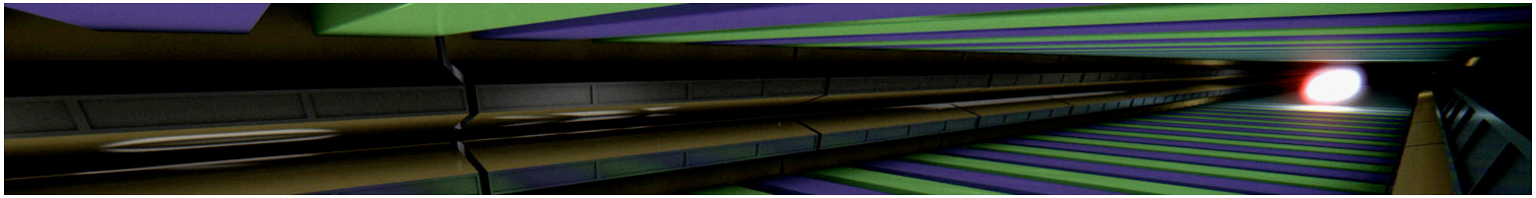


The Single Particles, clusters and Biomolecules (SPB) Instrument of the European XFEL: The Conceptual Design

Adrian Mancuso

Single Particles, clusters and Biomolecules (SPB)

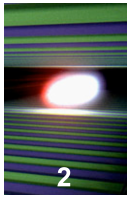
European XFEL

European XFEL

Outline

- Single particle imaging science–an ultrafast introduction
- The 3 canonical types of experiment
- Constraints on the design from these experiments
- Properties of the SASE 1 photon beam
- The SPB optical layout
- SPB Modeling program
- Sample delivery
- Detector requirements and detector specifications
- Conclusions

Outline



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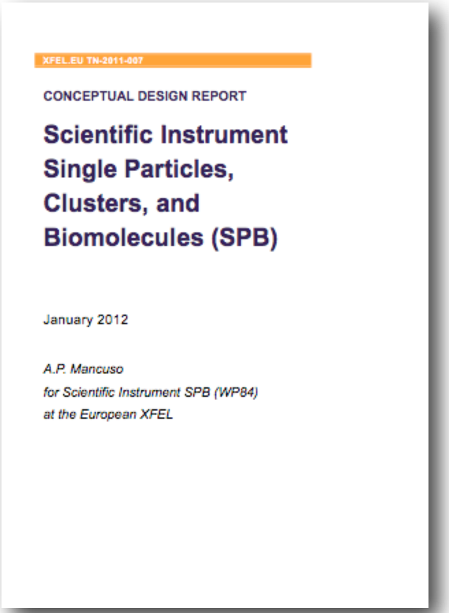
XFEL.EU TN-2011-007

CONCEPTUAL DESIGN REPORT

Scientific Instrument Single Particles, Clusters, and Biomolecules (SPB)

January 2012

A.P. Mancuso
for Scientific Instrument SPB (WP84)
at the European XFEL

European XFEL

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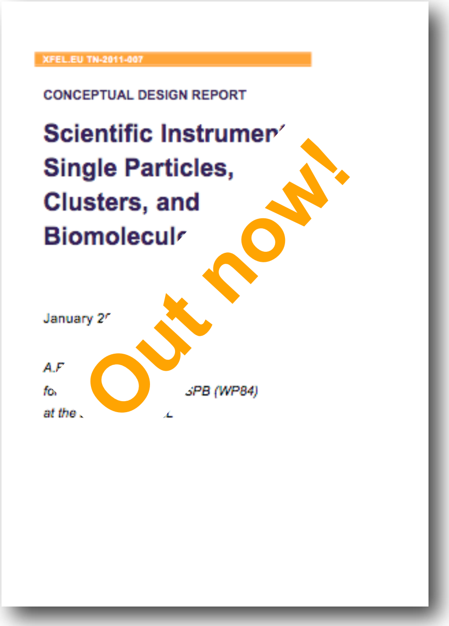

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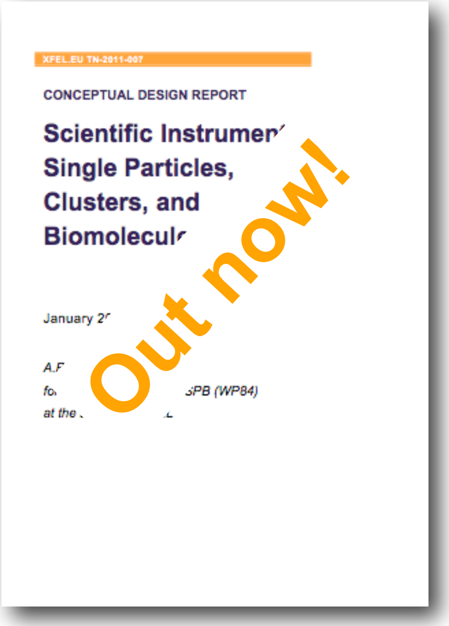

http://www.xfel.eu/documents/technical_documents

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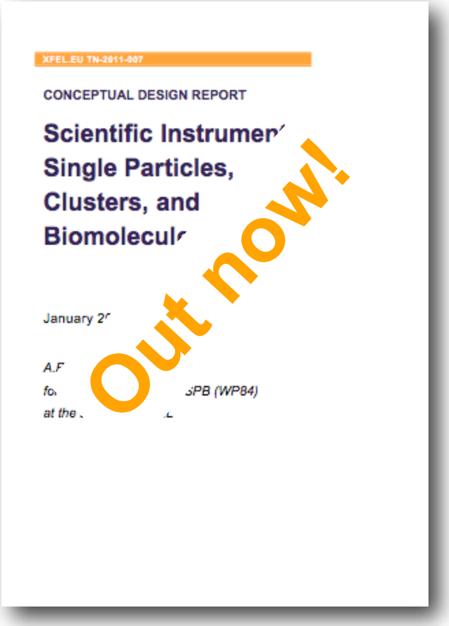

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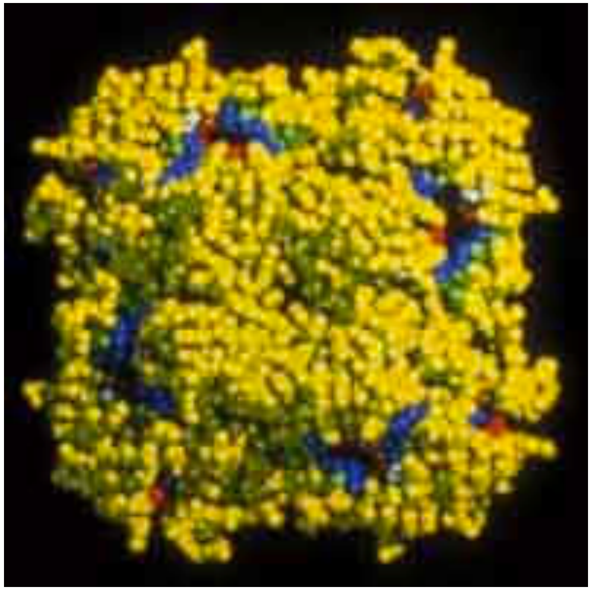
A New(ish) Imaging Technique: The Why of Coherent Imaging with Ultrashort Pulses

- Structure of a molecule -> function
- Structure allows, eg, Rational Drug Design, Understanding of human biochemistry.
- Photons (X-rays) allow depth information from intact systems.
- Coherent Diffraction Imaging (CDI) seeks to image molecules and structures unable to be imaged by other means. These are structures < microns.

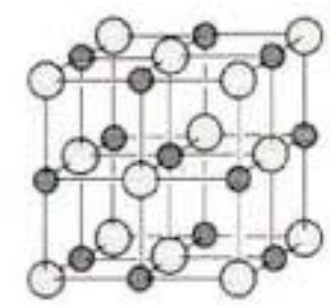


Influenza virus structure - A protein from the influenza virus

J. Varghese et al, CSIRO Health Sciences & Nutrition

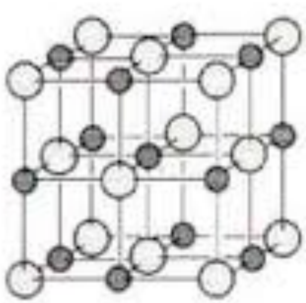
Review: A. P. Mancuso, *et al*, J. Biotechnol. **149** (2010) 229–237

Non-crystalline material scatters fewer x-rays than crystalline material



Scattered x-rays are proportional to N^2

Non-crystalline material scatters fewer x-rays than crystalline material



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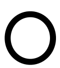

One guy scatters like... 1
(~ a lot less less than above)

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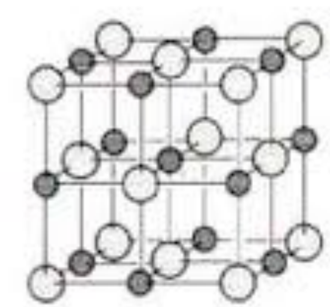

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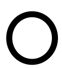

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Conclusion: Need a lot more x-rays to see a single particle

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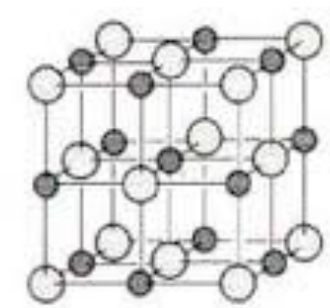

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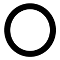

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(~ a lot less less than above)

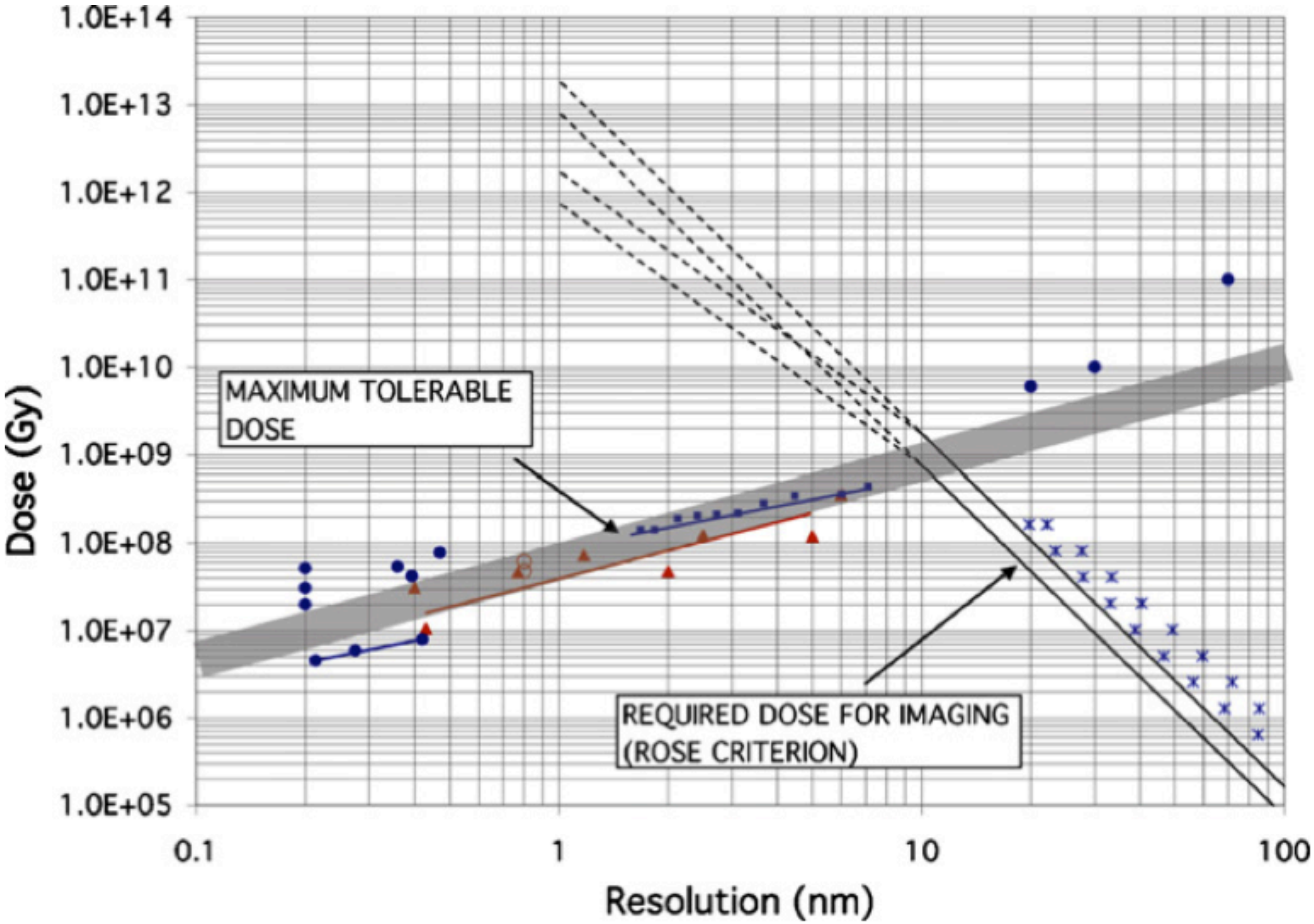
Conclusion: Need a lot more x-rays to see a single particle

First guess solution: Just leave the x-rays on for longer!

The problem of radiation damage

- M.R. Howells, et al, *Journal of Electron Spectroscopy and Related Phenomena 170 (2009)*

