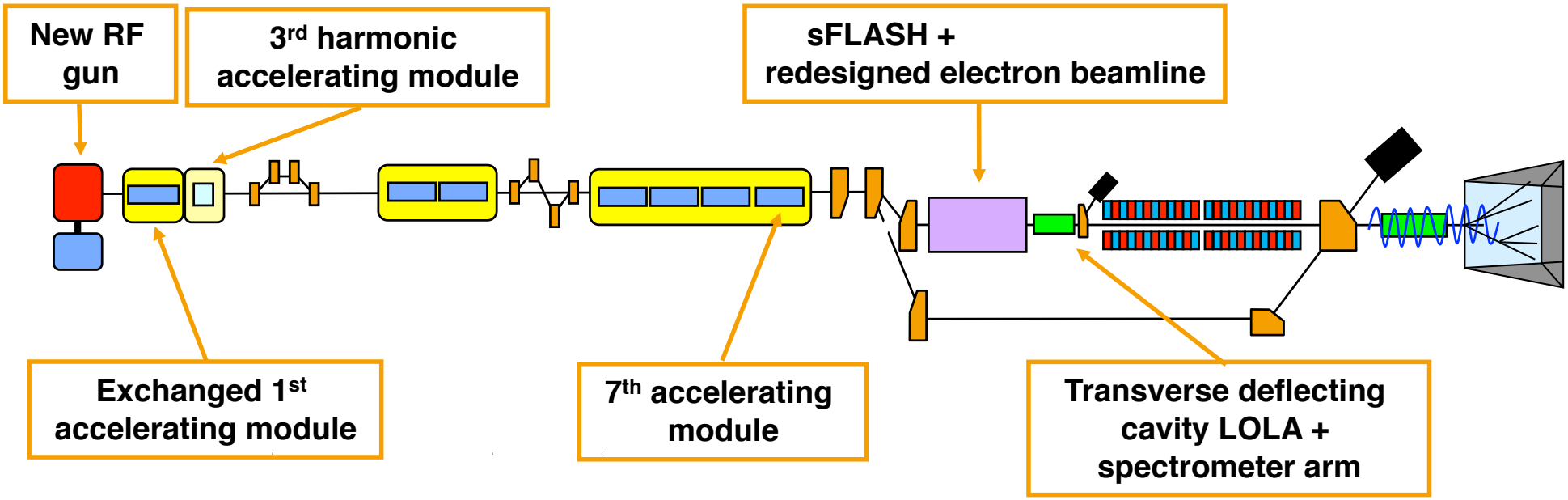
electron energy:	1.2 GeV
wavelength:	4.1-47 nm
average pulse energy:	50-200 µJ
peak pulse energy:	300 µJ
pulse duration:	10-150 fs
bunch train rep. rate	10 Hz
max. bunches/train	800
total bunch rep. rate	8000/s

