

# High Pulse Rate Experiments at the European X-ray Free-electron Laser



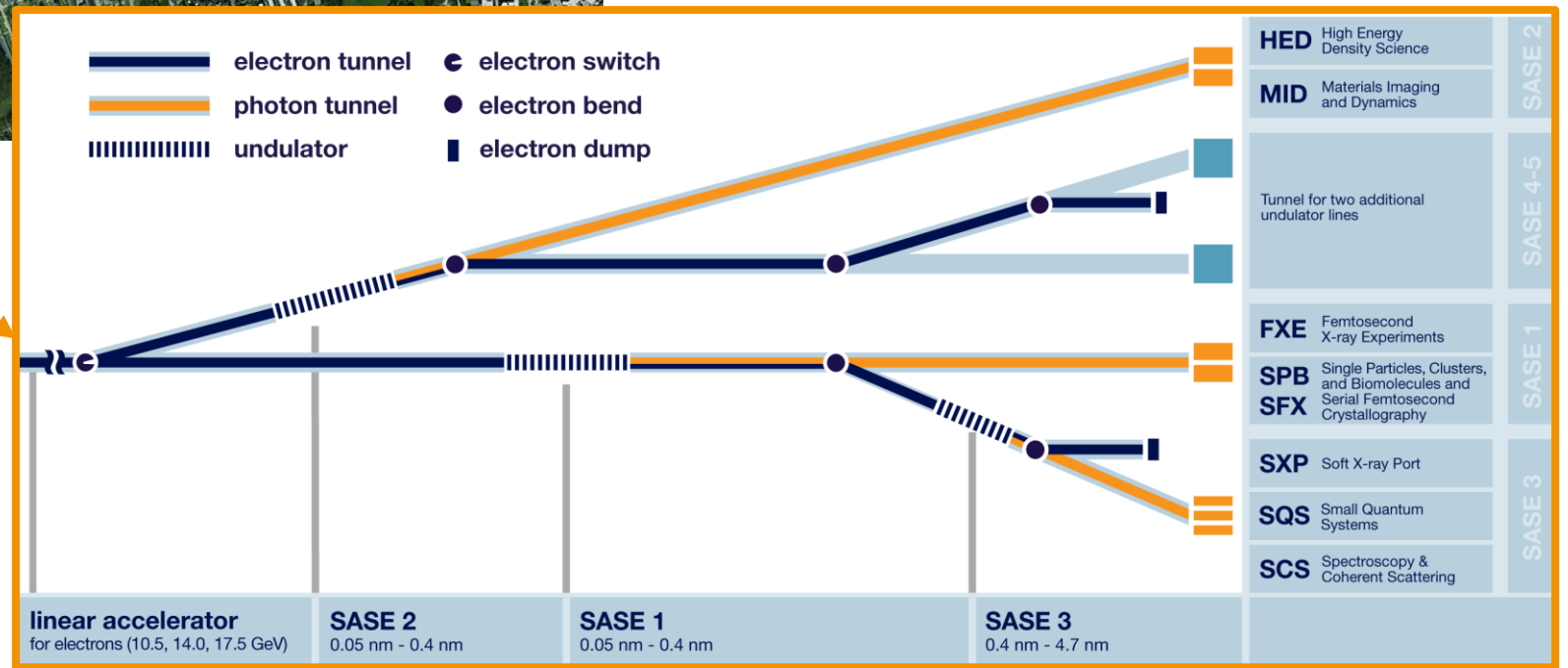
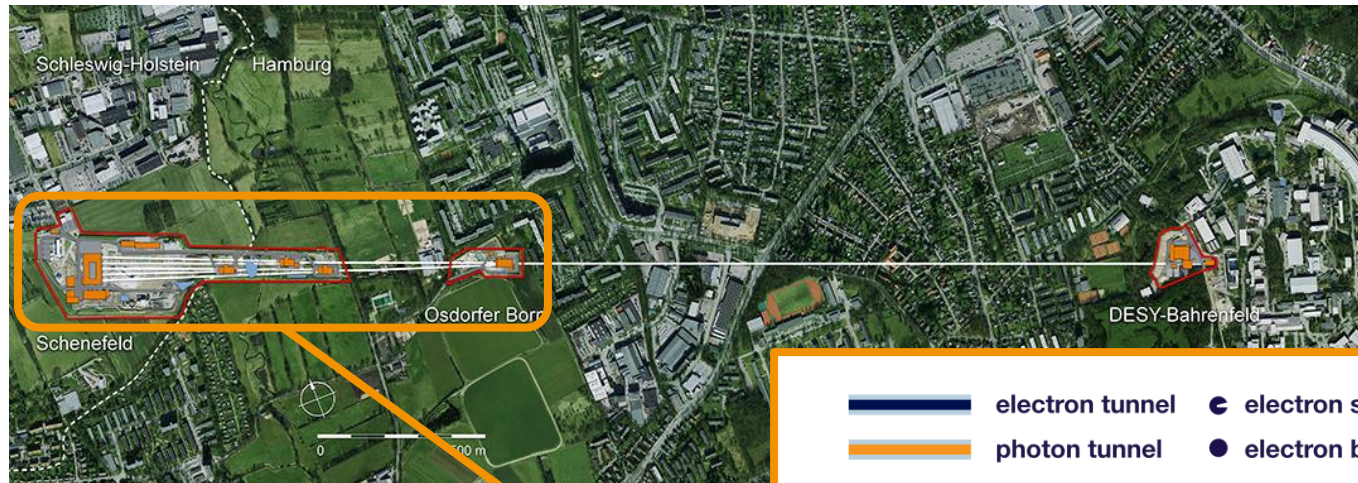
Romain Letrun