The problem of radiation damage



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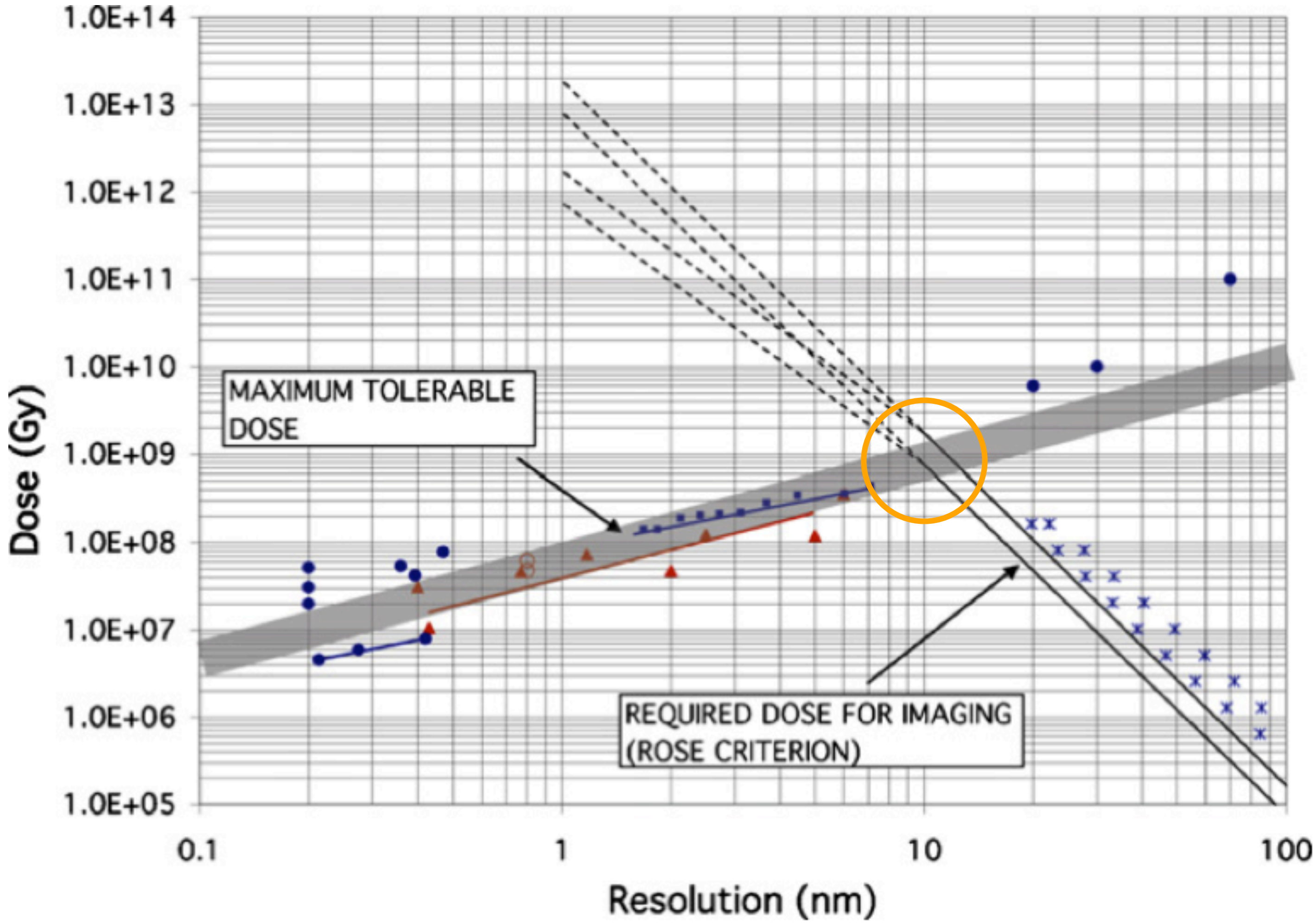
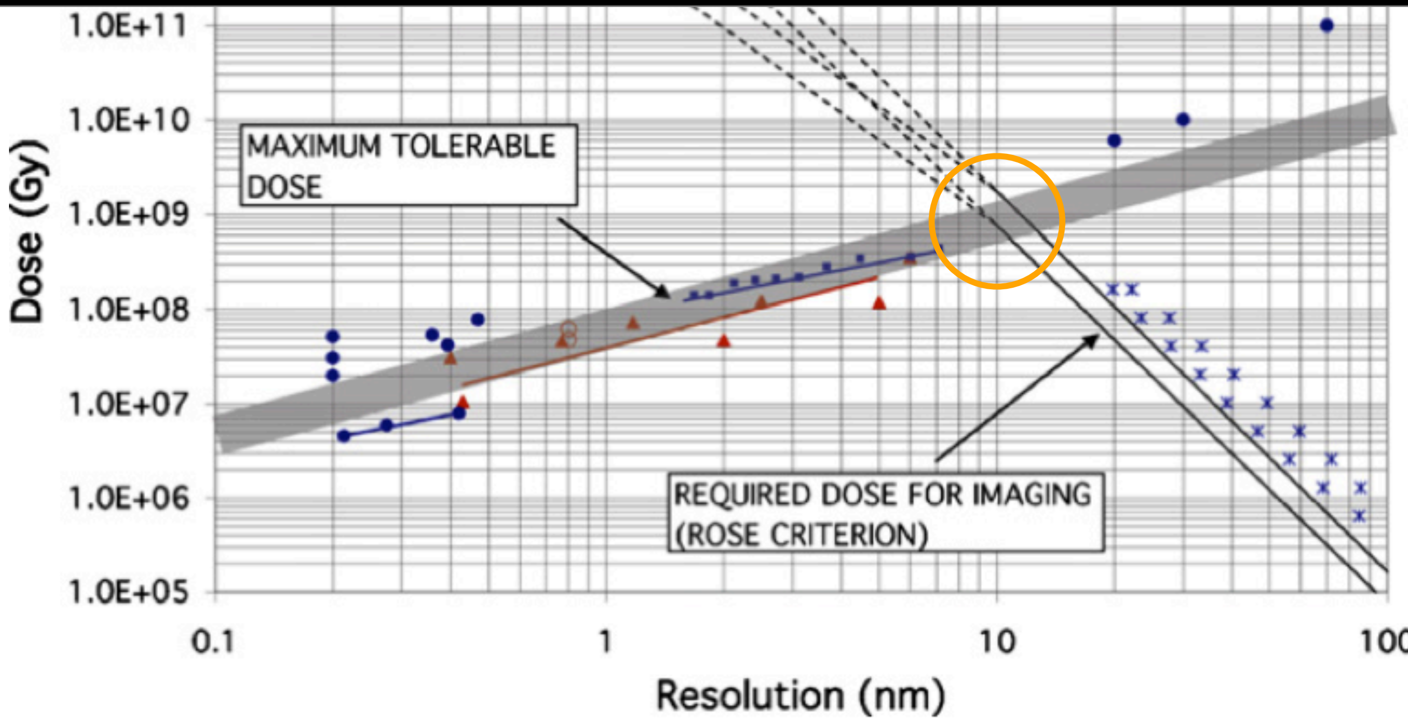


- M.R. Howells, et al, *Journal of Electron Spectroscopy and Related Phenomena 170 (2009)*

The problem of radiation damage

"The principal conclusion of this paper is that for unique, frozen hydrated biological objects with only natural X-ray contrast the resolution of XDM at Rose-criterion image quality will be limited by radiation damage to be not better than 10 nm."

"We have made a case that the 10-nm limit is not insurmountable..."



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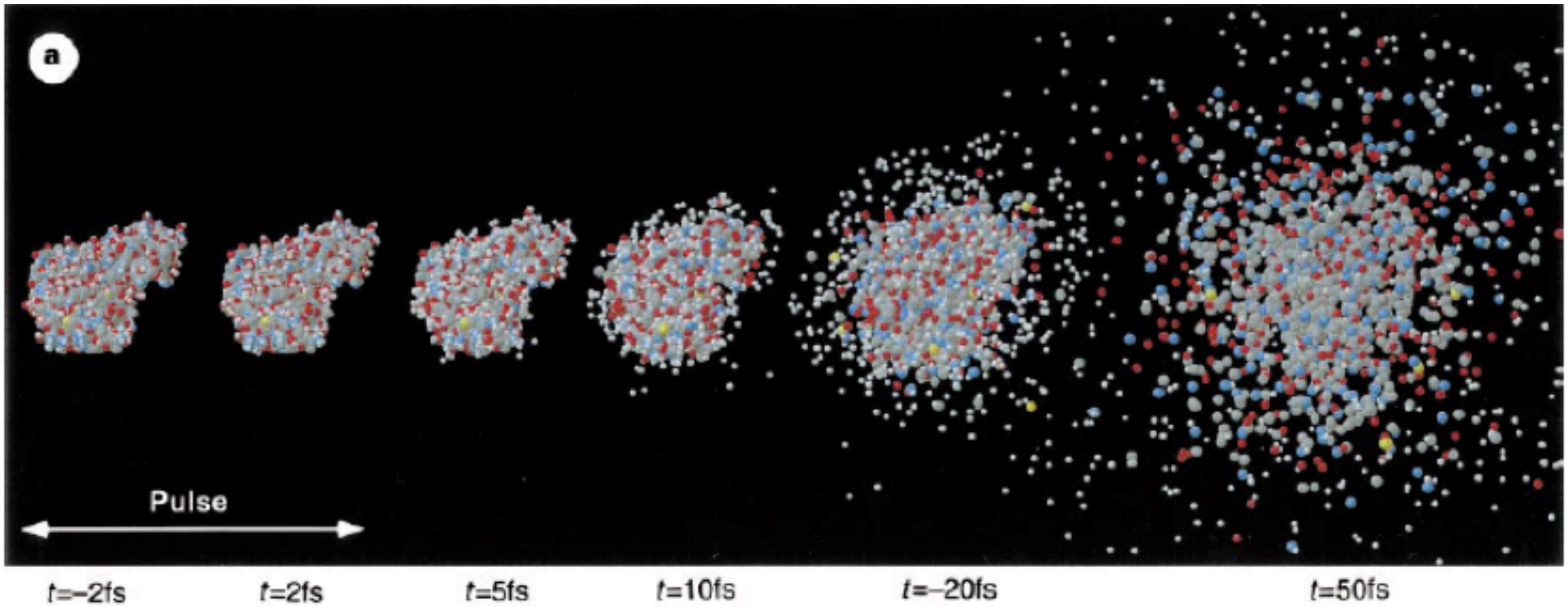
Overcoming Radiation Damage

- R. Neutze, et al., Nature (2000) 406, 752

European XFEL

Overcoming Radiation Damage



"...experiments using very high X-ray dose rates and ultrashort exposures may provide useful structural information before radiation damage destroys the sample..."

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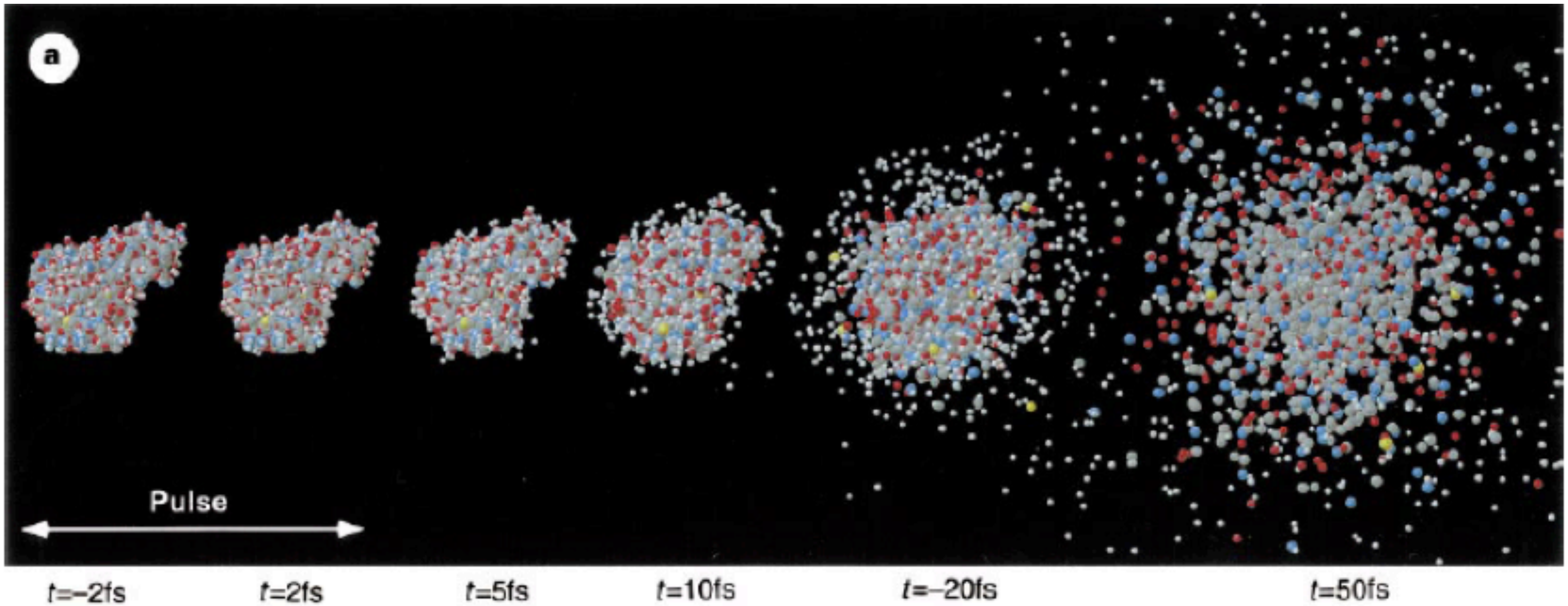
Overcoming Radiation Damage

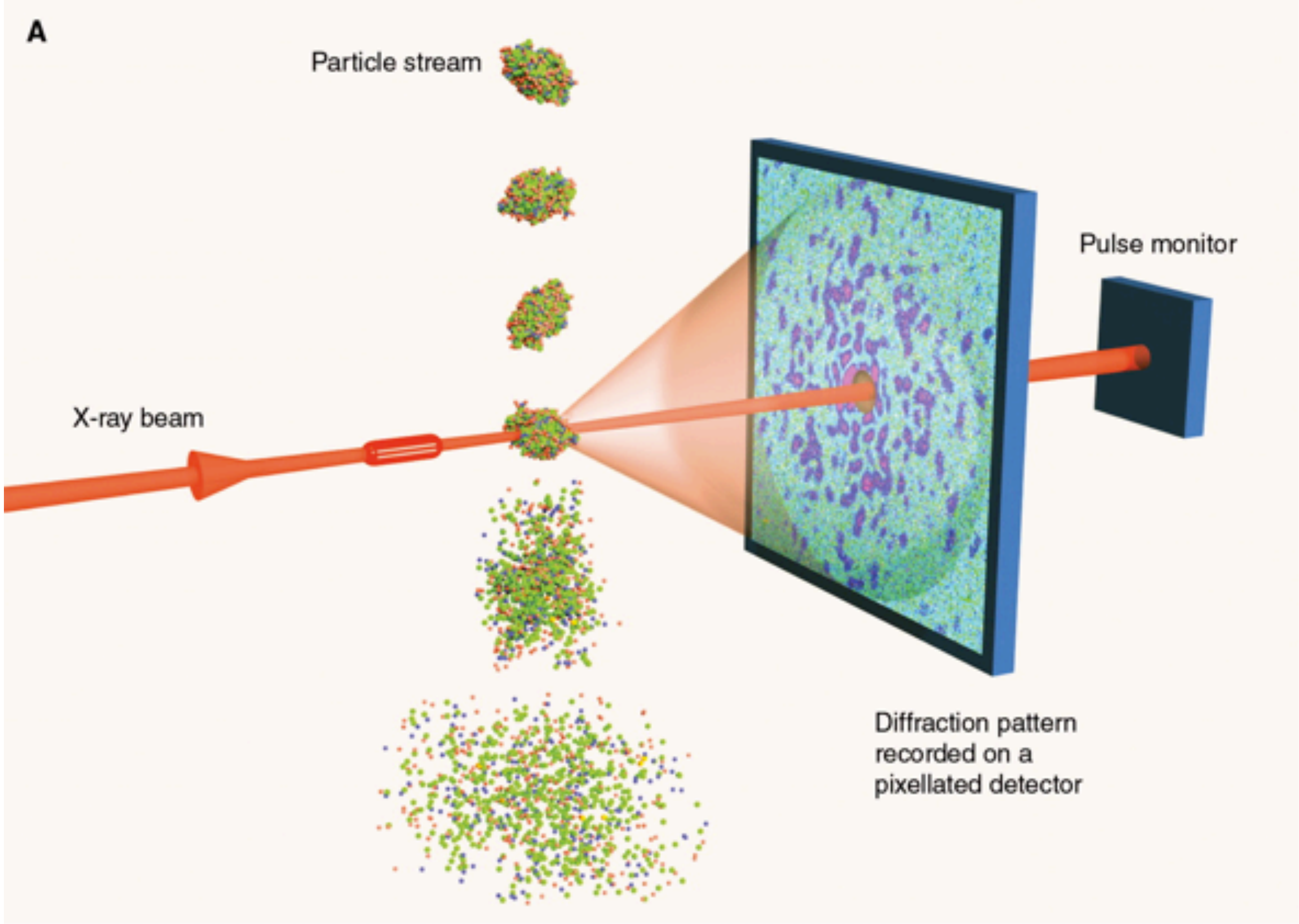


"...experiments using very high X-ray dose rates and ultrashort exposures may provide useful structural information before radiation damage destroys the sample..."

If we can illuminate these biomolecules with very bright and ultrashort pulses of x-rays, we might just be able to image them.