user operation:	since 2005
user beam time:	~ 3500 h/a

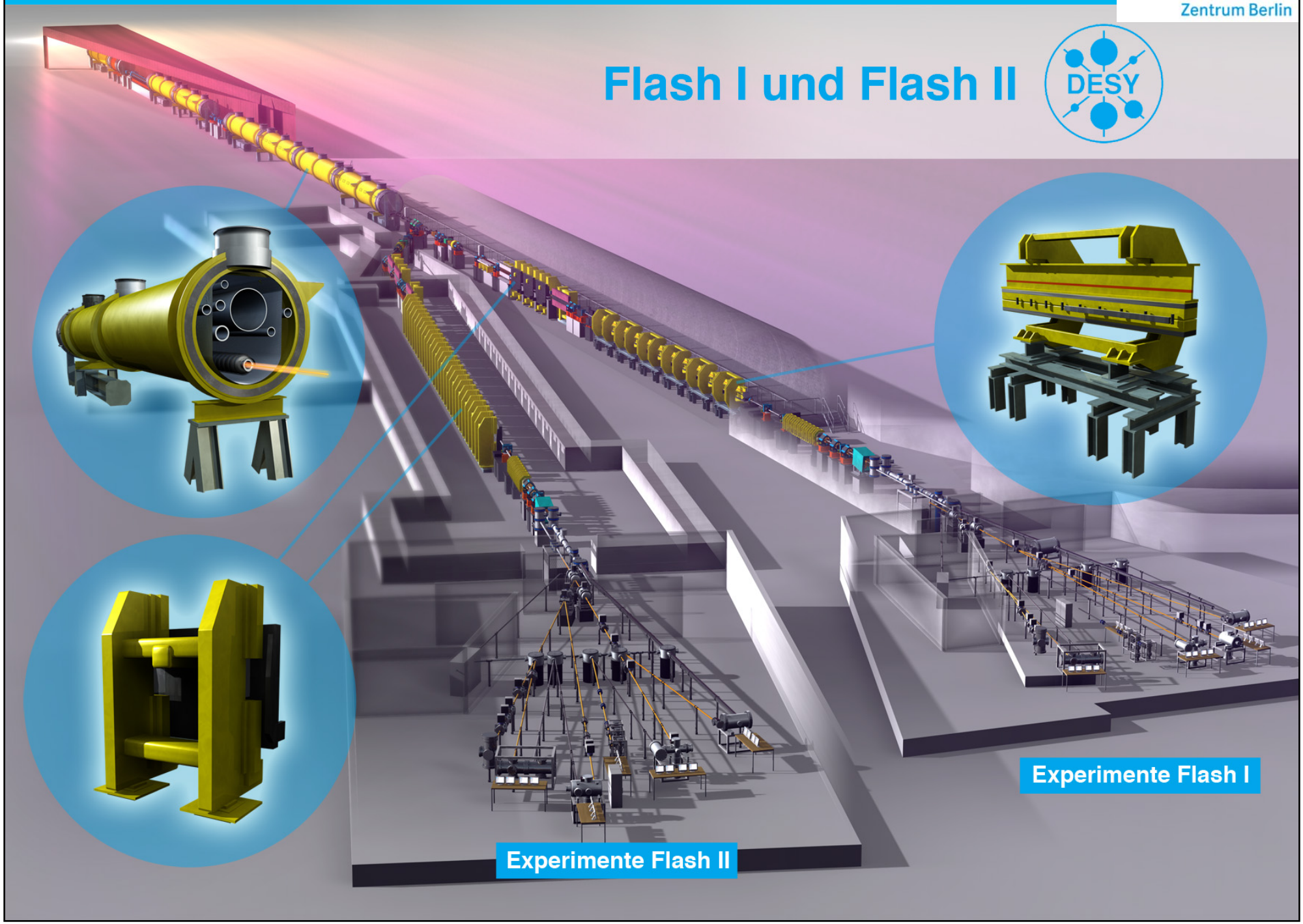
No. of beamlines:	5

FLASH: schematic layout

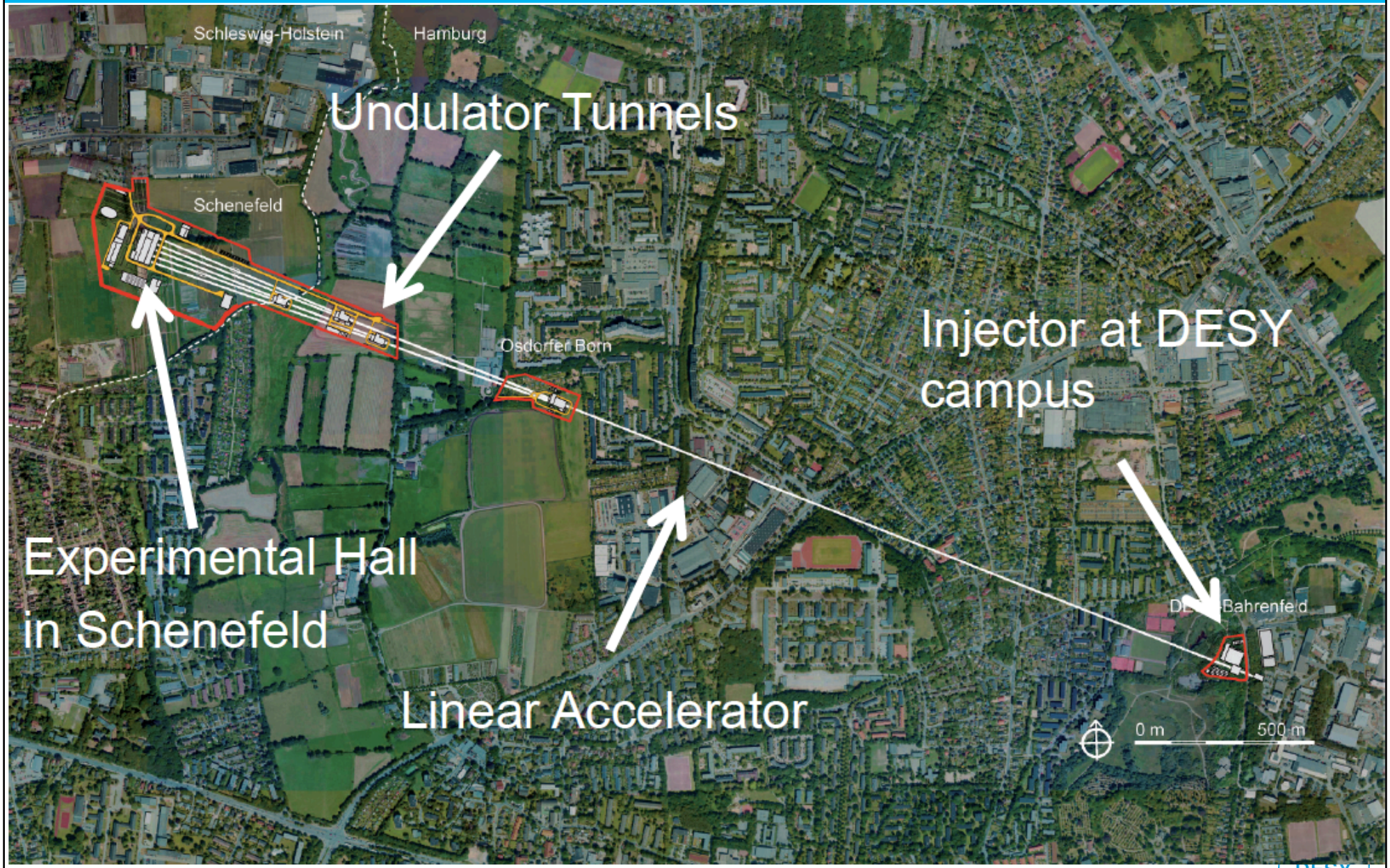
FLASH Upgrade



Flash I und Flash II

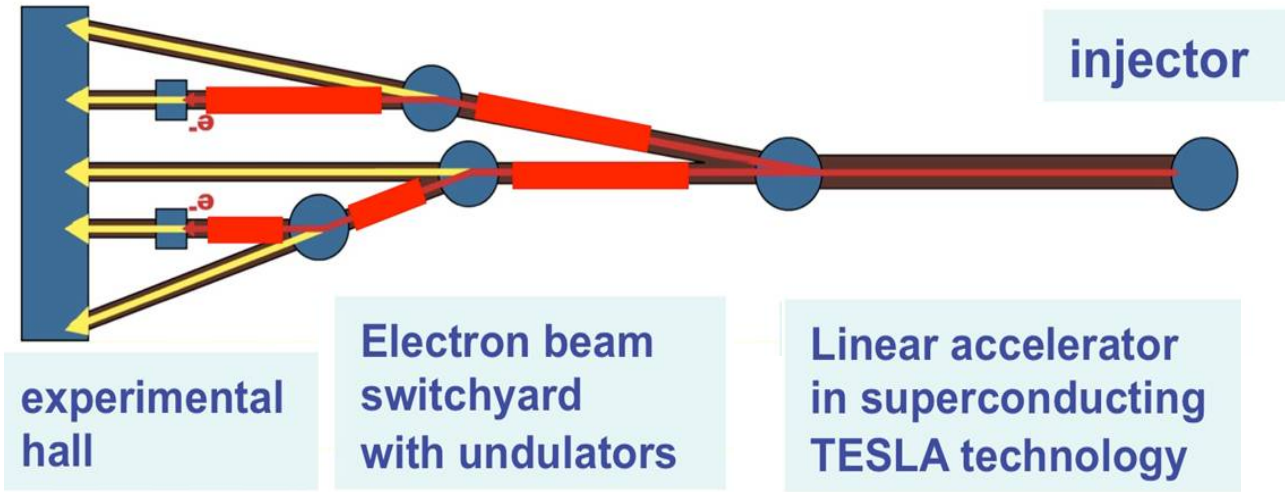


European XFEL Facility



European XFEL Facility

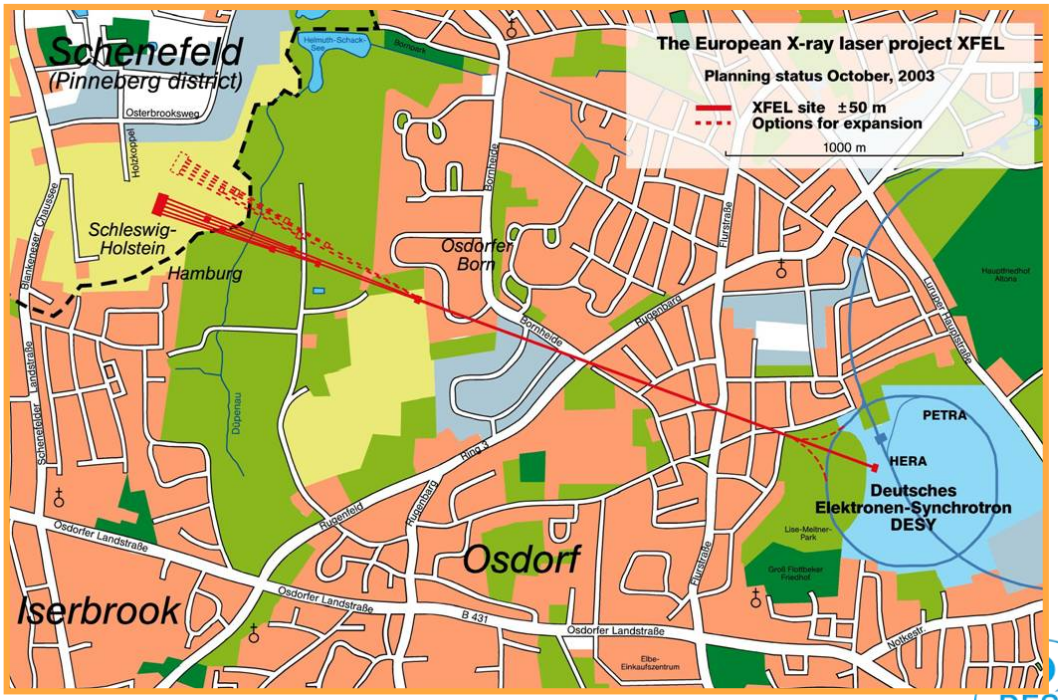
XFEL: Schematic Layout



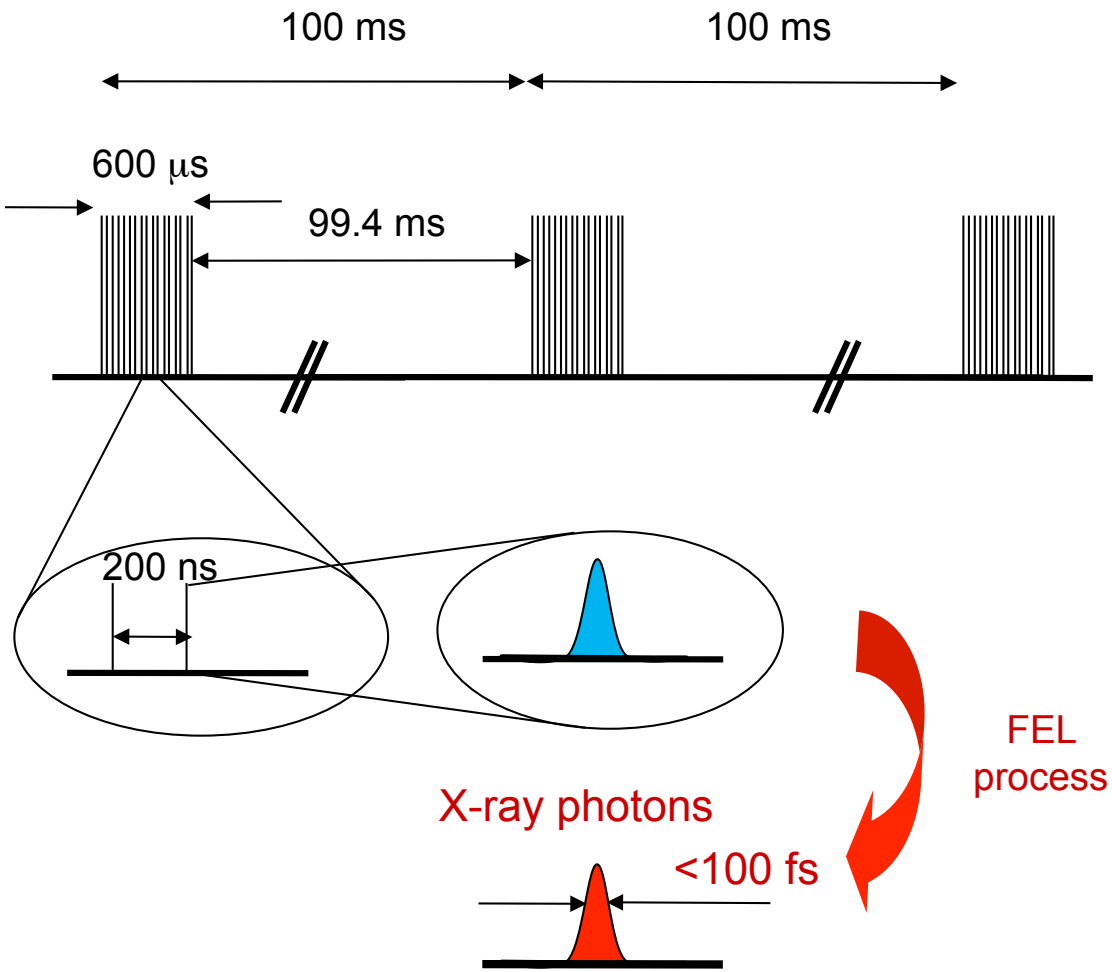
Linac: 17.5(14) GeV
min. wavelength: <1 Å
photons per pulse: ~10^{12}
pulse length: ~10-100 fs
No. of bunches: 30000 1/s

2 X-ray SASE FELs,
1 SASE XUV-FELs, and
2 beamlines; not in phase I

10 experimental stations

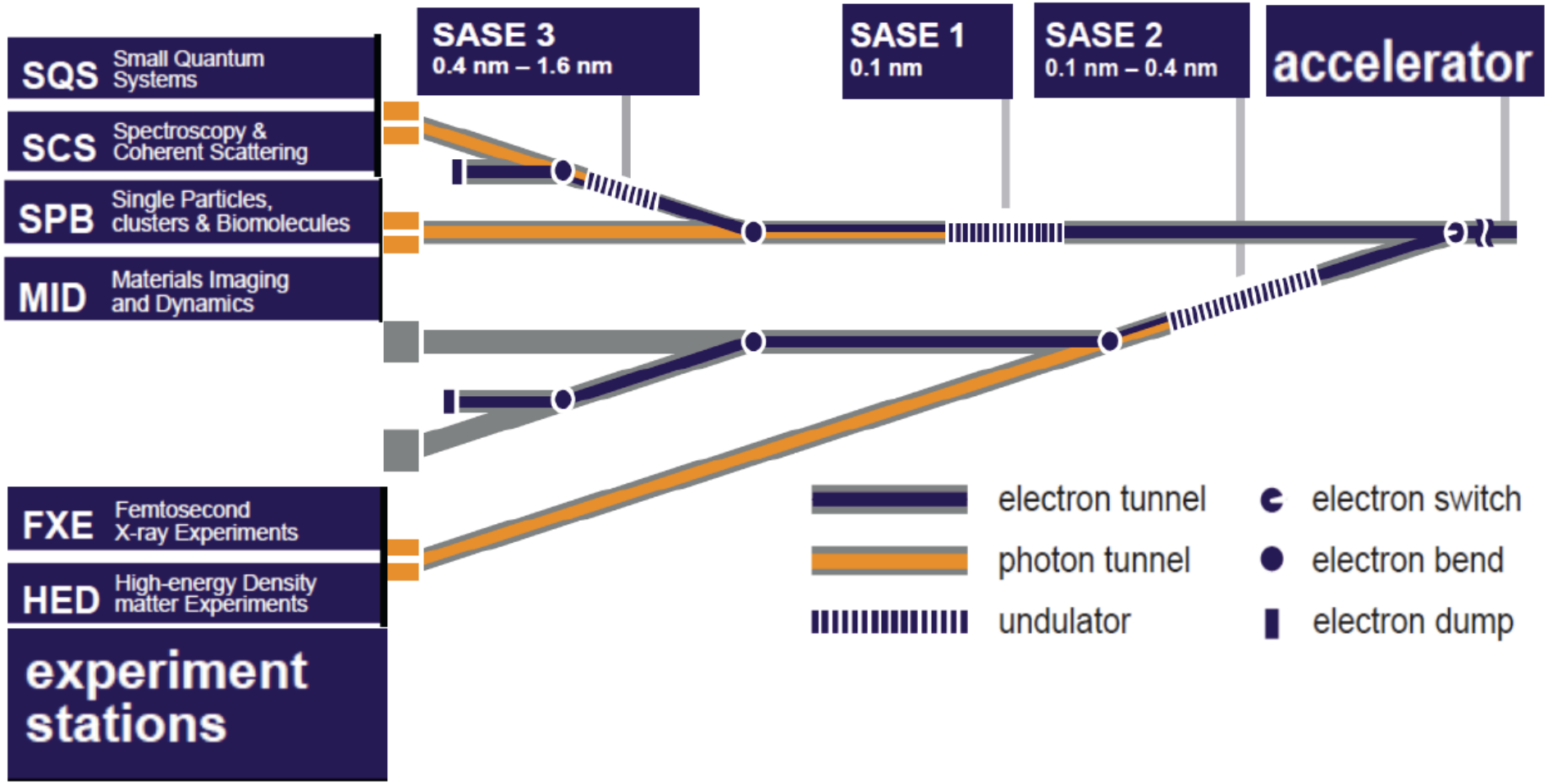


European XFEL: Bunch Structure



- up to 30,000 bunches per second
- very high intensities (up to 10^{12}/bunch)
- very high repetition rates (up to 5 MHz)
- large variability
  - pulse patterns
  - pulse to pulse variations
- future options
  - 30000 bunches in 25 Hz bunch trains
  - CW operation at lower gradient