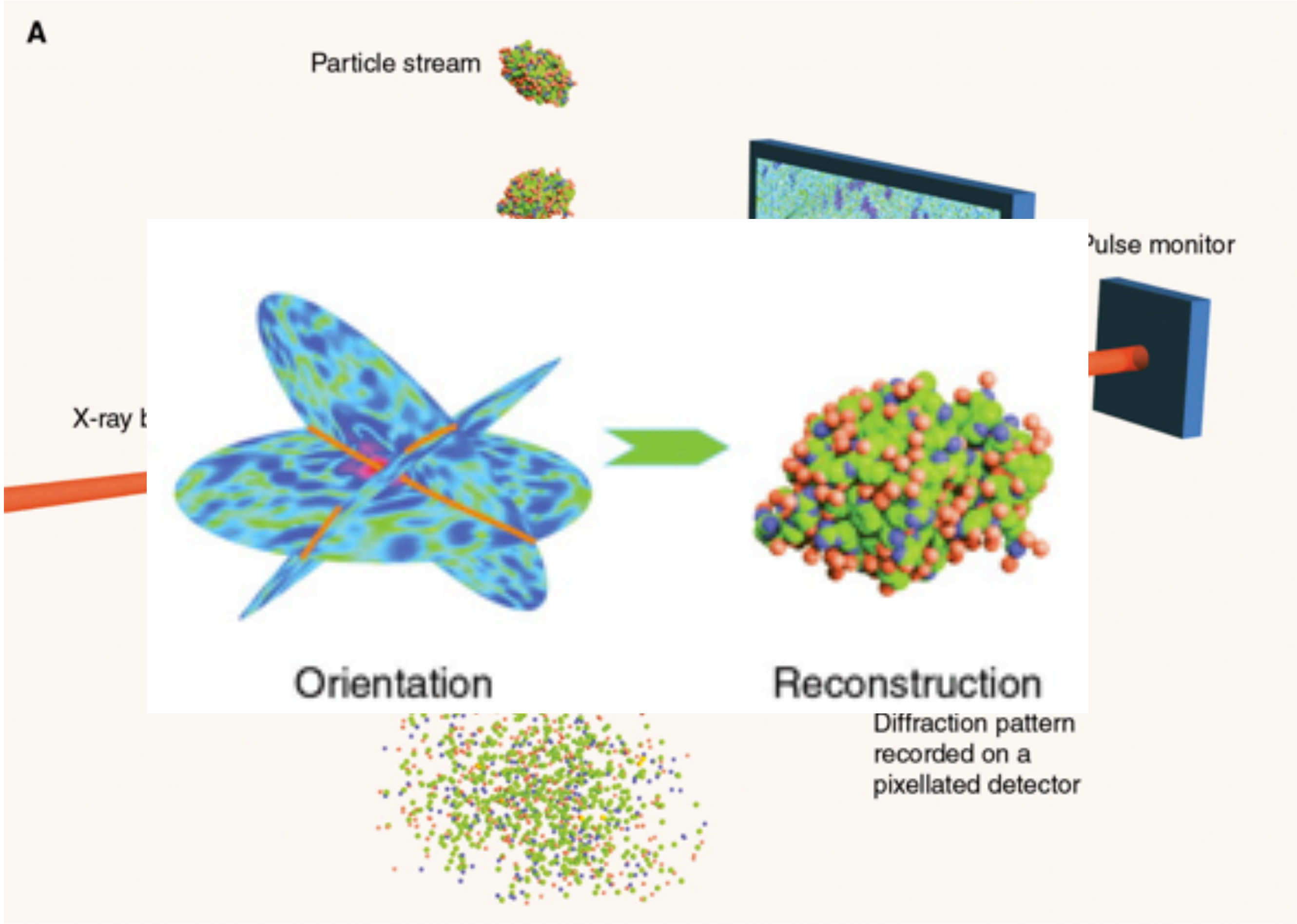
- R. Neutze, et al., Nature (2000) 406, 752

The Canonical CDI Experiment



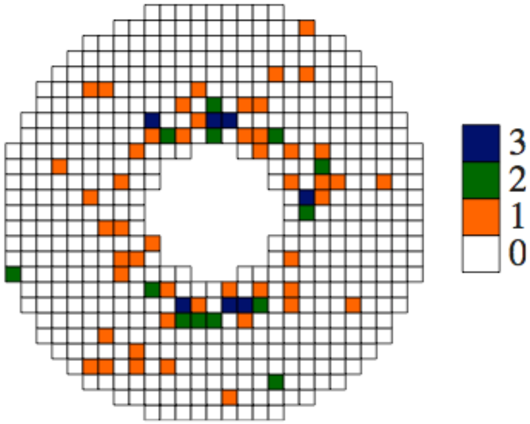
K.J. Gaffney and H.N. Chapman, Science, **316**, 1444 (2007)

The Canonical CDI Experiment



K.J. Gaffney and H.N. Chapman, Science, **316**, 1444 (2007)

The 3 Canonical SPB-type Experiments



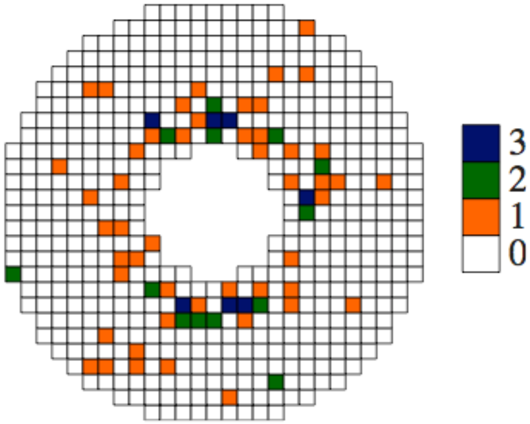
- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

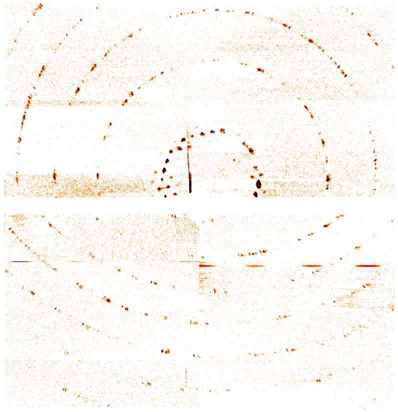
A

B

C

The 3 Canonical SPB-type Experiments





- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)
- Measured diffraction pattern produced from a nanocrystal (CFEL)

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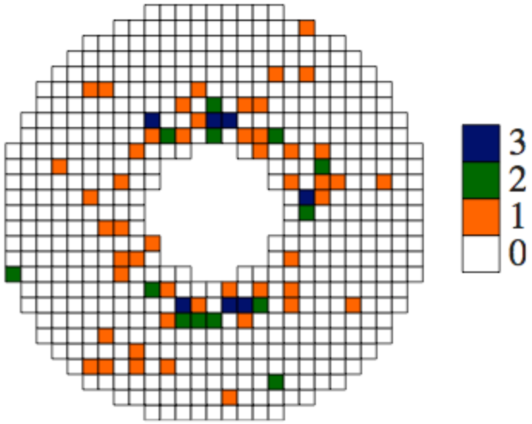

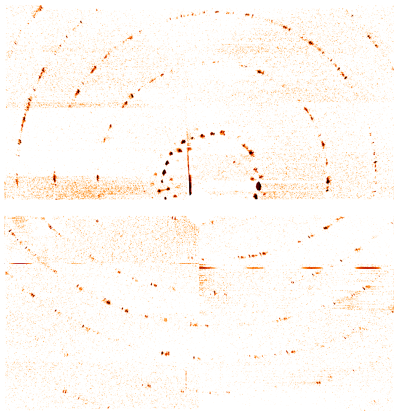

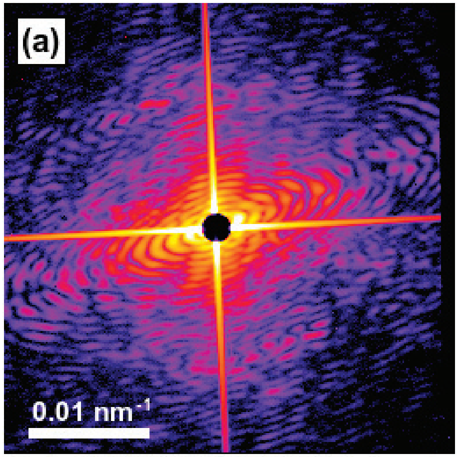

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- A. P. Mancuso et al, New J. Phys. (2010)

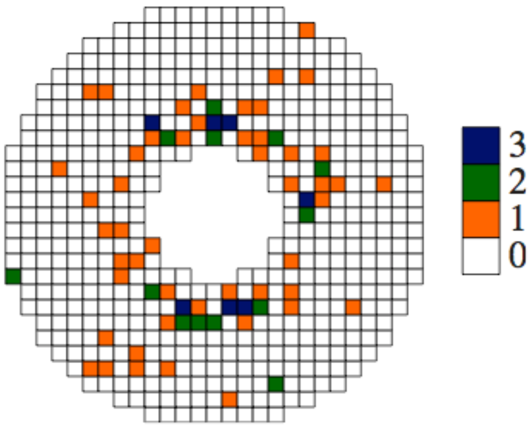
A

B

C

The 3 Canonical SPB-type Experiments

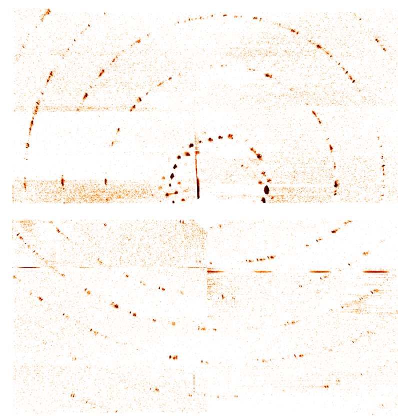
Weakly scattering



- N. Loh and V. Elser, Phys. Rev. E, **80**, 026705 (2009)

A

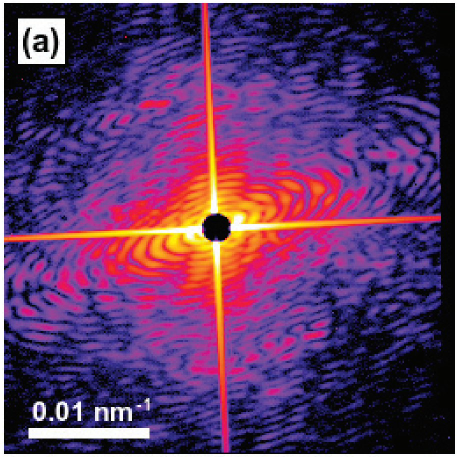
Nanocrystal



- Measured diffraction pattern produced from a nanocrystal (CFEL)

B

Not so weakly scattering



- A. P. Mancuso et al, New J. Phys. (2010)

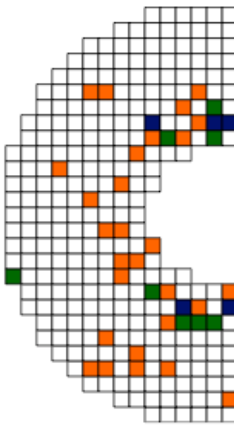
C

The 3 Canonical SPB-type Experiments

Weakly scattering

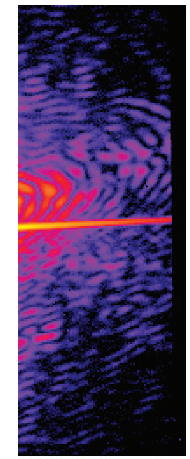
Nanocrystal

Not so weakly scattering



And of course many more...

- FCDI
- In-line Holography
- FTH
- Small angle scattering
- etc
- Pump-probe version of all these



- N. Loh a
Phys. Re
026705 (

so et al,
. (2010)

A

B

C

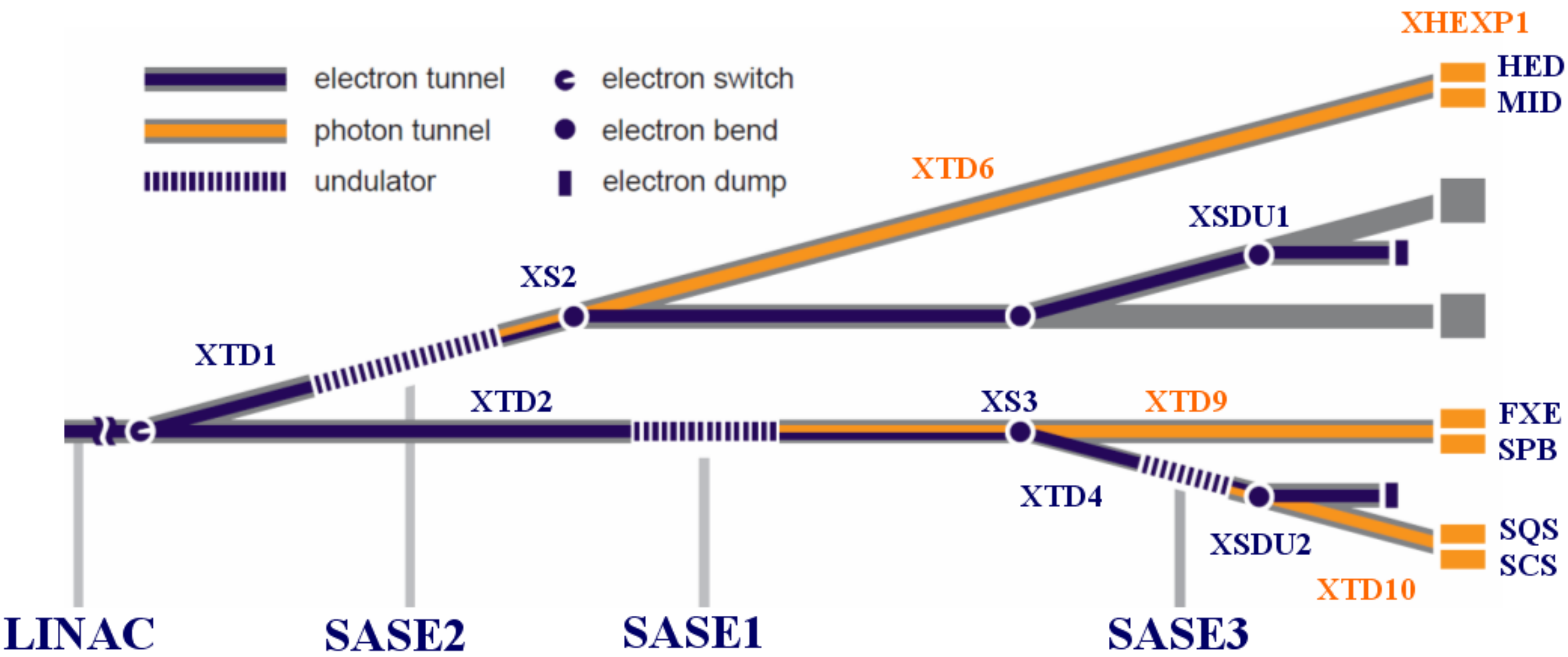
Requirements imposed by the 3 canonical experiments

- Maximum flux to sample (A, B, C)
- Wavefront preserving (or characterisable) (A, B*, C)
- Spot size(s) comparable to sample size(s) (A, B, C)

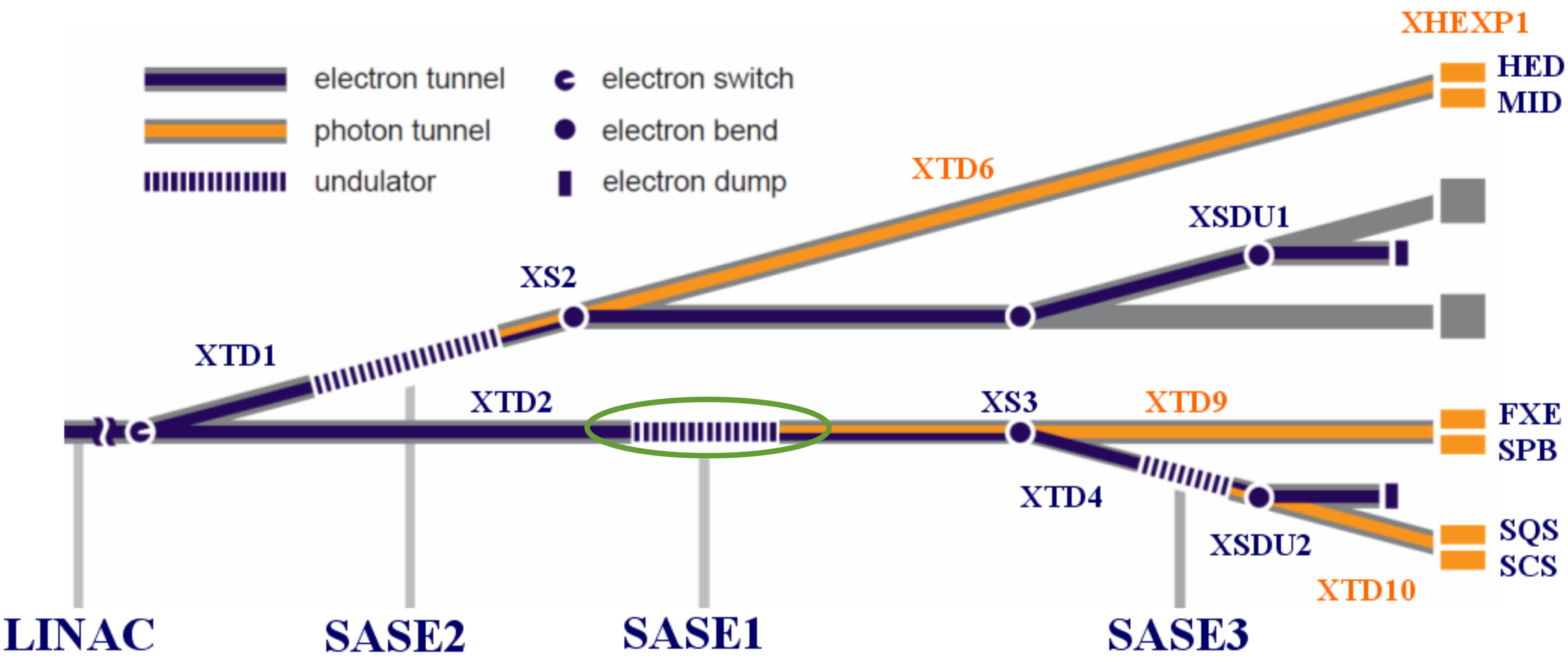
- Single photon counting detector (A)
- High dynamic range detector (B, C)
- Large number of pixels in detector (B, A*, C*)

- Single shot beam diagnostics (A, B, C)

SPB @ SASE1


electron tunnel
photon tunnel
undulator
electron switch
electron bend
electron dump
XHEXP1
HED
MID
XTD6
XSDU1
XS2
XTD1
XTD2
XS3
XTD9
FXE
SPB
XTD4
XSDU2
SQS
SCS
XTD10
LINAC
SASE2
SASE1
SASE3

SPB @ SASE1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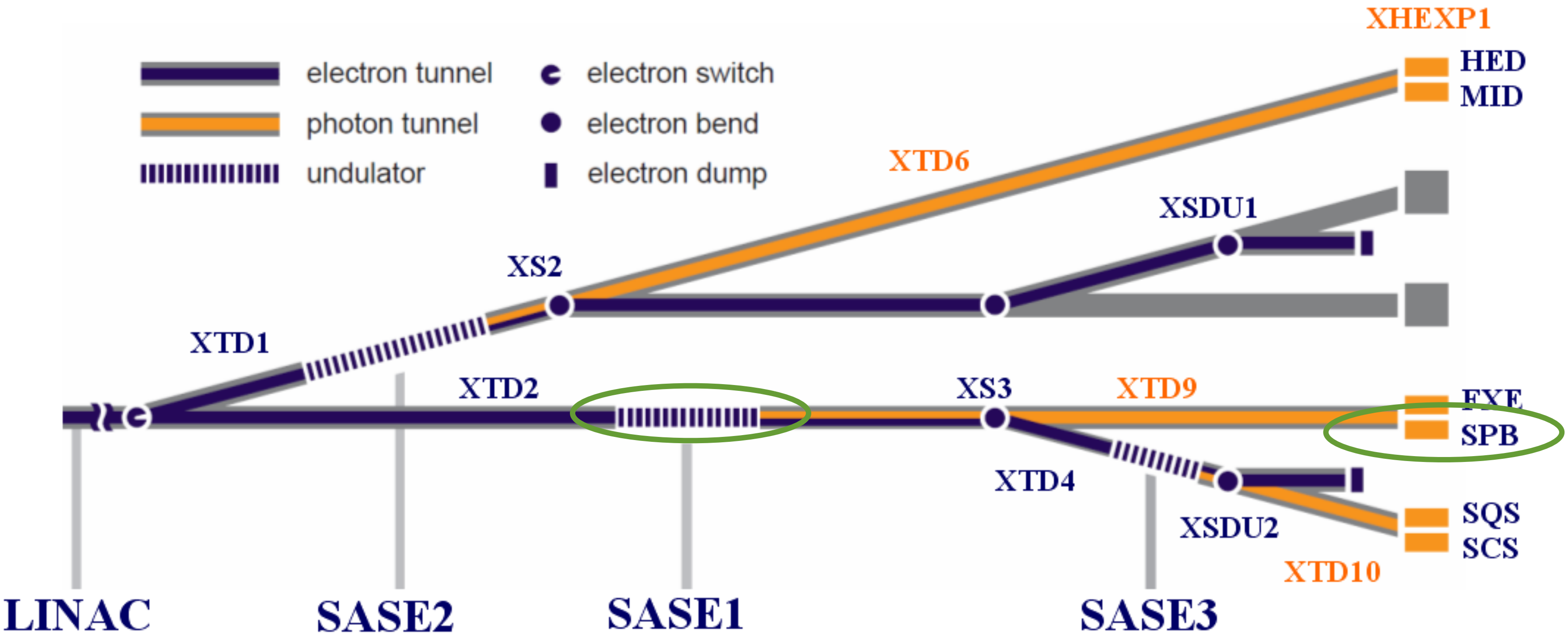
LINAC
SASE2
SASE1
SASE3

European XFEL

SPB @ SASE1



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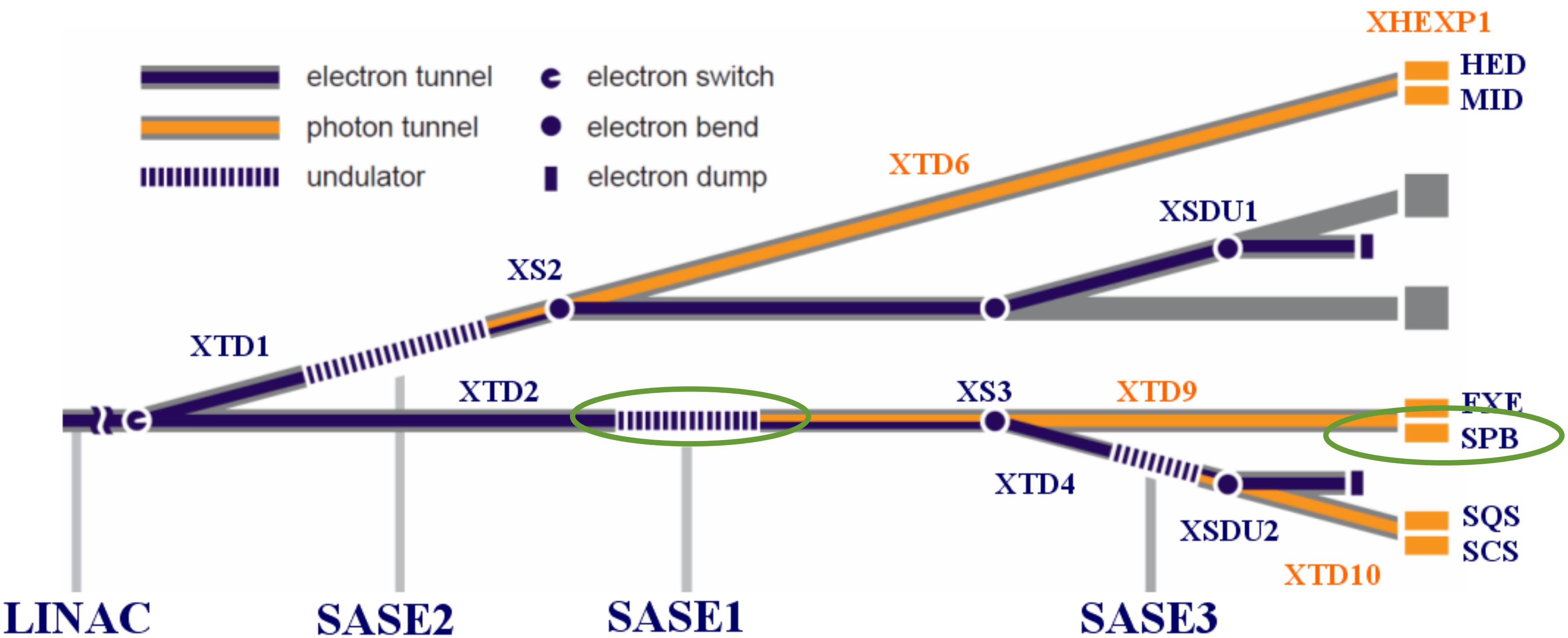
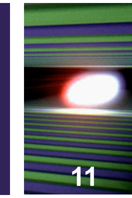


SASE1 undulator and beam transport deliver photons ≥ 3 keV

XFEL.EU delivers 2700 pulses / train (27 000 pulses / s)

Photon beam parameters at SASE 1 (at saturation)



Parameter	Unit	Value								
Photon energy	keV	7.75			12.4			15.5		
Radiation wavelength	nm	0.16			0.10			0.08		
Electron energy	GeV	14			14			14		
Bunch charge	nC	0.02	0.25	1	0.02	0.25	1	0.02	0.25	1
Peak power	GW	46	37	24	35	24	12	29	15	9
Average power	W	2	23	69	2	15	34	1	9	27
Source size (FWHM)	µm	31	39	46	29	37	49	29	35	54
S. divergence (FWHM)	µrad	2.8	2.3	1.9	1.9	1.5	1.3	1.5	1.3	1.0
Spectral bandwidth	1E-3	2.3	1.9	1.4	1.9	1.4	1.0	1.6	1.3	0.8
Coherence time	fs	0.16	0.20	0.27	0.13	0.17	0.23	0.12	0.15	0.23
Coherence degree		0.96	0.96	0.91	0.95	0.91	0.71	0.96	0.84	0.57
Photons/pulse	1E11	0.6	7.0	20.7	0.3	2.8	6.4	0.2	1.4	4.0
Pulse energy	µJ	76	864	2570	58	549	1260	49	347	991
Peak brilliance	1E33*	2.38	2.41	1.96	3.54	3.17	1.6	4.26	2.46	1.6
Average brilliance	1E23*	1.1	15.1	56.8	1.6	19.9	46.4	1.9	15.5	46.2

* In units of photons/(mm^2 mrad^2 0.1% bandwidth s)

Table: T. Tschentscher, XFEL.EU TN-2011-001

Photon beam parameters at SASE 1 (at saturation)

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European XFEL

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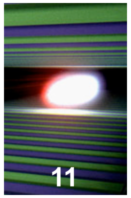
Table: T. Tschentscher, XFEL.EU TN-2011-001

Measured at LCLS. See Vartanyants, Singer, Mancuso, et al, Phys. Rev. Lett. (2011).

Photon beam parameters at SASE 1 (at saturation)



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Average power	W	2	23	69	2	15	34	1	9	27
Source size (FWHM)	µm	31	39	46	29	37	49	29	35	54
S. divergence (FWHM)	µrad	2.8	2.3	1.9	1.9	1.5	1.3	1.5	1.3	1.0
Spectral bandwidth	1E-3	2.3	1.9	1.4	1.9	1.4	1.0	1.6	1.3	0.8
Coherence time	fs	0.16	0.20	0.27	0.13	0.17	0.23	0.12	0.15	0.23
* Coherence degree		0.96	0.96	0.91	0.95	0.91	0.71	0.96	0.84	0.57
Photons/pulse	1E11	0.6	7.0	20.7	0.3	2.8	6.4	0.2	1.4	4.0
Pulse energy	µJ	76	864	2570	58	549	1260	49	347	991
Peak brilliance	1E33*	2.38	2.41	1.96	3.54	3.17	1.6	4.26	2.46	1.6
Average brilliance	1E23*	1.1	15.1	56.8	1.6	19.9	46.4	1.9	15.5	46.2

* In units of photons/(mm^2 $mrad^2$ 0.1% bandwidth s)

Table: T. Tschentscher, XFEL.EU TN-2011-001

Measured at LCLS. See Vartanyants, Singer, Mancuso, et al, Phys. Rev. Lett. (2011).

Photon beam parameters at SASE 1 (at saturation)

Parameter	Unit	Value								
Photon energy	keV	7.75			12.4			15.5		
Radiation wavelength	nm	0.16			0.10			0.08		
Electron energy	GeV	14			14			14		
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Participants of the inaugural SPB Workshop in Uppsala, Sweden (November 2008)

A. P. Mancuso and H. N. Chapman, Report from "International workshop on science with and instrumentation for ultrafast coherent diffraction imaging of Single Particles, clusters and Biomolecules (SPB) at the European XFEL", (2008), http://www.xfel.eu/events/workshops/2008/spb_workshop_2008/

Goals of the Optical Layout

- The maximum number of photons are delivered to the samples in spot sizes comparable to the sample sizes
- Focal spots to match samples of different sizes, as outlined in the SPB Workshop summary (ie ~1 µm & 100 nm)*
- A minimally perturbed wavefront in the focal plane is delivered.