European XFEL: experimental stations



First experiments: 2014/2015

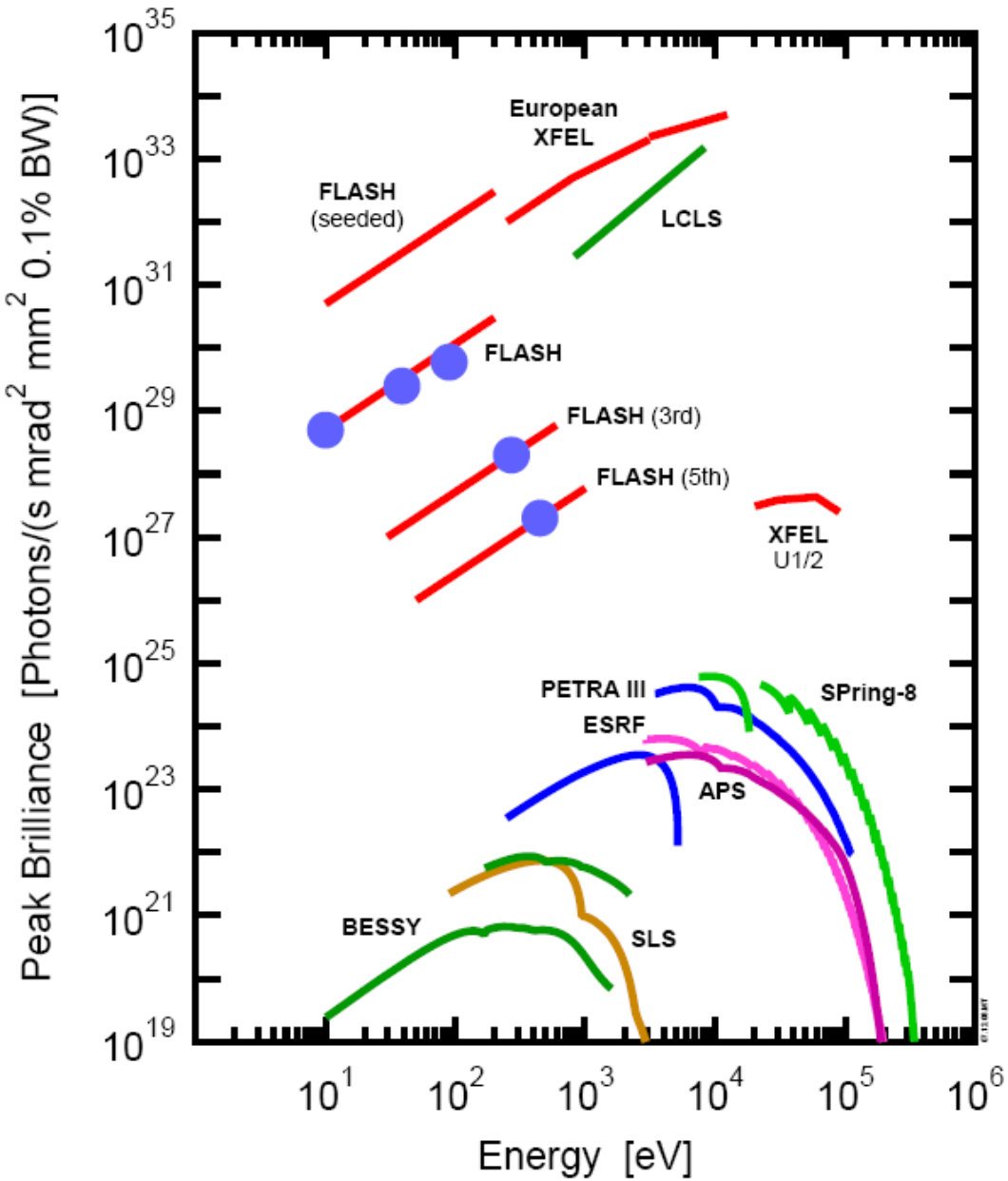
European XFEL: first tunnel segment finished

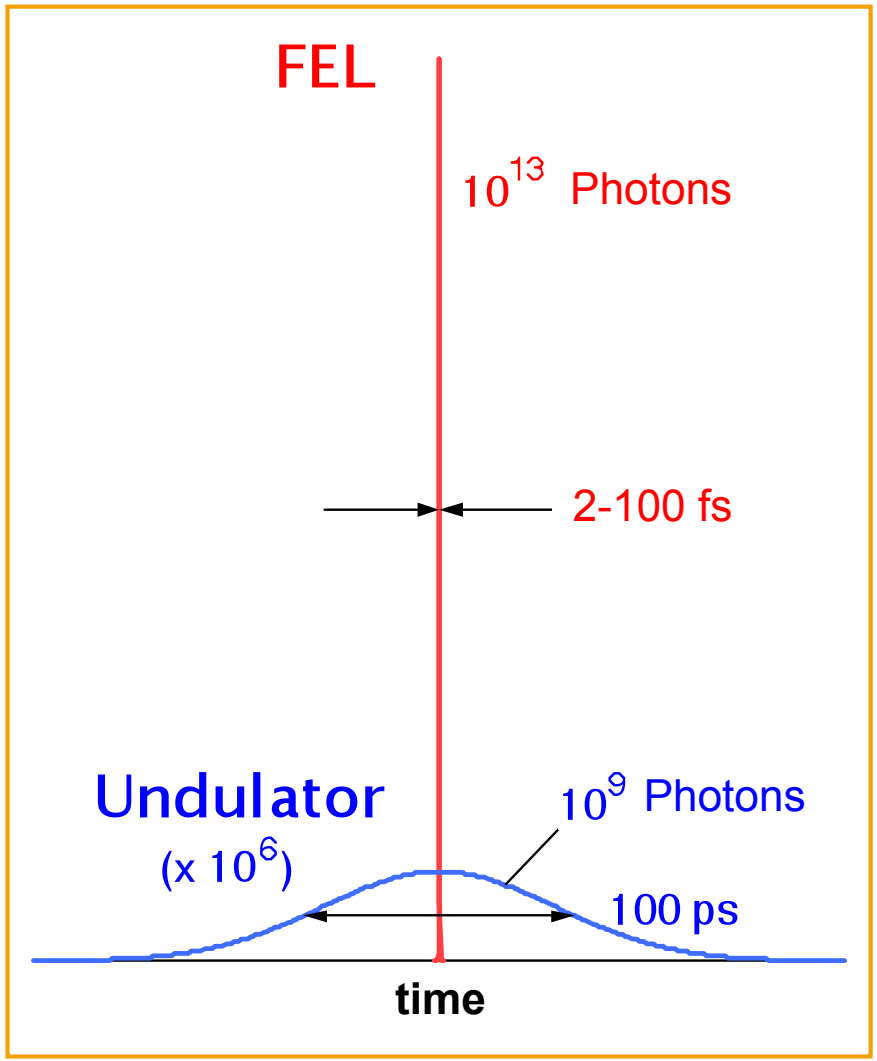
European XFEL: first tunnel segment finished

Properties of XFEL radiation

> **Extremely high peak brilliance due to pulse durations from ~ 2-5 fs to 100-200 fs**

Properties of FEL radiation





Properties of XFEL radiation

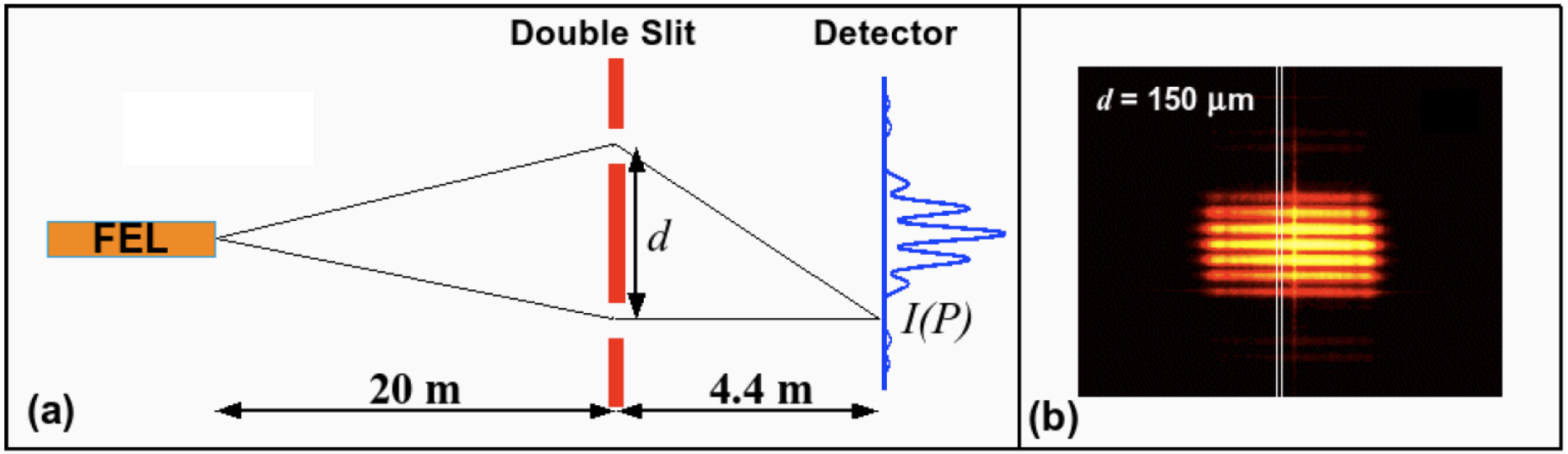
- Extremely high peak brilliance due to pulse durations from ~ 2-5 fs to 100-200 fs
  - ~ 1000 times shorter than at storage rings (SR)
  - one pulse provides the same number of photons as a SR in 0.1-1 s

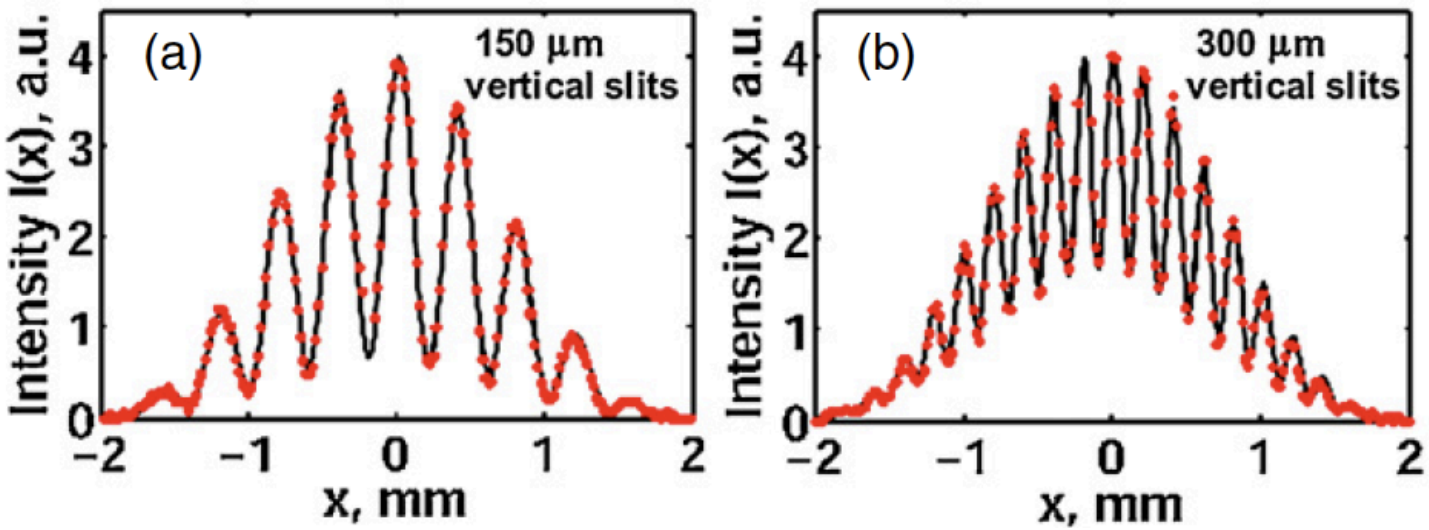
  ➔ investigation of phenomena on ultra short time scales down to atomic length scales, e.g.:
  - reaction dynamics
  - non equilibrium states of matter

- Very high degree of transfers coherence

Coherence properties of XFEL radiation

Vartanyants et al., J. Phys. B. 43 (2010) 194016





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- reaction dynamics
- non equilibrium states of matter

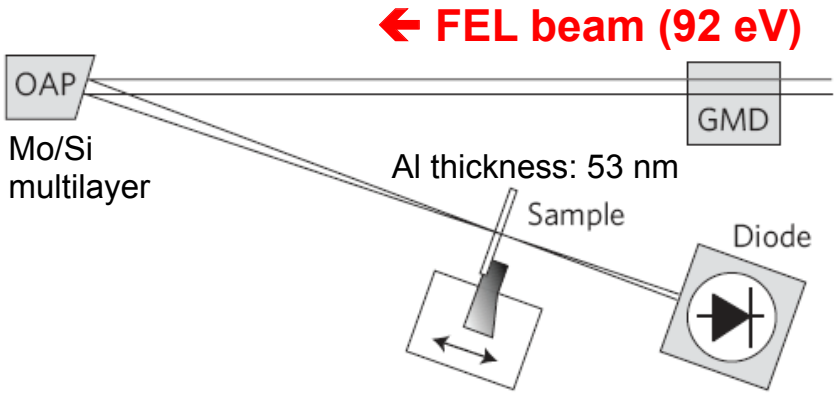
> Very high degree of transverse coherence
- 35 - 85 % degree of transverse coherence measured (SR: <1%)