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- ~930 m source to interaction region distance
  - ➔ Large (~mm) beam at focusing optics
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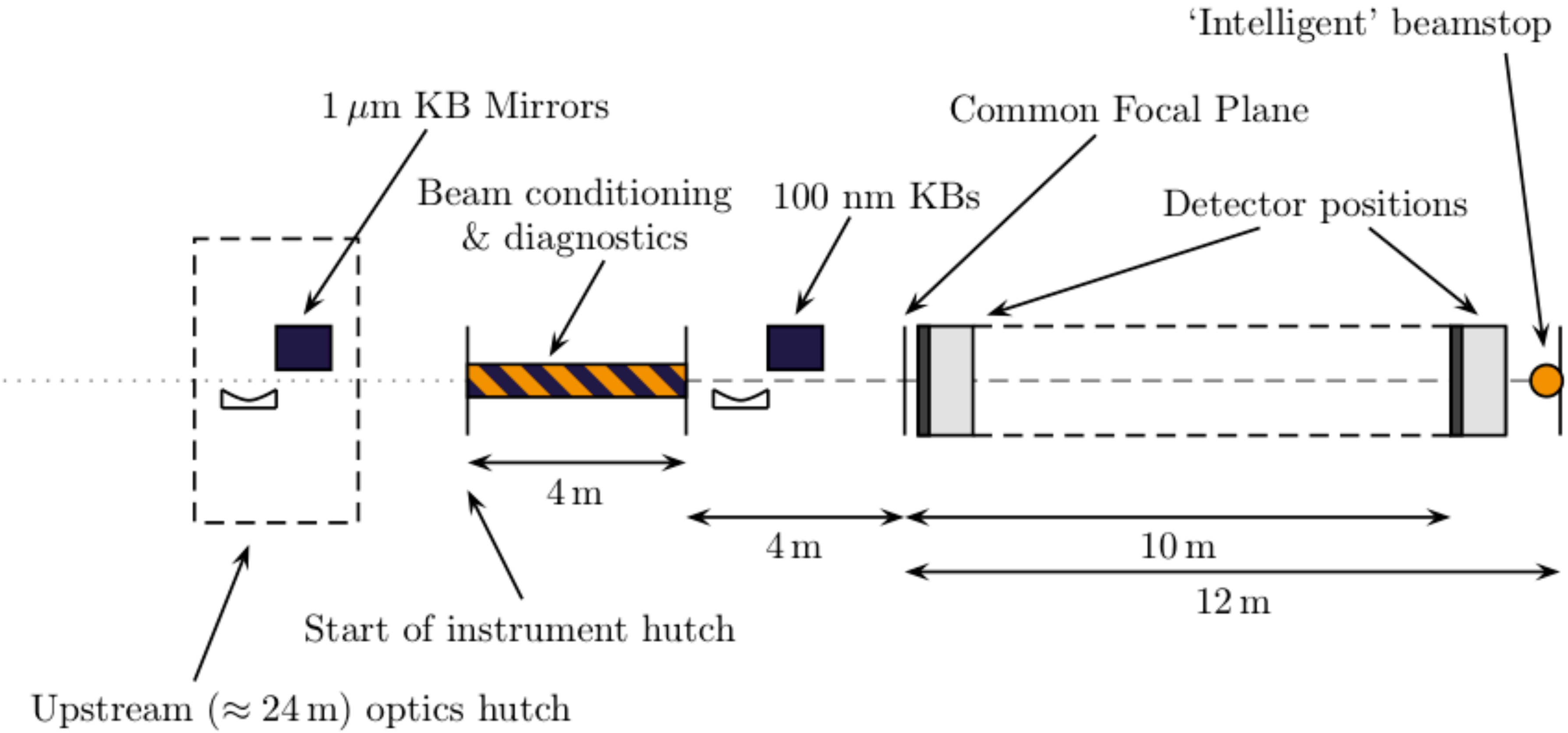
Outline of the SPB instrument



Choice of focusing technology

- Mirror technology has been chosen here for a variety of reasons that satisfy the requirements outlined above. Mirrors are:
  - Efficient, reflecting the vast majority of radiation incident on them, provided their graze angles are respected.
  - Damage resistant (for appropriate fluences)
  - Wavefront preserving (if length and figure error specifications are achieved)
  - Achromatic, making for simple (and hence faster) alignment of the instrument
- Mirrors need to be long enough to transmit most of the beam and avoid diffraction effects from aperturing the beam

Required mirror lengths

	3 keV	8 keV	12 keV	18 keV
C coating	1087 mm	1260 mm	1339 mm	1485 mm
Pd coating	652 mm	756 mm	803 mm	891 mm
Pt coating	481 mm	558 mm	593 mm	658 mm

Minimum mirror length for a vertical KB mirror that collects 4σ of the beam in the experimental hall as a function of mirror coating.Table taken from [Sinn, XRBT, 2011].

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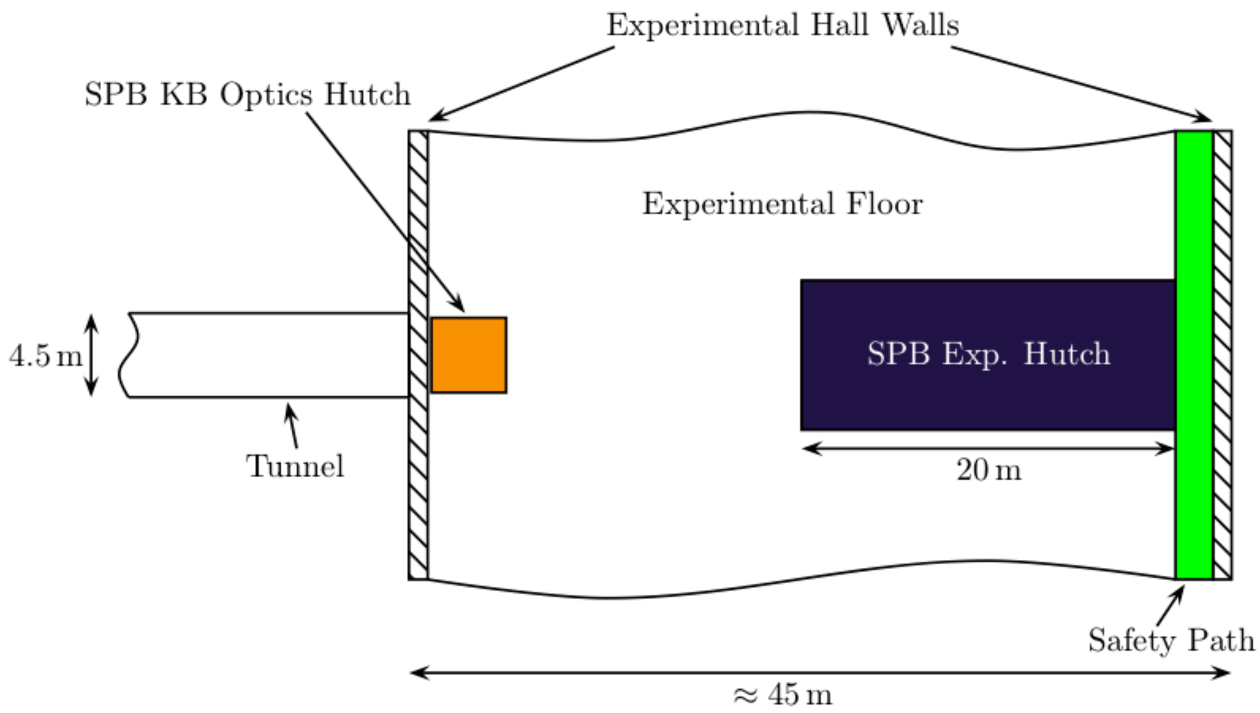
The calculated deposited energy per atom for Palladium coated KB mirrors at angles between 2.3 and 5 mrad has, in all cases, a deposited energy per atom of less than 10 meV/atom/mJ in simulations that neglect the cooling effect of photo-electron transport.

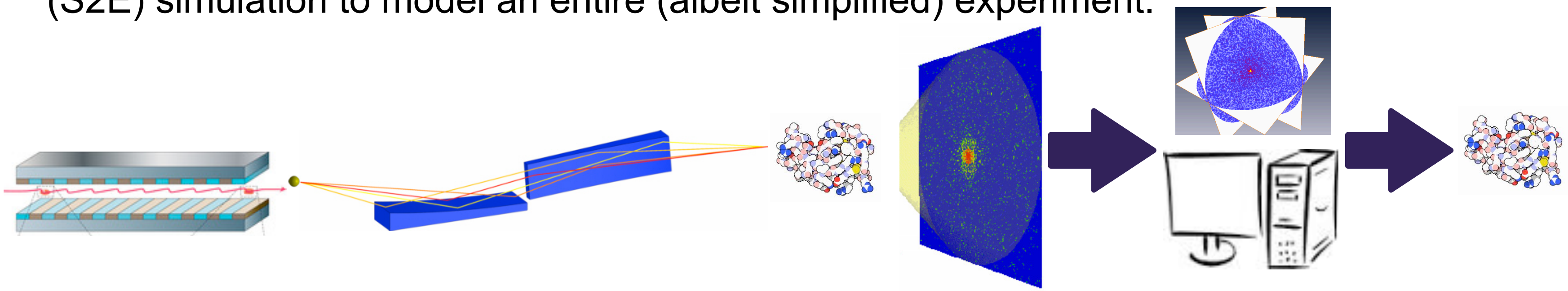
Experimental Layout



- 10 m propagation distance limits sample size to ~1 μm (sampling)
- To deliver 1 μm spot, optics are located as far upstream as possible on exp. floor
- Depth of focus is excellent (see later modeling)
- Distance between 100 nm optics and interaction region very comfortable at > 1 m
- Beam size varies considerably over the length of the hutch

The SPB Modelling Program: Informing the SPB design (and more)

- Modeling will help inform the conceptual & technical design of the instruments.
  A modeling program for SPB has been started that aims to achieve these goals through simulating the different stages of the experiment
  - starting with the generation of the radiation,
  - modeling its transport to the interaction region,
  - modeling the photon-matter interaction between the FEL beam and a model sample,
  - the propagation of the radiation to the 2D detector system and it's measurement in that detector system
  - and finally the interpretation of the measured data.
- This ambitious program is modular in design with modules focusing on each of the above stages of the overall system. This allows the project participants to work independently on each of the stages listed above, which can then be combined into a complete Start-to-End (S2E) simulation to model an entire (albeit simplified) experiment.



Images: *Nature Photonics* **4**, 814–821 (2010), x-ray-optics.de, pdb.org, J. Phys. B: At. Mol. Opt. Phys. 43 (2010) 194016, SPB CDR

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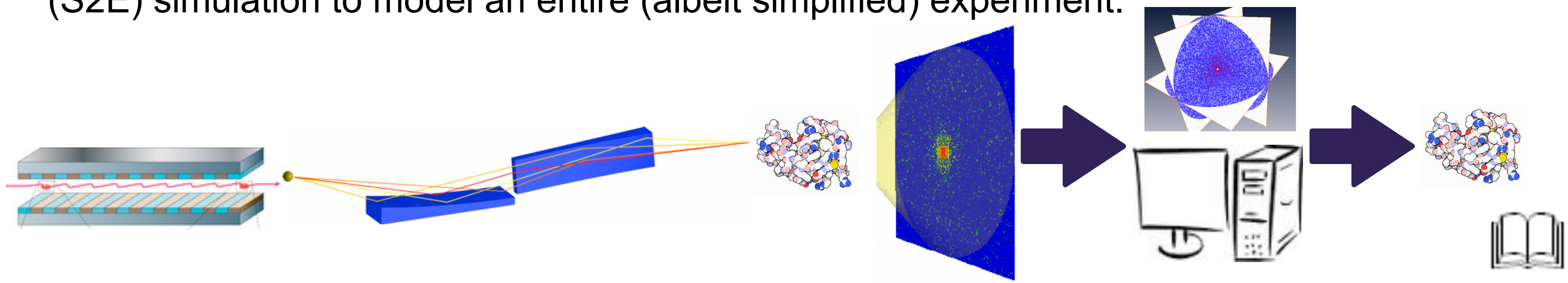

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Focal properties

- Modelled both focii for 12 keV & 5 keV radiation
- Model contains some simplifying assumptions
- Produces 1 μm focal spot with high transmission
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Nanofocusing optic example:
For a 250 pC bunch charge with the accelerator operating at 14 GeV electron energy, one expects to produce about 1.3×10^{12} photons / pulse at 5 keV [Schneidmiller & Yurkov]. Assuming no further losses than those considered in the model (apertures, height errors), this amounts to about 2.6×10^{11} photons / pulse in a 100 nm focal spot.

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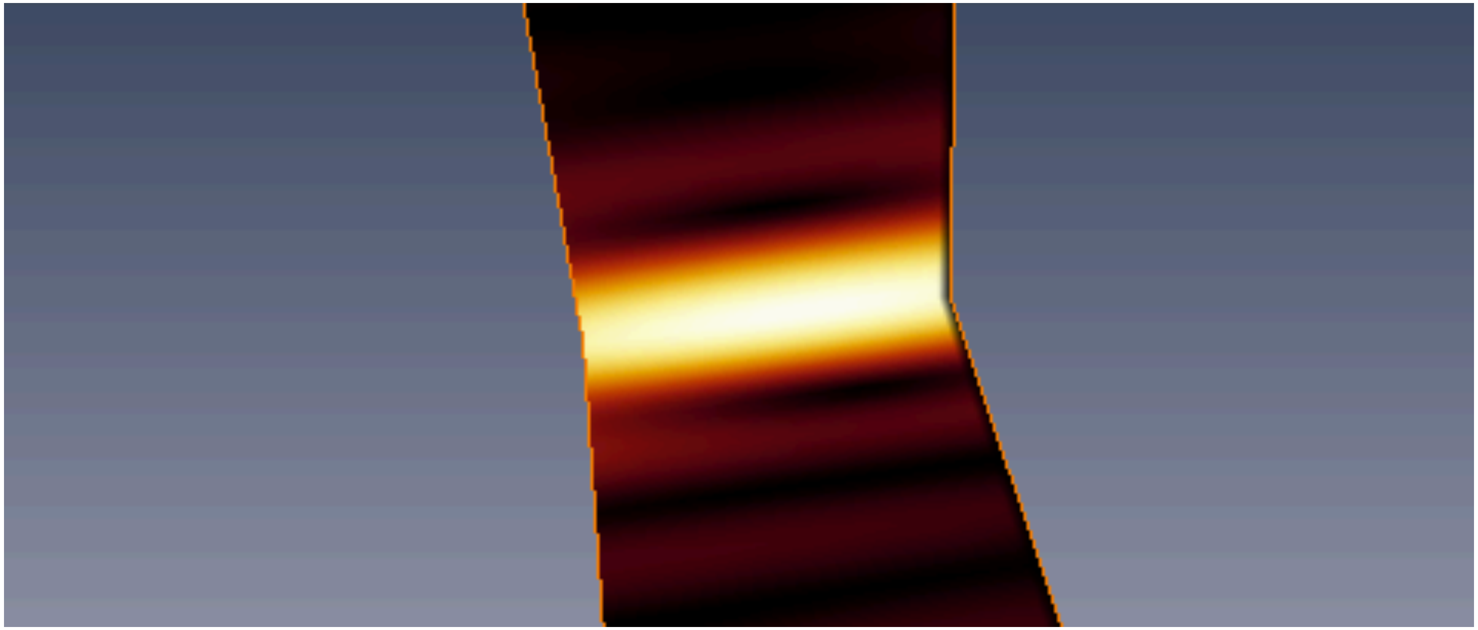
Simulations: L. Samoylova, European XFEL

Expected beam profile @ 12 keV along the focus



Longitudinal profile of the nominally 1 μm focal spot for 12 keV radiation and Pd-coated mirrors. The longitudinal dimension is 14.5 mm. Note the extremely long depth of focus (even longer than shown here), which is of great benefit for the coherent imaging of injected samples.