➔ diffraction from non-translation periodic objects

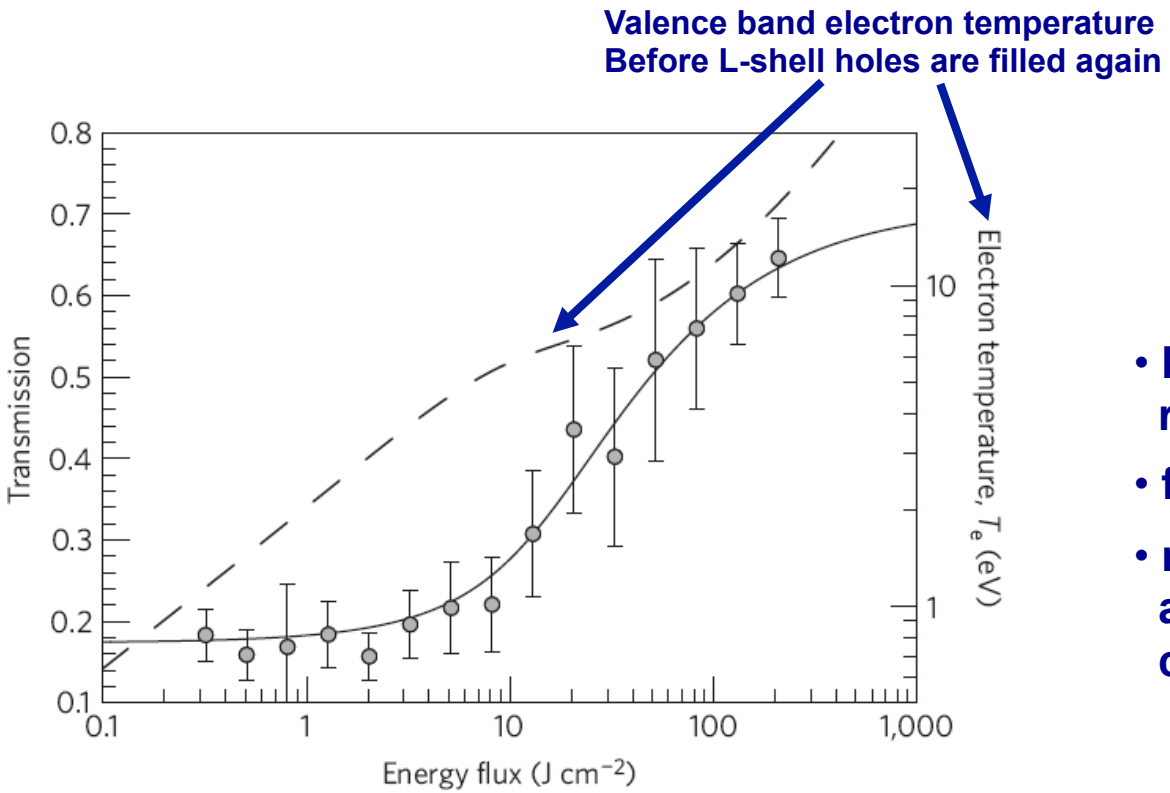
➔ holographic imaging techniques

Generating and exploring non-equilibrium states of matter

- after X-ray pulse: all Al-atoms have an L-shell hole, valence band ~ 9 eV
- L-hole life time: ~ 40 fs
- reduced screening ➔ E_L is increased > 92 eV
- Auger decay heats VB e^- to ~ 25 eV
- ➔ homogenous warm dense matter



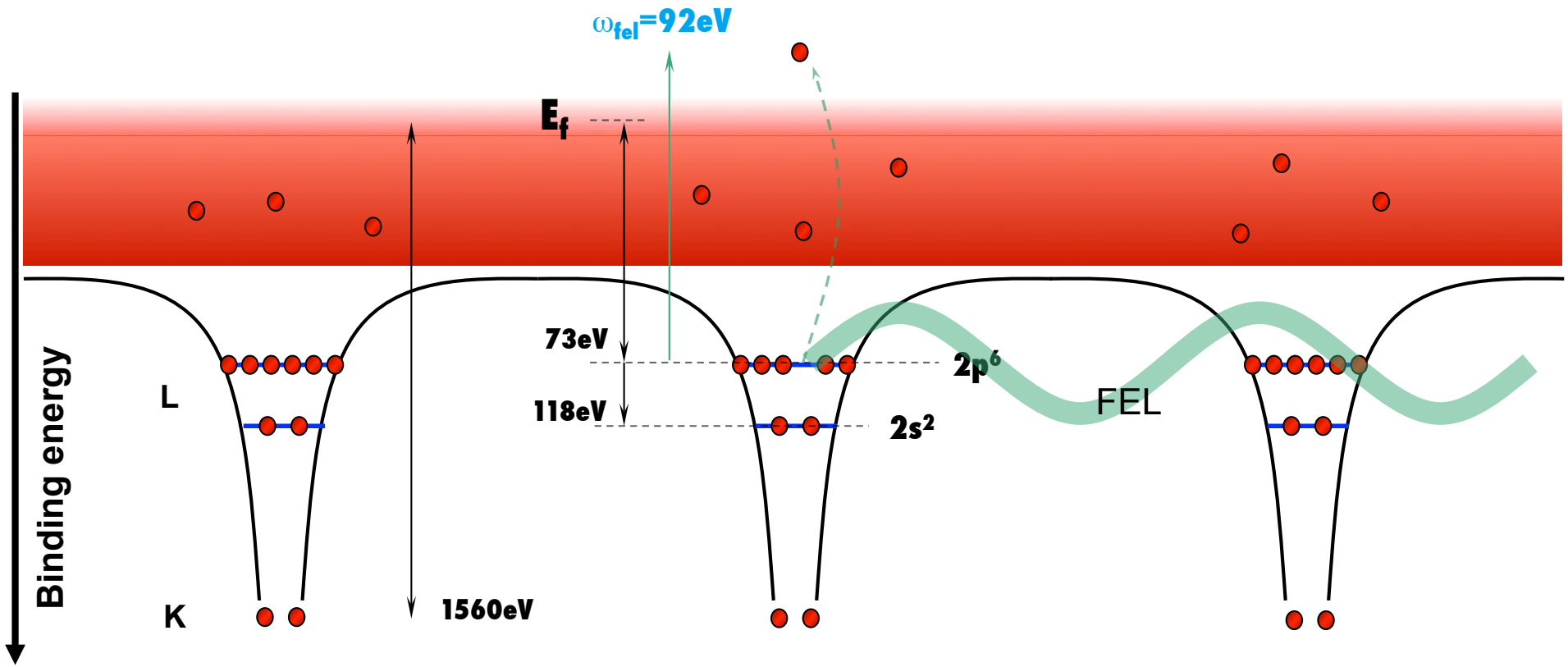
focus: 1.5 – 45 µm
up to > 10^{16} W/cm^2



B. Nagler et al., Nature Physics (2009)

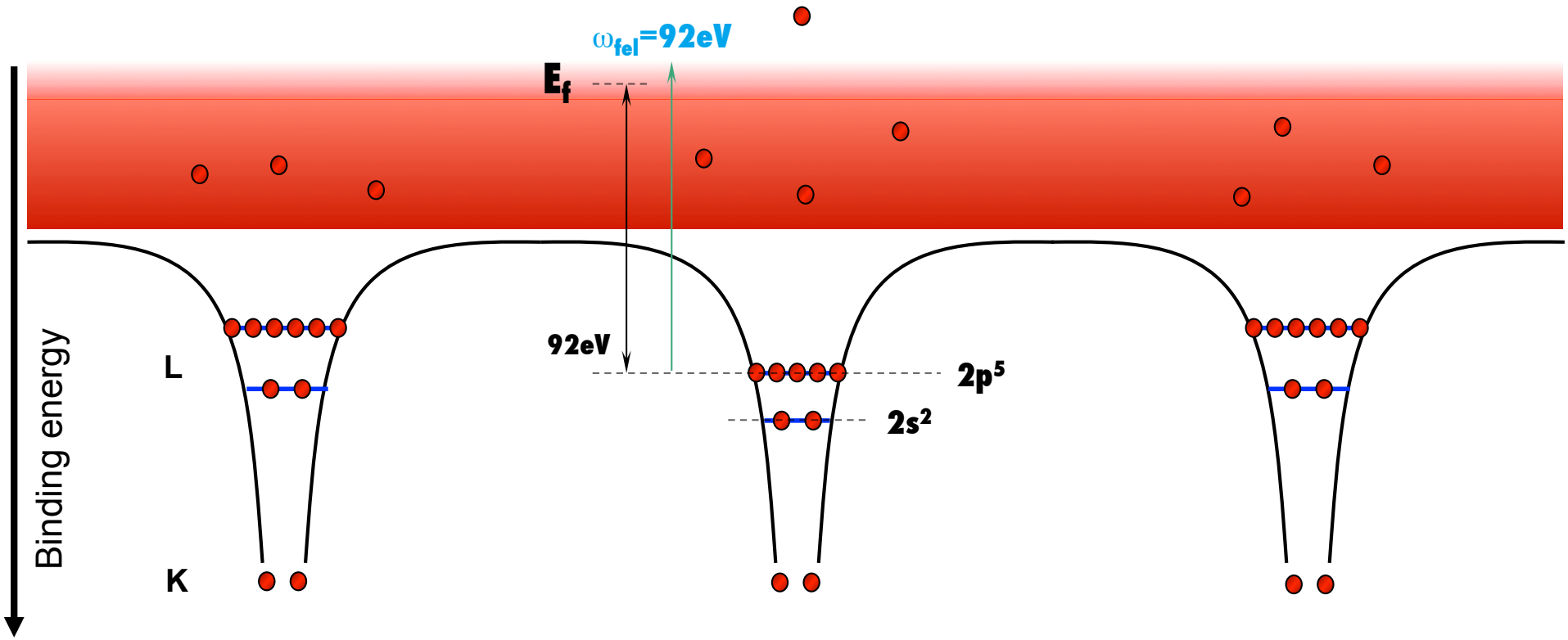
- known effect in optical or infra-red experiments
- first observation for core levels
- relevant to planetary science, astro physics and inertial confinement fusion