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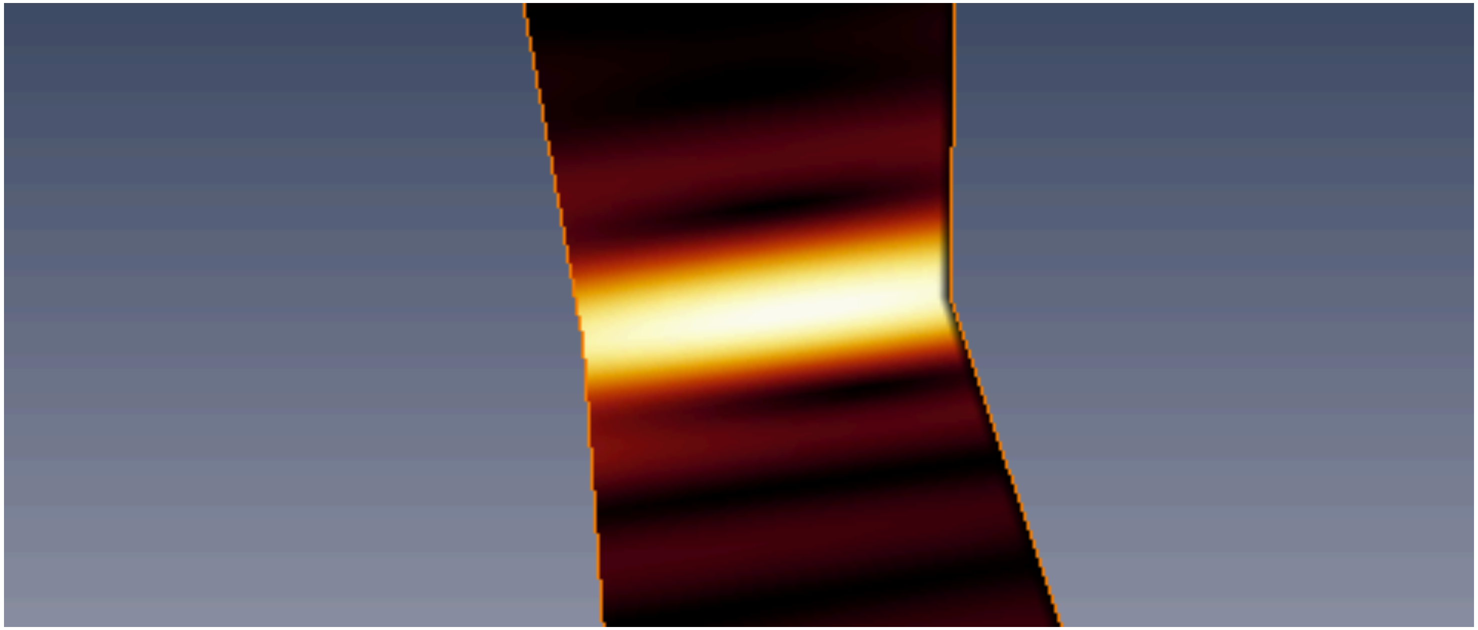

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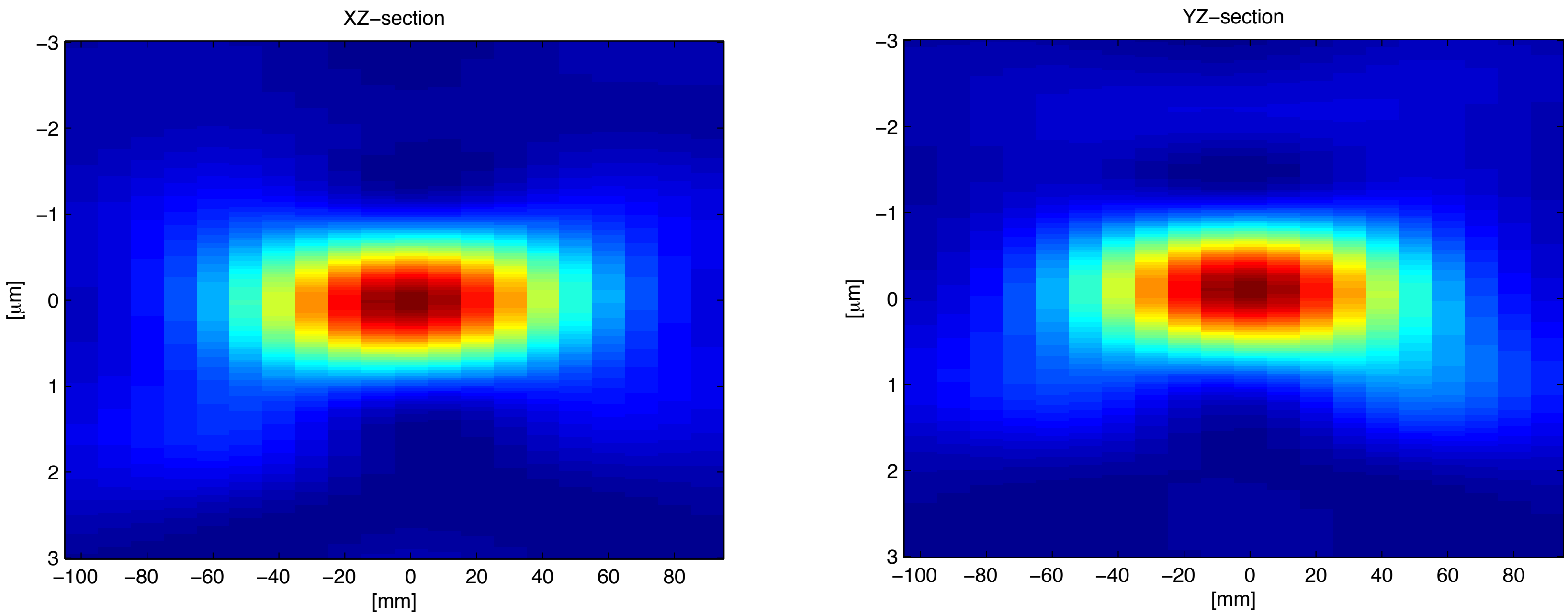

Longitudinal profile of the nominally 1 µm focal spot for 12 keV radiation and Pd-coated mirrors. The longitudinal dimension is ~200 mm. Note the extremely long depth of focus (~4 cm), which is of great benefit for the coherent imaging of injected samples.

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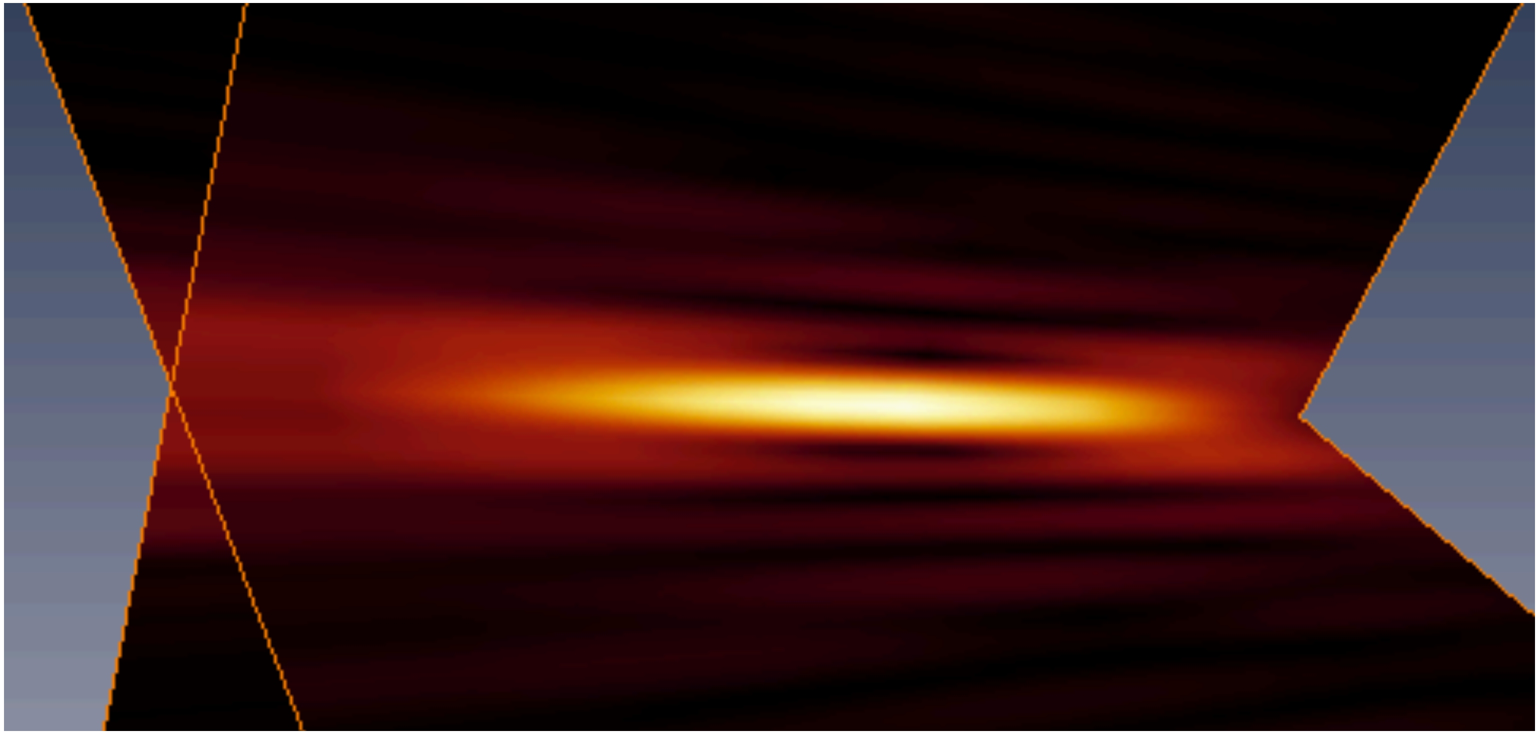

Longitudinal profile of the nominally 100 nm focal spot for 12 keV radiation and Pd-coated mirrors. The longitudinal dimension is 1 mm. Note again the long depth of focus

The three key ways of getting the sample to the interaction region

- Liquid Jet
- Aerodynamic Jet
- Fixed target

Short Conclusion

- Sample injection speeds are compatible with European XFEL pulse rate
- The XFEL.EU's 27,000 pulses per second improves the data rate and minimises sample waste compared to other facilities
- There are cases where fixed target samples will also be necessary (samples requiring orientation, samples for beam characterisation, etc)

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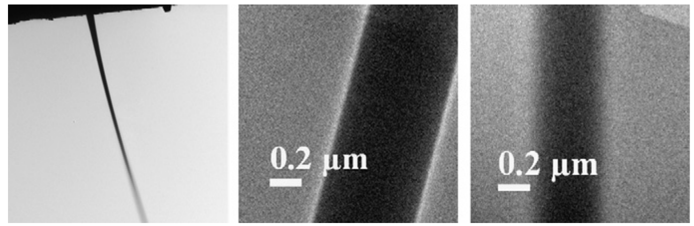
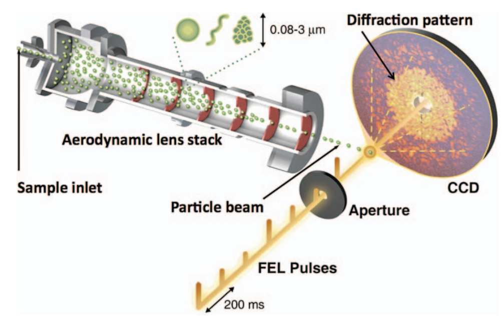


Fig. 3. TEM micrographs of a liquid jet. Left—low-magnification image of water jet showing transition from unbroken jet to droplet stream; middle—high-magnification image of IPA jet, 600 nm diameter and right—high-magnification image of IPA jet, 350 nm diameter.

D. DePonte, et al, Ultramicroscopy, (2010)



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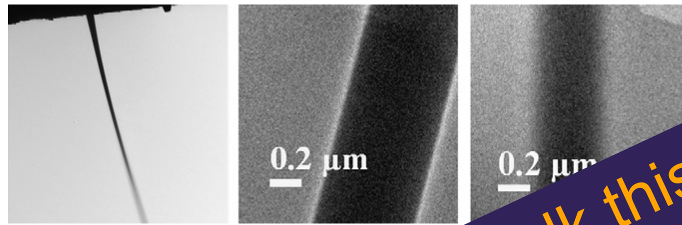

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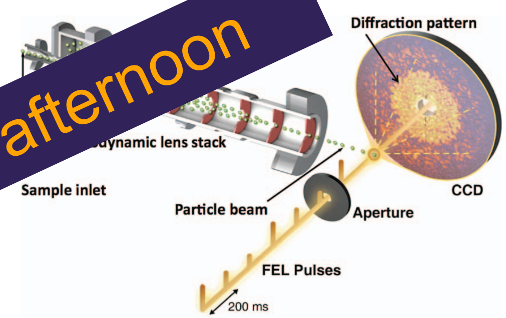

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See J. Schultz's talk this afternoon

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Requirements on detection: What we want

- The key properties that a 2D area detector for coherent imaging applications at the European XFEL should ideally satisfy:
  - Compatibility with the 4.5 MHz repetition rate within individual pulse trains of FEL radiation
  - Ability to read out, or store for read out between trains, an entire train length (2700 pulses) of images, a third of this number when the accelerator is multiplexing to three beamlines or as many as is technically feasible.
  - High quantum efficiency across the operating range (for SPB 3–16 keV)
  - Single photon sensitivity (> 5 σ) across the operating range of the detector (that is, less than one false positive per megapixel)

Requirements on detection: What we want 2

- High dynamic range (preferably as much as six (6) orders of magnitude [ref-SPB-Workshop-Report], but as high as is practicable). This can be mitigated by the use of a second detector in a single experiment.
- Pixel size that allows appropriate sampling of the diffraction data for the proposed sample sizes and propagation distances
- A number of pixels that is commensurate with the number of resolution elements required (ie at least 1k x 1k).

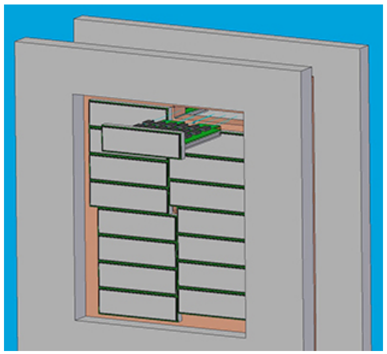
$$N_{res} = \frac{N_{detector}}{2\sigma}$$

- A well-calibrated (but not necessarily linear) response, which is accurate to better than Poissonian noise.
- An adjustable sized hole that can be matched to the size of the direct beam for different beam sizes.
- In-vacuum operation that allows the direct beam to pass through the detector's central hole and propagate further downstream throughout this propagation in-vacuum.

European XFEL

XFEL 2D Imaging Detectors

AGIPD Adaptive Gain Integrating Pixel Detector (AGIPD)



Energy range

3 - 13 keV

Dynamic range

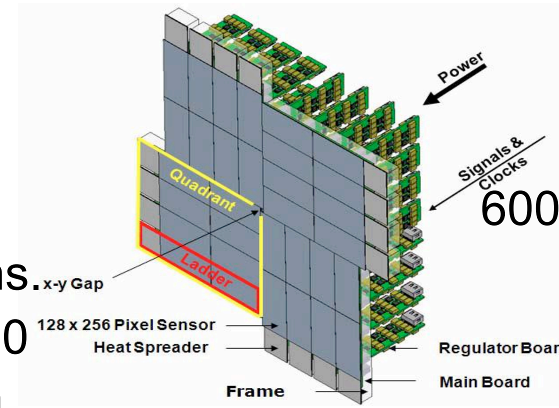
10^4@12 keV

Single Photon Sens.

Storage Cells ≈ 300

Pixel size 200 µm

DEPFET Sensor with Signal Compression (DSSC)



Energy range

0.5 - 6 keV (25 keV)

Dynamic range

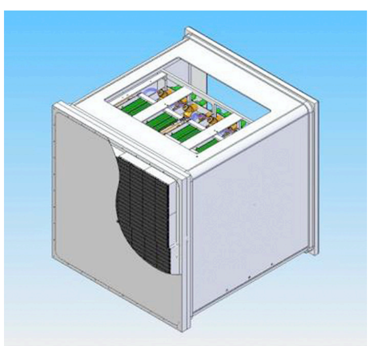
6000 ph/pix/pulse@1 keV

Single Photon Sens.

Storage Cells ≈ 640

Pixel size ~200 µm

Large Pixel Detector (LPD)



Energy range

5 (1) - 20 keV (25 keV)

Dynamic range

10^5@12 keV

Single Photon Sens.

Storage Cells ≈ 512

Pixel size ~500 µm

Other Detectors

- 0D/1D detectors for high repetition rate applications (e.g. veto, dispersive spectrometers)
- Small areas, low rep. rate, low energy 2D imaging detectors
- Particle detectors (eTOF, iTOF)

Slide courtesy M. Kuster

European XFEL

The three quarter-time slide

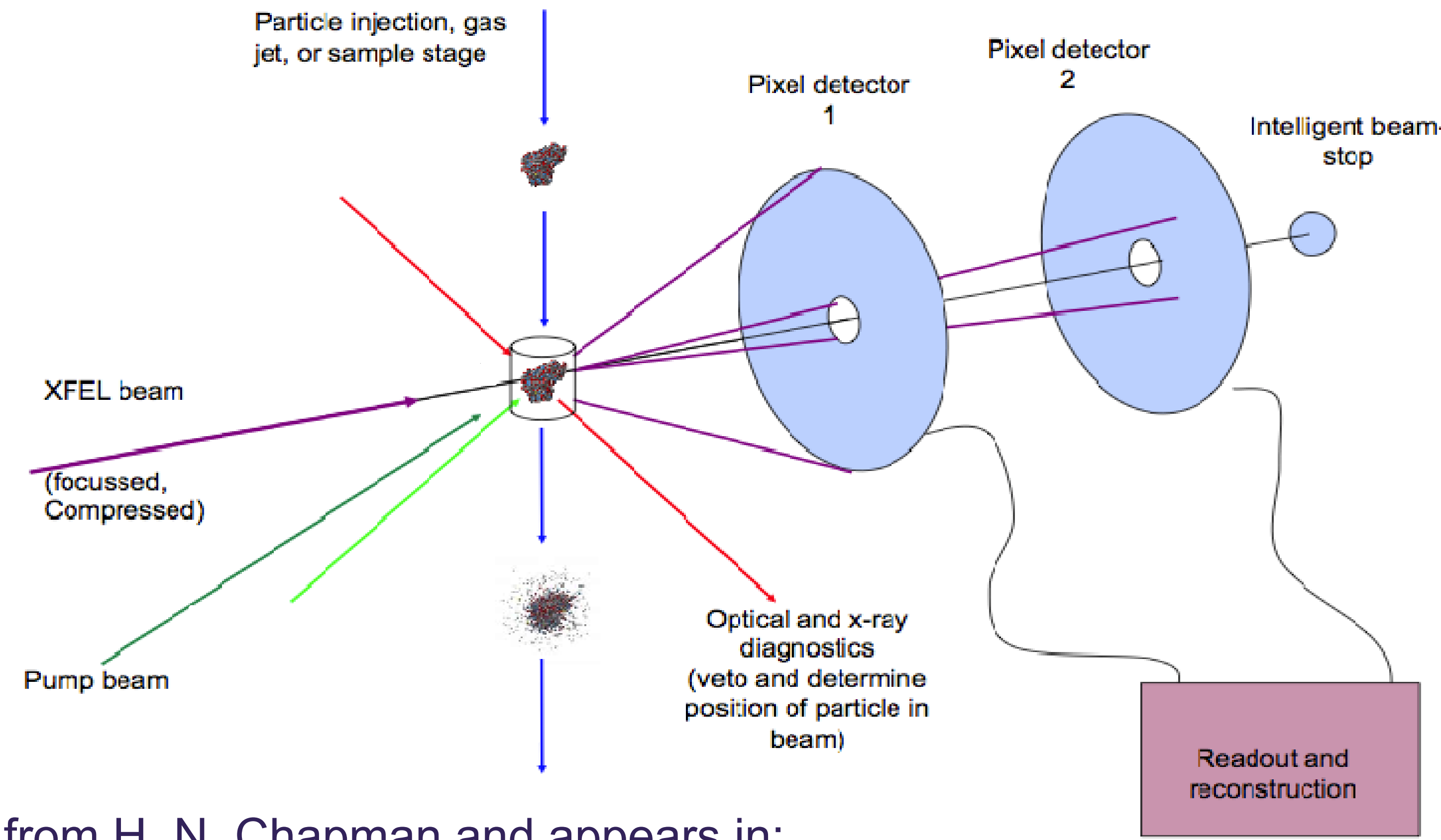


Image: from H. N. Chapman and appears in:

A. P. Mancuso and H. N. Chapman, International Workshop on Science with and Instrumentation for Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules (SPB) at the European XFEL (2011).

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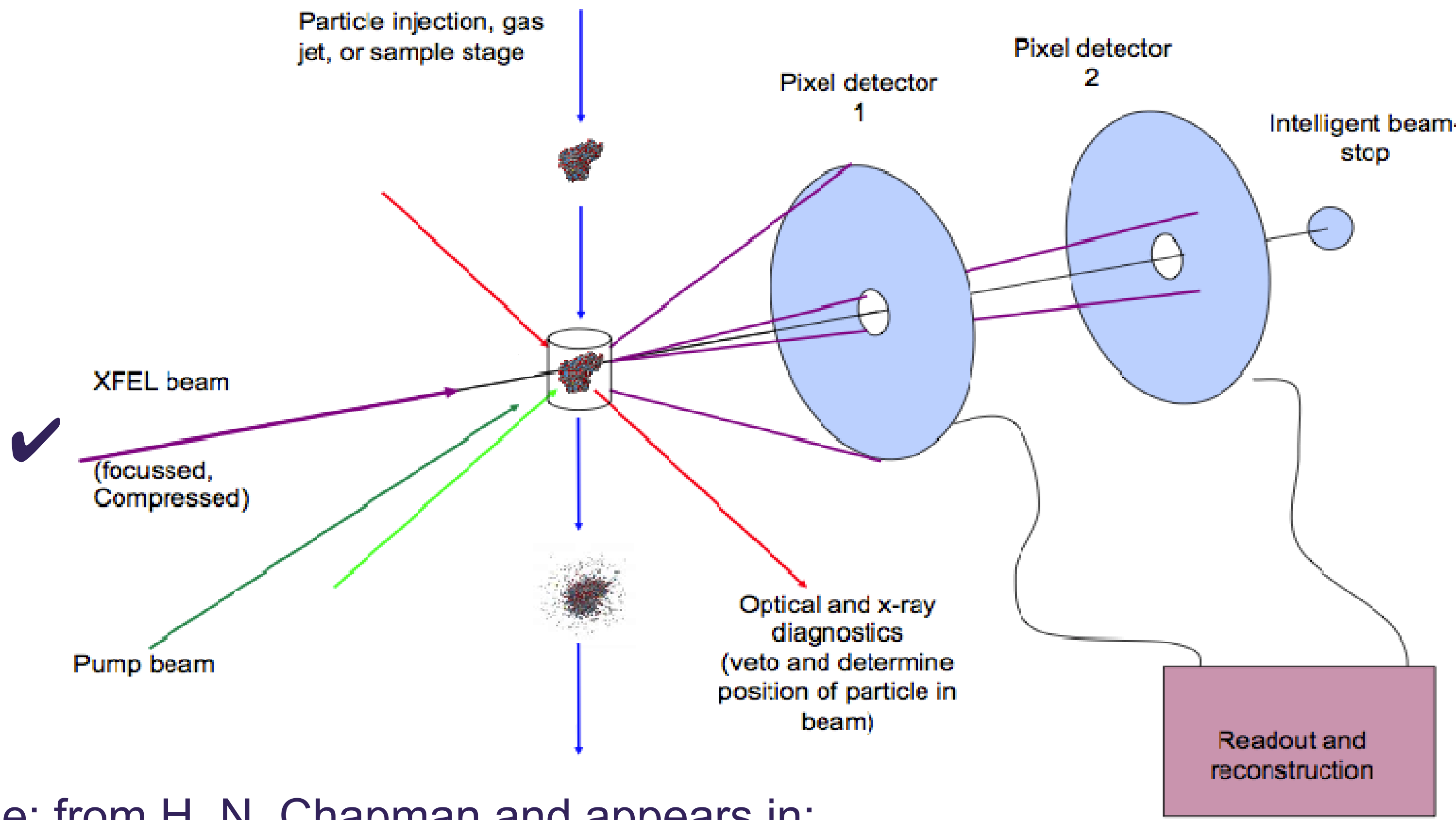

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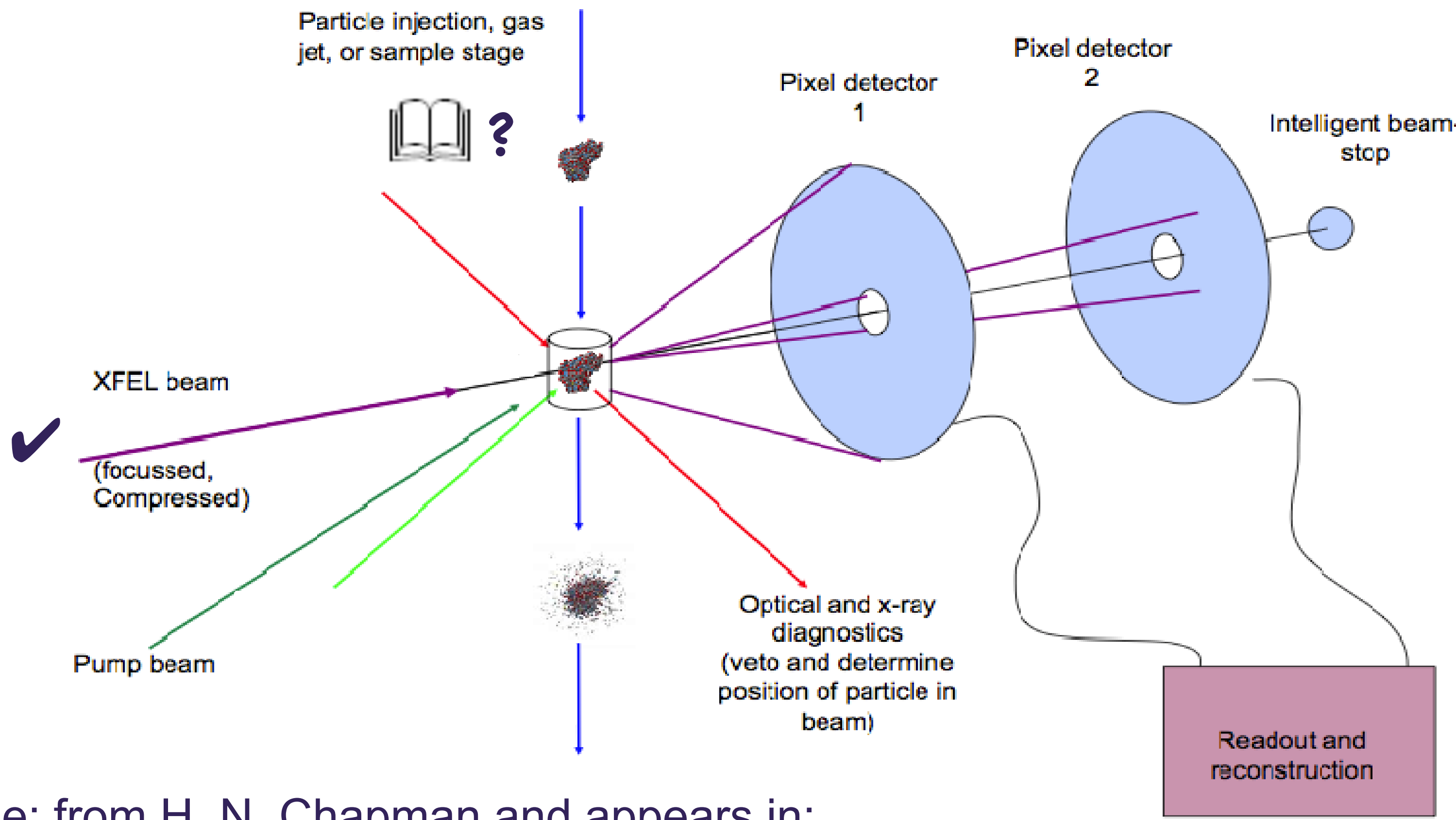

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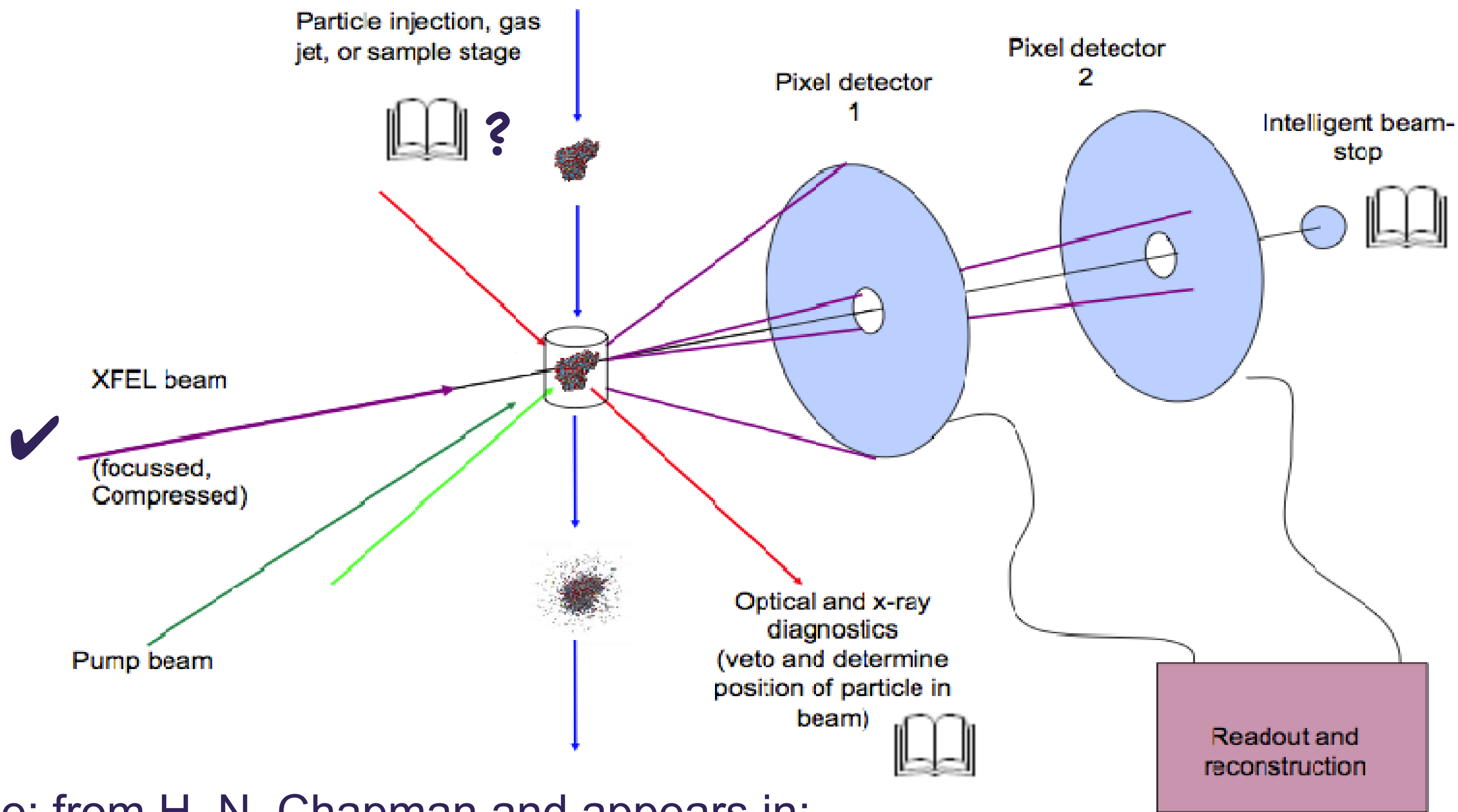