A single FEL pulse ionizes all Al atoms



Absorption of FLASH photons in the L shell: photoionization

Level shift due to core hole ➔ reduced absorption



L core hole life time: 40 fs

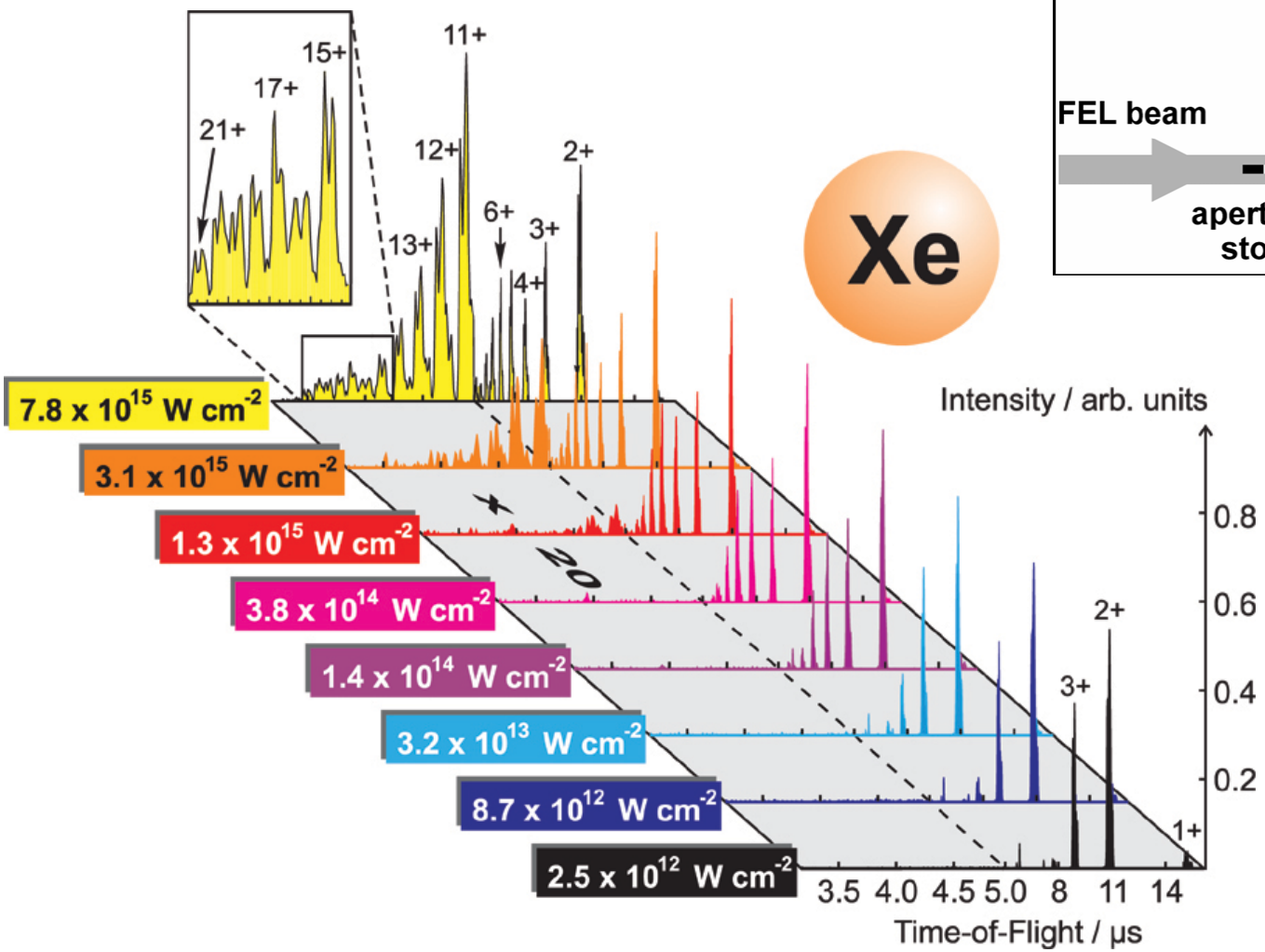
➔ Level shift of L absorption edge

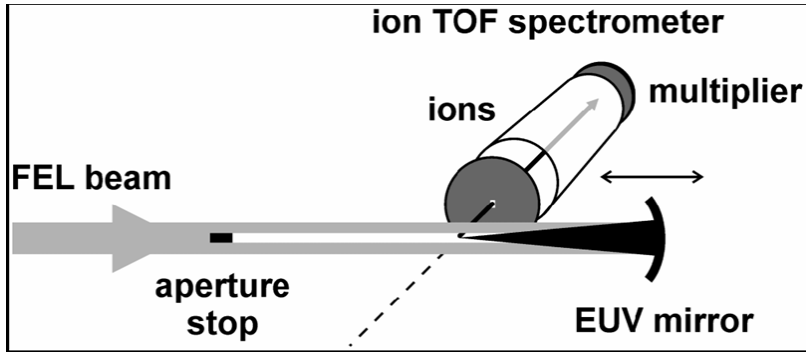
➔ Strongly reduced absorption

➔ ‚transparent' aluminium

➔ energy deposition: one core hole per atoms

Nonlinear Interaction of Light and Matter





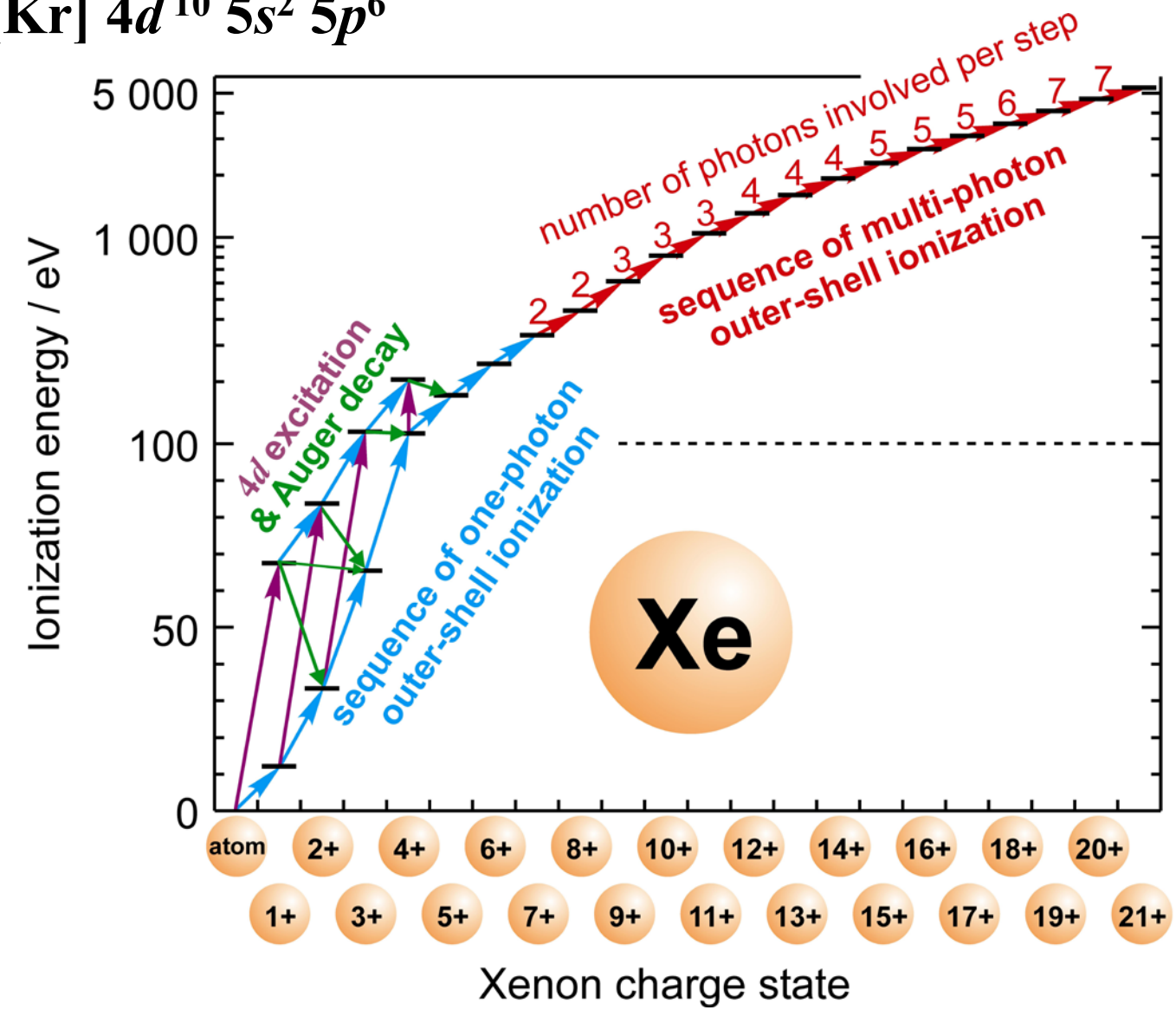
focus size < 3µm

Xe^{21+} requires
> 5keV energy
i.e. absorption of
> 50 photons@93eV
in ~10fs

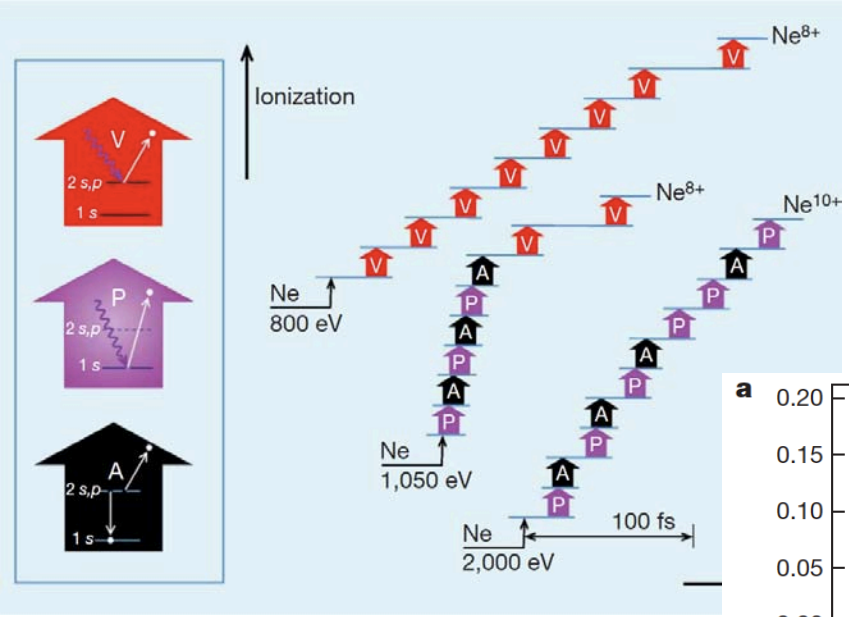
A. A. Sorokin et al., Photoelectric Effect at Ultrahigh Intensities, PRL 99, 213002 (2007) collaboration PTB, Ioffe Institute, Fraunhofer Jena, DESY

Nonlinear Interaction of Light and Matter: Xe^{21+}

Xe: [Kr] $4d^{10}\,5s^2\,5p^6$

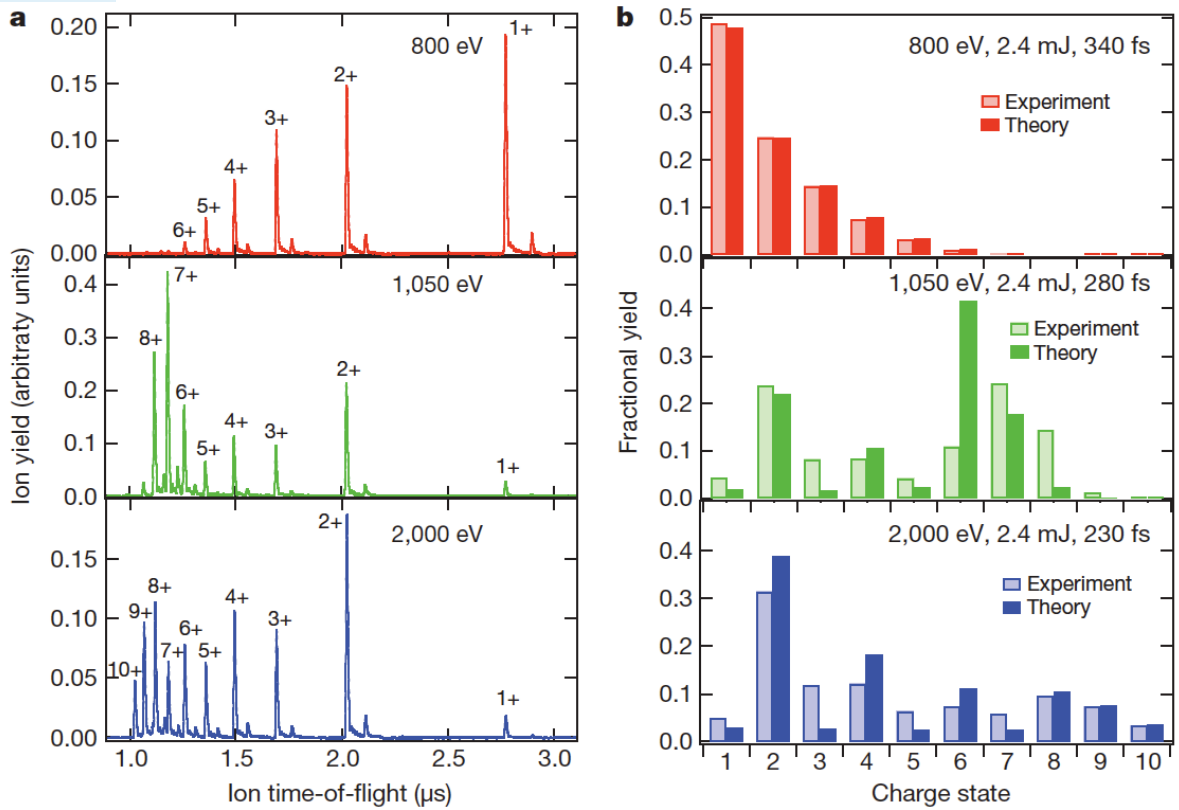


Ionization dynamics of Ne



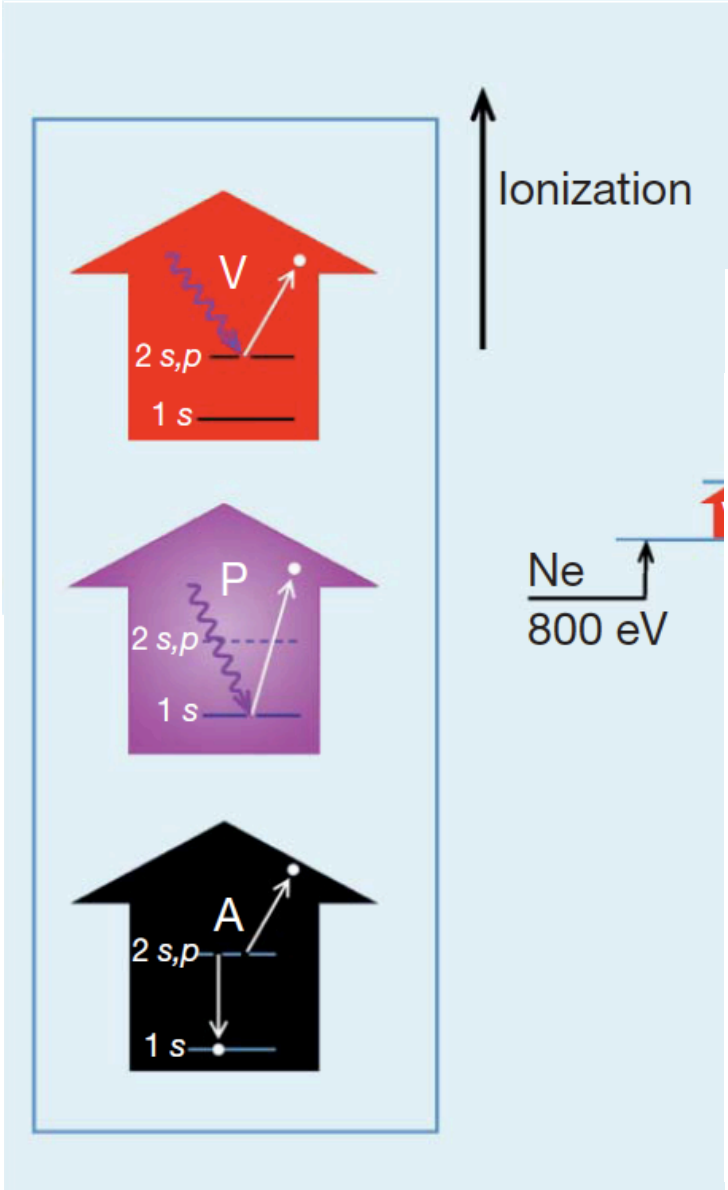
- **Reasonable agreement between theory and experiment**
- **Ratio between single and double core hole provides indication on the photon pulse length**

LCLS at about 2.3 mJ/pulse



L. Young et al., Nature 446 (2010) 57-62

Ionization dynamics of Ne



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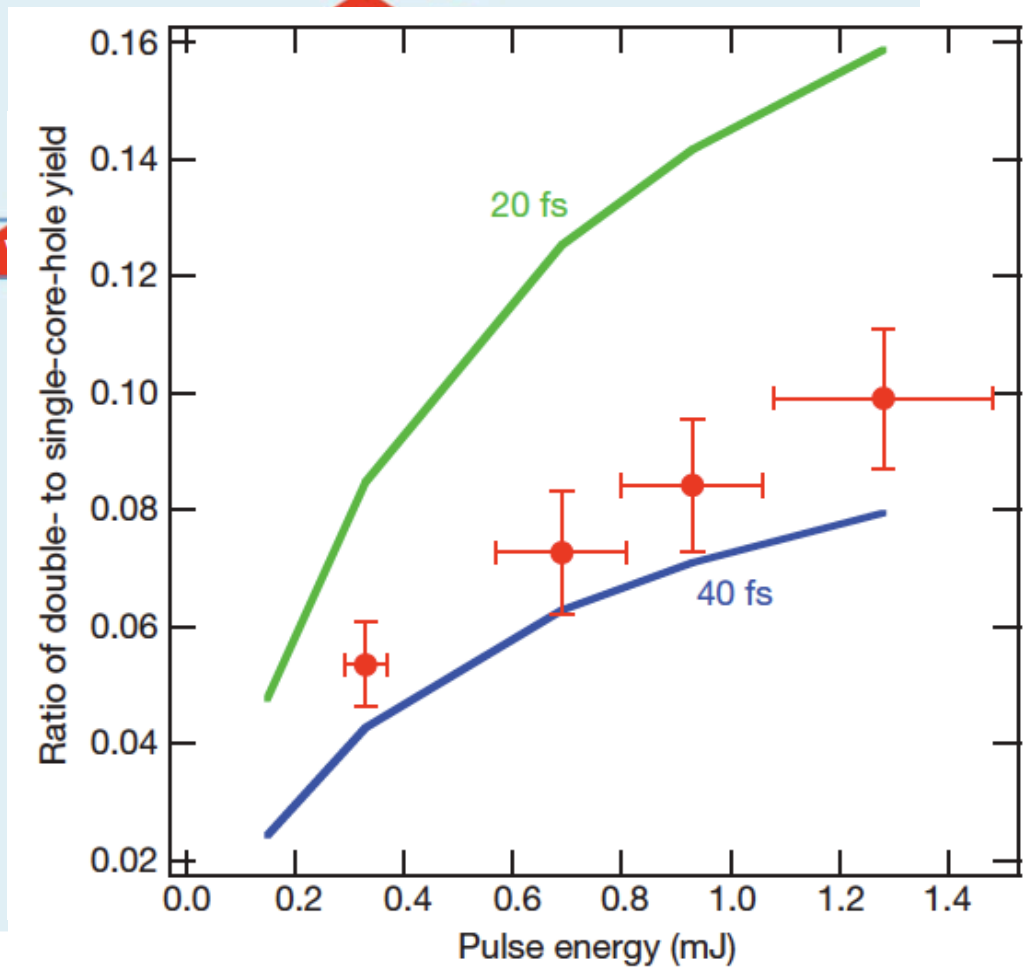


L. Young et al., Nature 446 (2010) 57-62

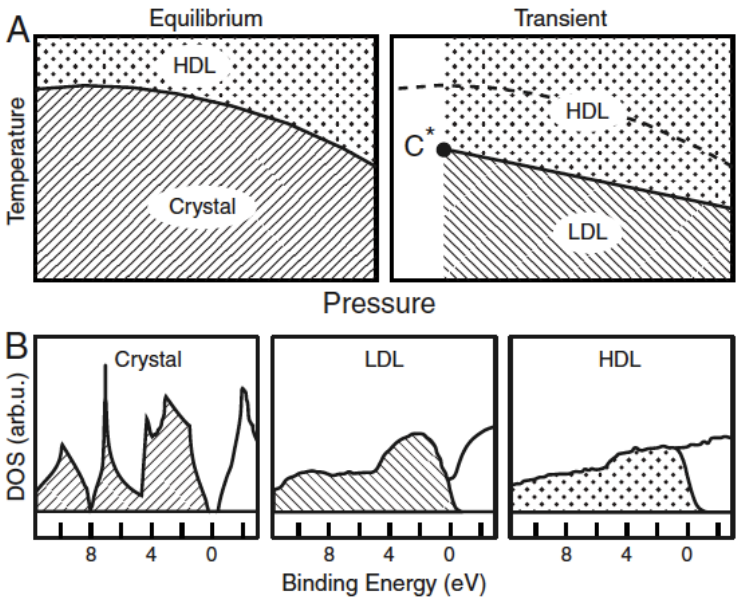
Optical laser pump - FEL probe experiments

The liquid-liquid phase transition in silicon revealed by snapshots of valence electrons

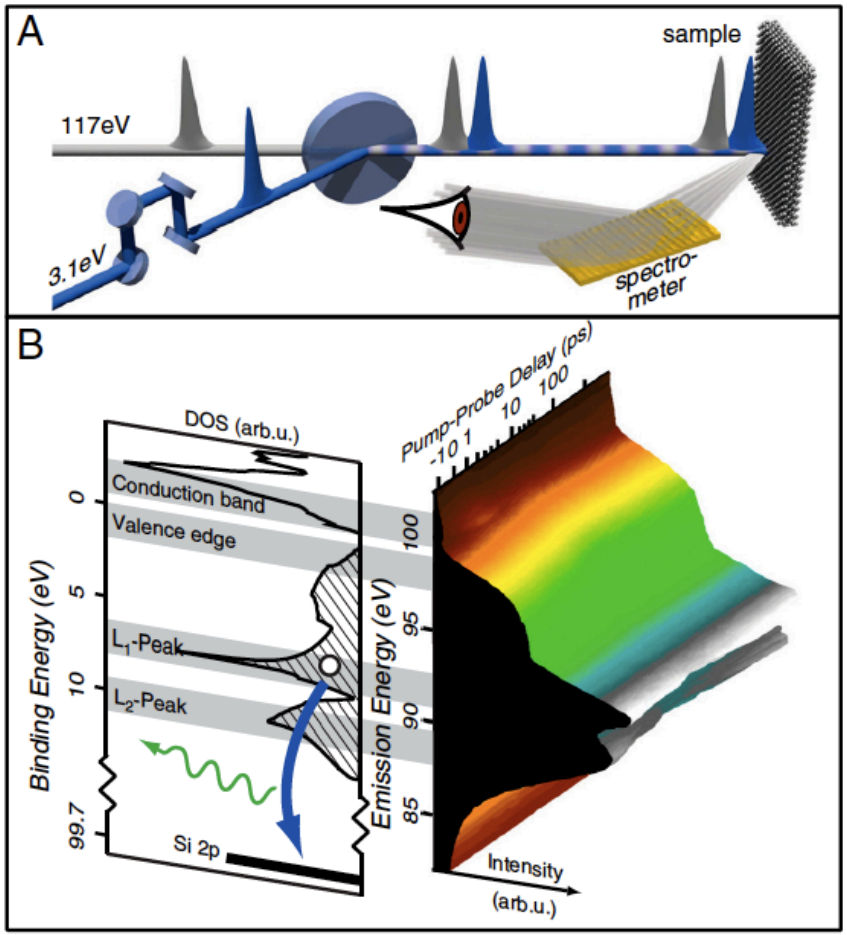
Martin Beye[1,2], Florian Sorgenfrei, William F. Schlotter[3], Wilfried Wurth, and Alexander Föhlisch[2]

Institut für Experimentalphysik, Universität Hamburg and Centre for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany

PNAS 107, 16772-16776 (2010)



As the relevant phases are easily distinguishable in their electronic structure, we track how silicon melts into the low-density-liquid phase while a second phase transition into the high-density-liquid phase only occurs after the latent heat for the first-order phase transition has been transferred to the atomic structure. Proving the existence of the liquid-liquid phase transition in silicon, the hypothesized liquid-liquid scenario for water is strongly supported.