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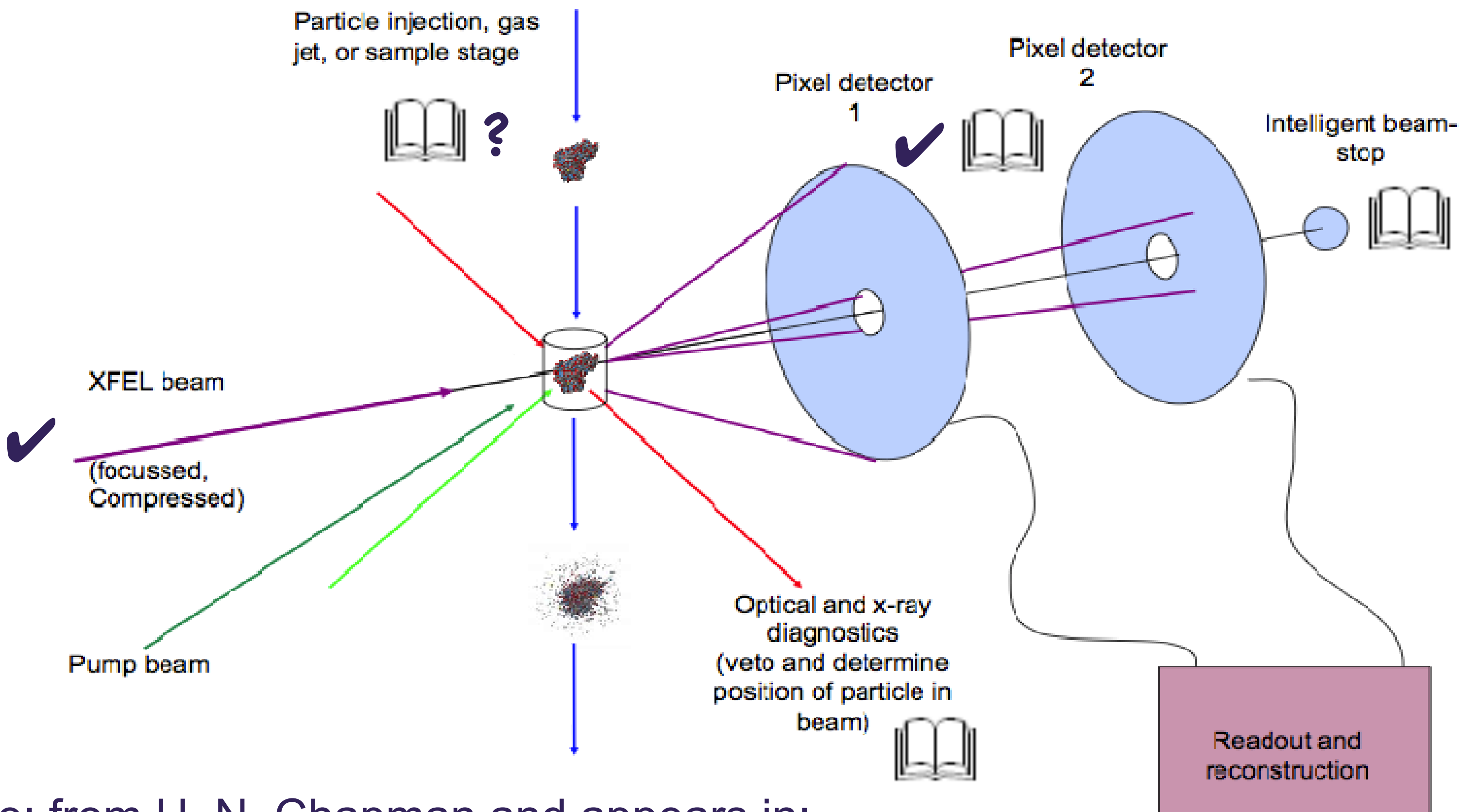

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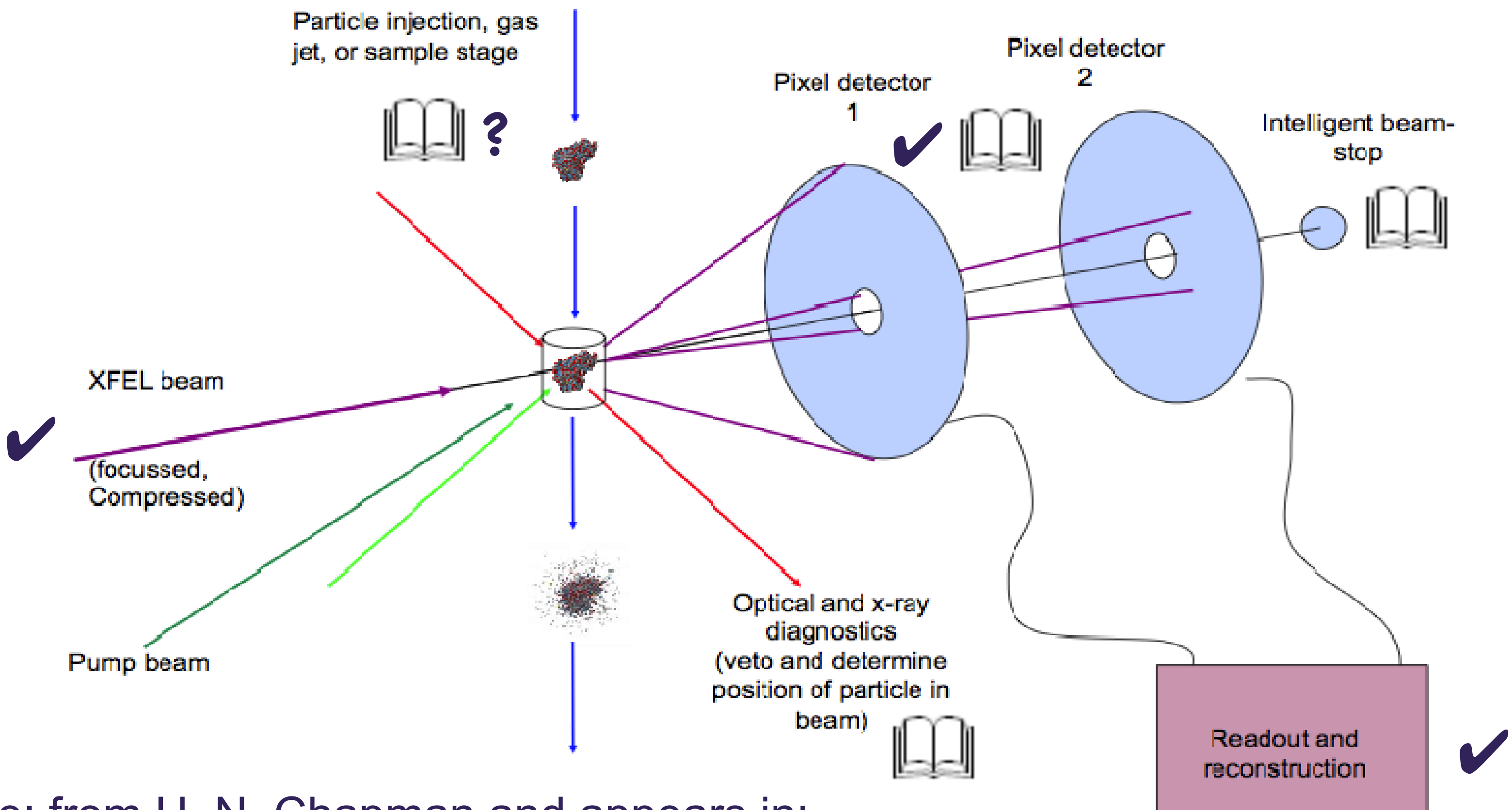

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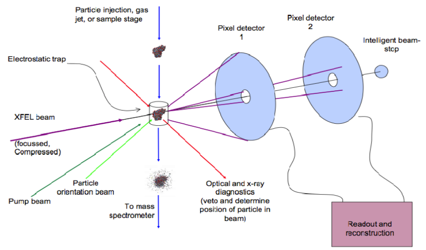
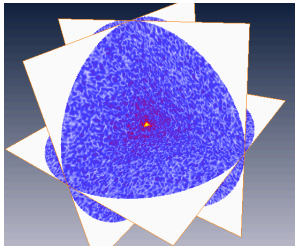
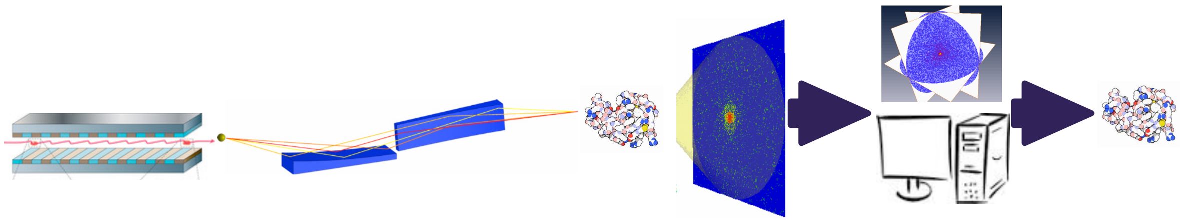
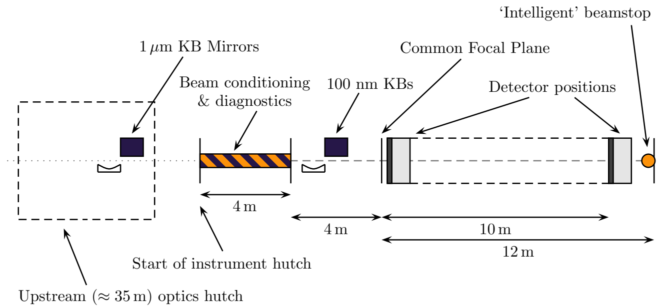
Conclusions

- Flux, wavefront, focal size are key parameters
- Metal coated (or SiC on metal) KB Mirrors as focusing optics
- Custom (XFEL rep rate) detector(s) required
- Modeling and Scientific Computing to be tightly integrated to the SPB instrument



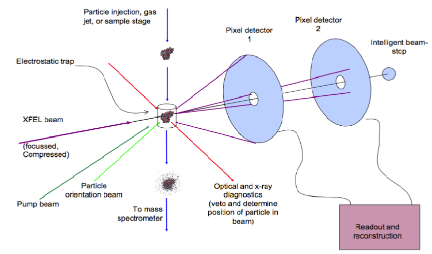






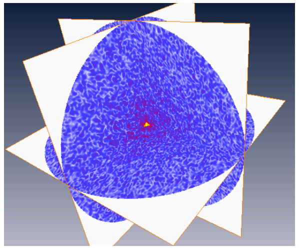
Conclusions

- Flux, wavefront, focal size are key parameters



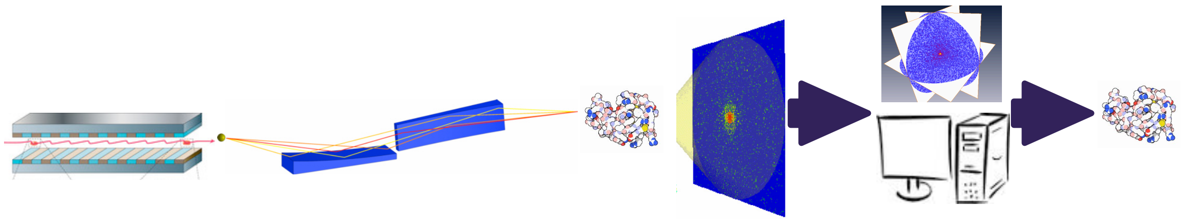
- Metal coated (or SiC on metal) KB Mirrors as focusing optics

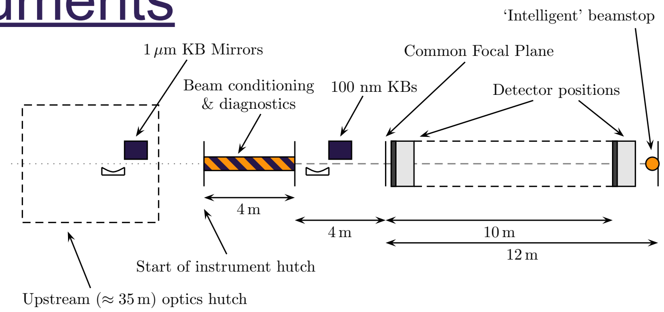
- Custom (XFEL rep rate) detector(s) required



- Modeling and Scientific Computing to be tightly integrated to the SPB instrument

http://www.xfel.eu/documents/technical_documents





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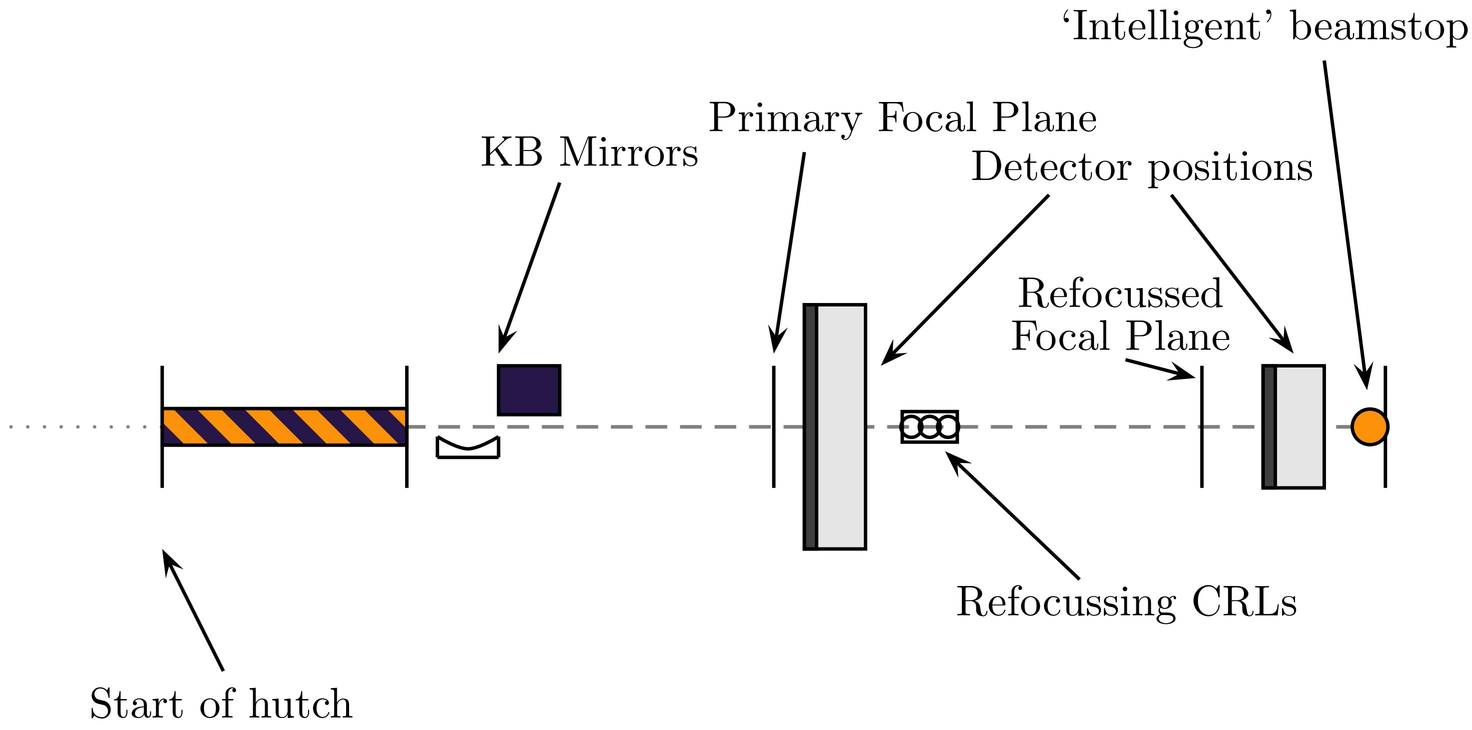
"Beyond Baseline" Optics Options



Beyond baseline

Potentially accommodates SFX UC EoI with minimal changes

Not yet modeled with propagation code

Requires circa 2–4 m longer hutch than baseline