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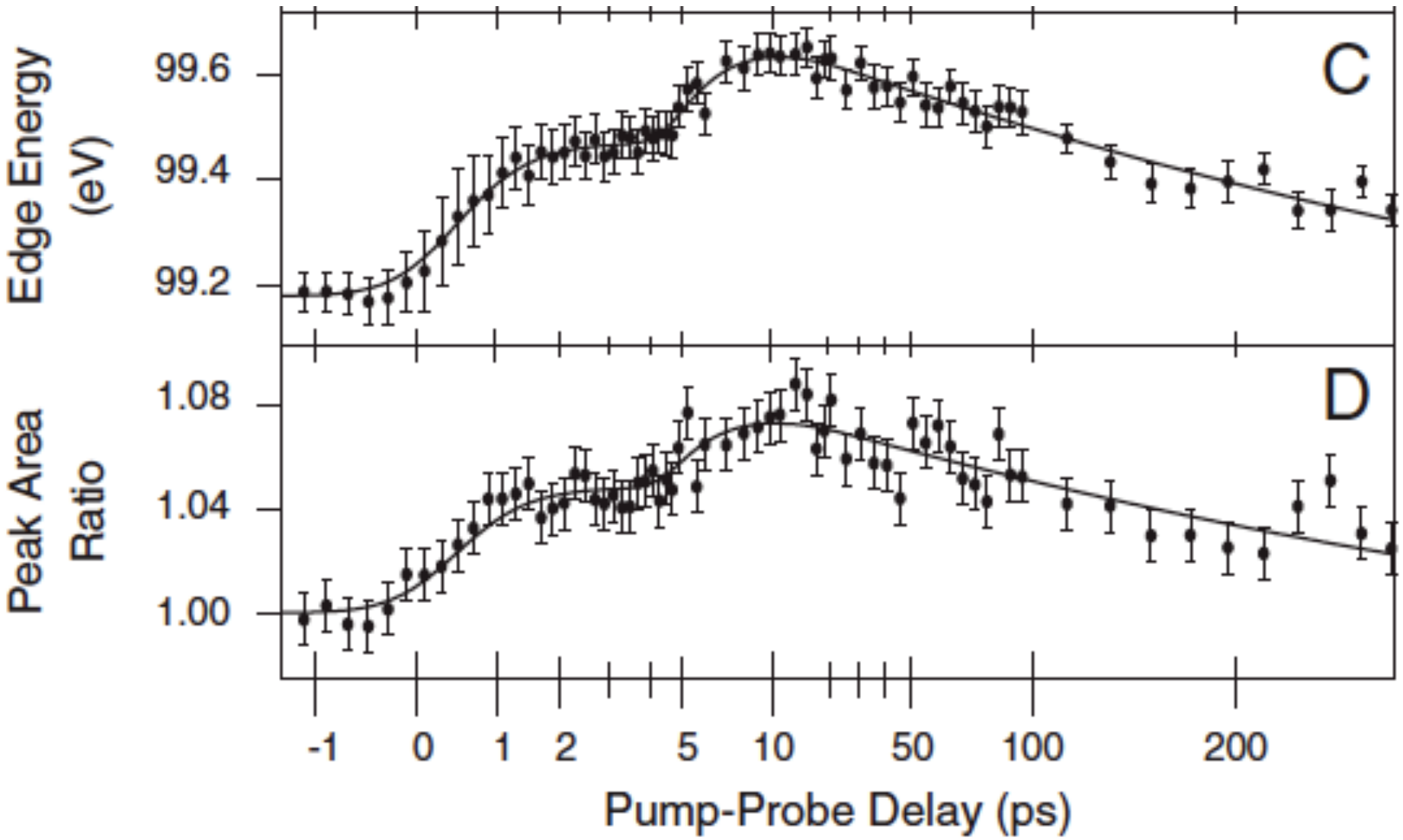
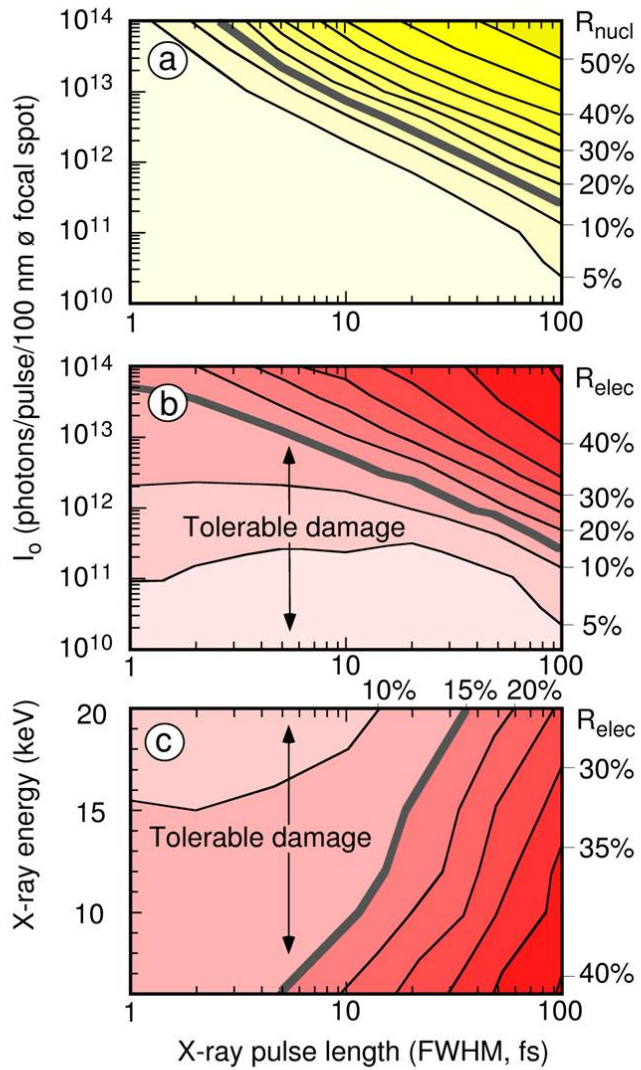


Single particle imaging: Dynamics of radiation damage

Estimates for radiation damage:

- **Under the assumptions made: damage remains 'tolerable' for a 50-100 fs pulse of 3-10x10^{11}ph/(100nm)^2**
- **If the samples are smaller than the mean free path of a photo electron and under assumption that also half of the Auger electrons escape: 3x10^{10}ph/(100nm)^2 seem to be tolerable.**
- **At a pulse length of 2 fs more than 10^{13}ph/(100nm)^2 should be tolerable**

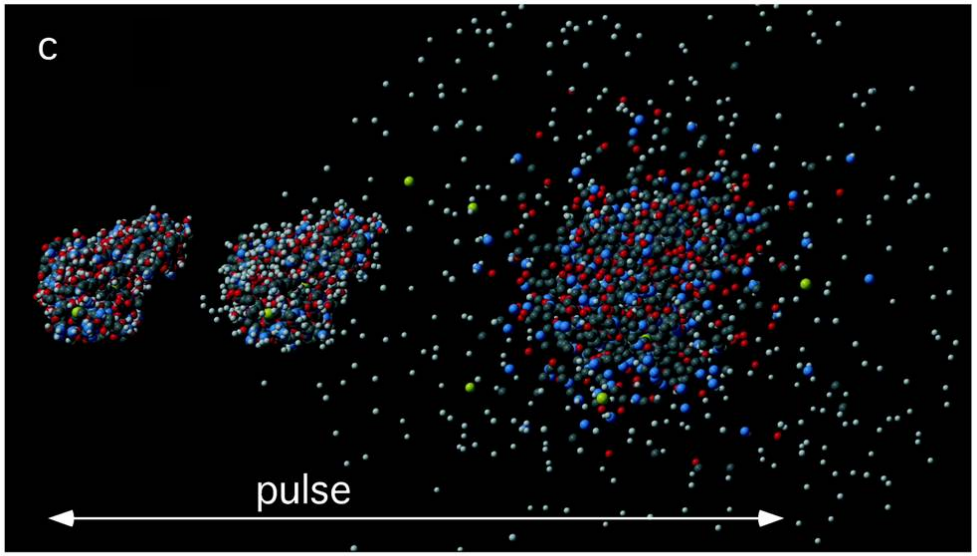


Neutze, Wouts, v. d. Spoel, Weckert, Hajdu , Nature **406** (2000) 752

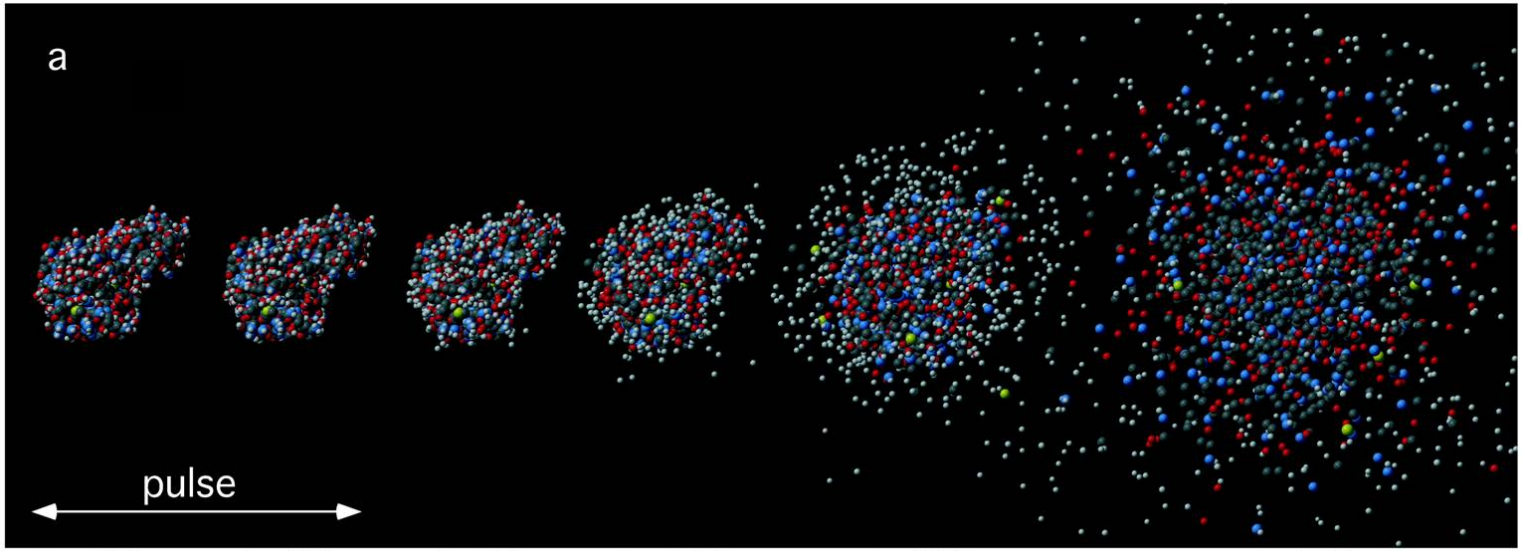
Single Particle Imaging: Dynamics of radiation damage

Neutze et al., Nature, (2000)

MD simulations:
$3x10^{12}$ph/(100nm)^2
per pulse



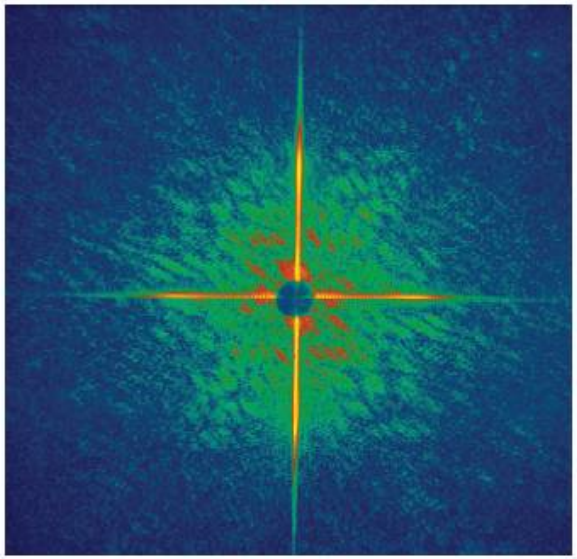
t=-50fs t=0fs t=50fs

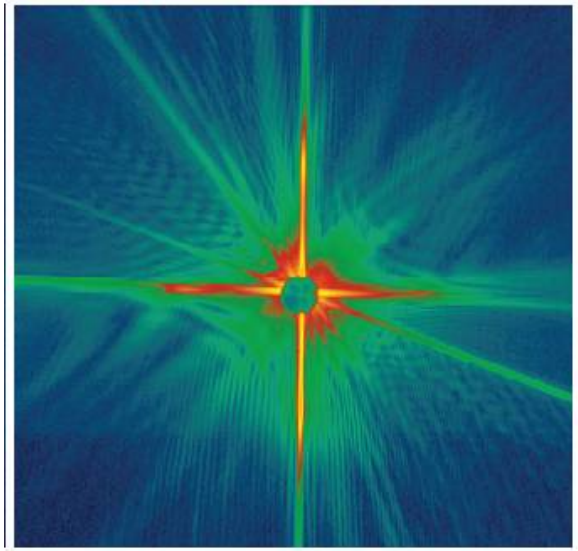


t=-2fs t=2fs t=5fs t=10fs t=20fs t=50fs

Ultrafast coherent diffraction

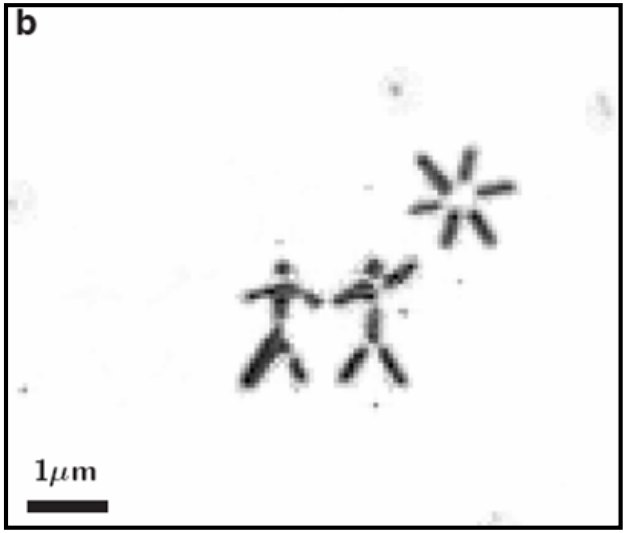
diffraction pattern from first pulse

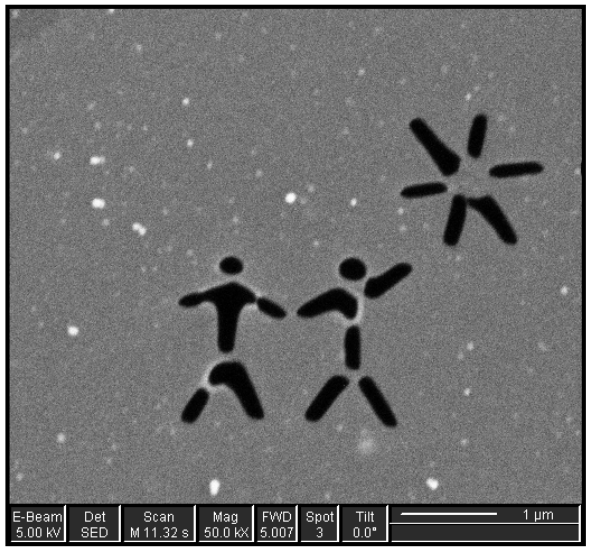




diffraction pattern from second pulse

reconstructed picture

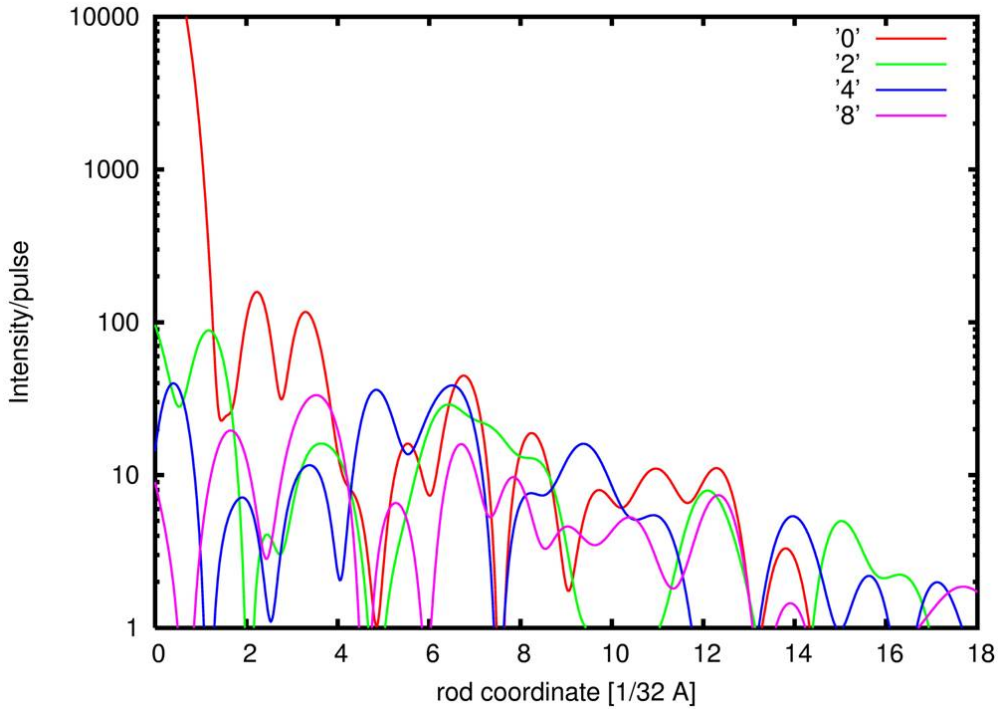


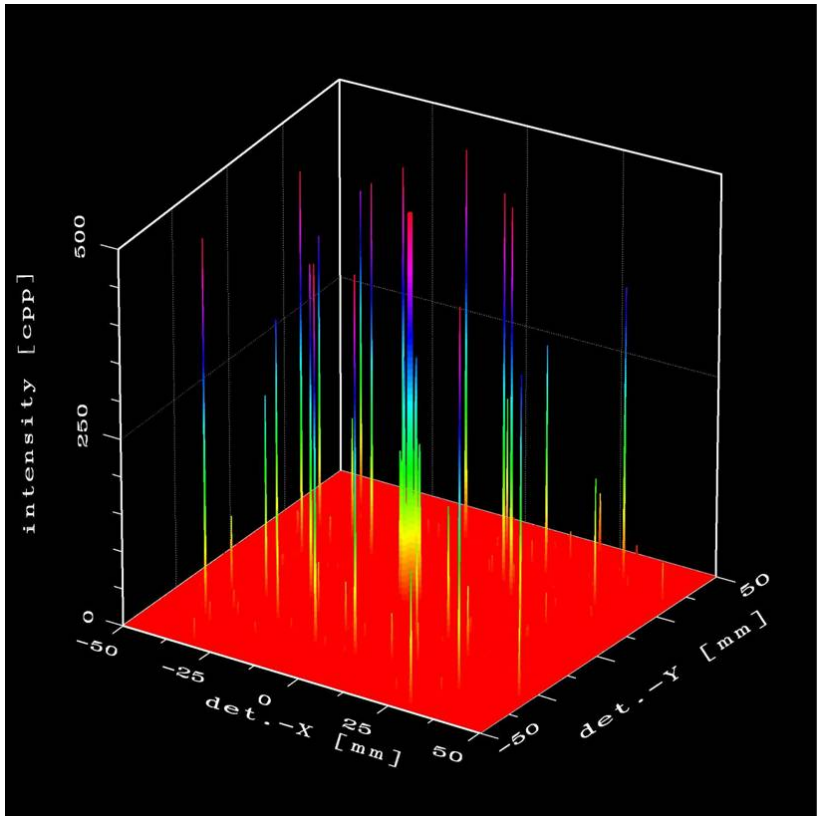


TEM picture from original structure

H. Chapman, J. Hajdu et al., Nature Phys., **2** (2006) 839

2D arrays of macromolecules and nano crystals



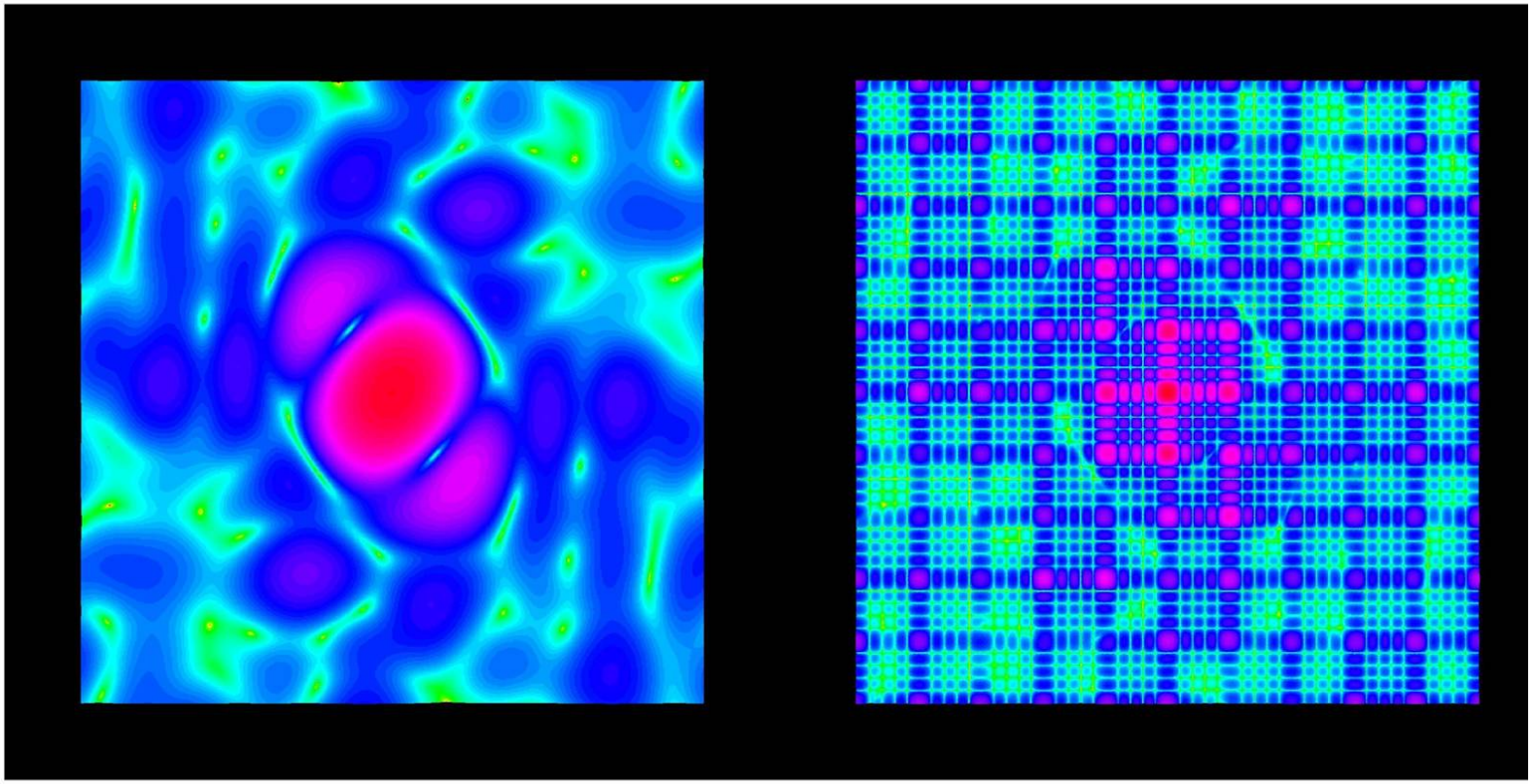


1500^2 molecules
single pulse with 10^{12}ph/(5μm)^2

50^3 molecules
single pulse with 3 x 10^{10} ph/(0.1μm)^2

Difference: crystal and non-translation periodic object

hk0 – plane in reciprocal space



single molecule **5 x 5 x 5 crystal (P – lattice)**

crystal: rather small coherence lengths are sufficient
non-translation periodic object: coherent illumination required

Conclusion

- X-ray FELs provide unprecedented possibilities for the structure and dynamics of matter

- fs - short and extremely intense photon pulses enable
  - to study states of matter far away from equilibrium
  - to follow the kinetics and structure of intermediates in chemical reactions
  - to overcome (slow) radiation damage in single pulse exposures
  - to explore non-linear phenomena
  - …

- transverse coherent radiation pulses enable
  - single particle diffraction experiments
  - holographic imaging techniques
  - …

- tbc …

Thank you for your attention