On behalf of the EuXFEL instrument groups

Luzern, 30.08.2023

67th ICFA Advanced Beam Dynamics Workshop on Future Light Sources: FLS 2023

# EuXFEL instruments overview

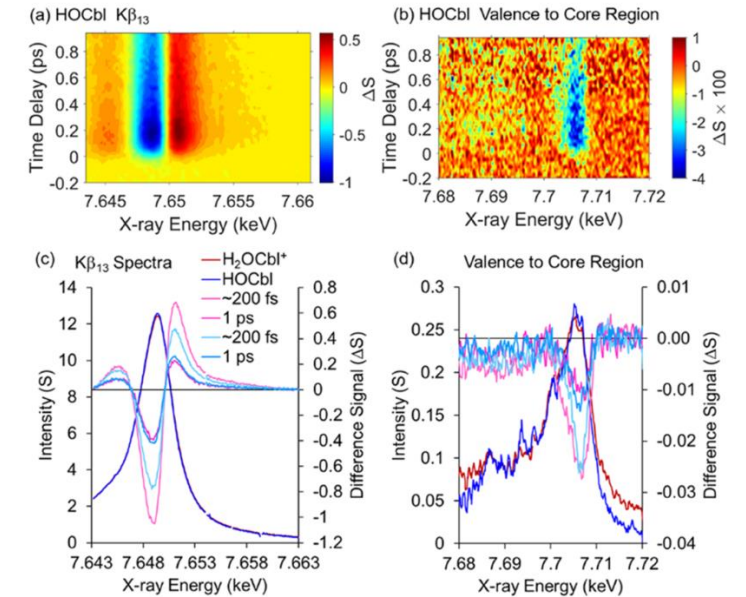


## Motivations for higher pulse rate

- Reduction of data acquisition time
  - Quickly reach sufficient signal-to-noise ratio
  - Evolution of existing techniques and development of new methods
  - Enlarge the scientific community
  
- Collection of very large datasets
  - Required for experiments with low hit rate
  - Classification into data subsets
  - Advanced data analysis methods
  
- Systematic studies
  - Lacking due to scarcity of beamtime

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Sension *et al.*, *JACS* **145** 14070–14086 (2023)

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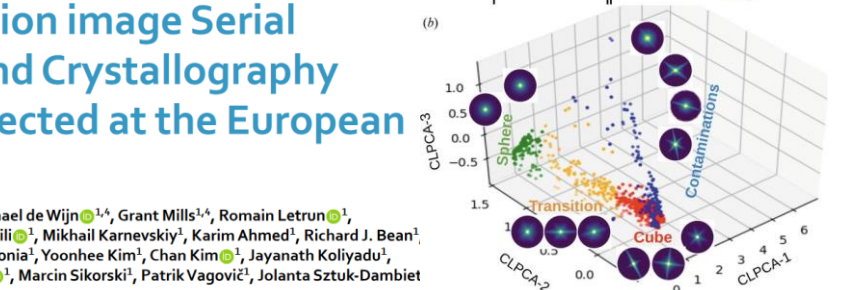
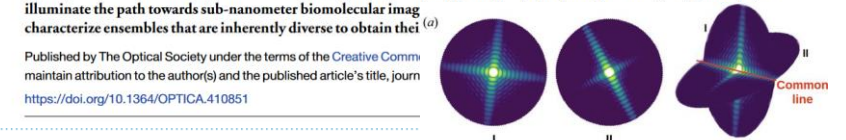
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### 3D diffractive imaging of nanoparticle ensembles using an x-ray laser

KARTIK AYYER,<sup>1,2,3,\*†</sup> P. LOURDU XAVIER,<sup>1,3,4,†</sup> JOHAN BIELECKI,<sup>5</sup> ZHOU SHEN,<sup>6</sup> BENEDIKT J. DAURER,<sup>6</sup> AMIT K. SAMANTA,<sup>4</sup> SALAH AWEL,<sup>4</sup> RICHARD BEAN,<sup>5</sup> ANTON BARTY,<sup>4</sup> MARTIN BERGEMANN,<sup>5</sup> TOMAS EKEBERG,<sup>7</sup> ARMANDO D. ESTILLORE,<sup>3</sup> HANS FANGOHR,<sup>5</sup> KLAUS GIEWEKEMEYER,<sup>5</sup> MARK S. HUNTER,<sup>8</sup> MIKHAIL KARNEVSKIY,<sup>5</sup> RICHARD A. KIRIAN,<sup>9</sup> HENRY KIRKWOOD,<sup>5</sup> YOONHEE KIM,<sup>5</sup> JAYANATH KOLYADU,<sup>5</sup> HOLGER LANGE,<sup>3,10</sup> ROMAIN LETRUN,<sup>5</sup> JANNIK LÜBKE,<sup>3,4,11</sup> THOMAS MICHELAT,<sup>5</sup> ANDREW J. MORGAN,<sup>12</sup> NILS ROTH,<sup>4,11</sup> TOKUSHI SATO,<sup>5</sup> MARCIN SIKORSKI,<sup>5</sup> FLORIAN SCHULZ,<sup>10</sup> JOHN C. H. SPENCE,<sup>9</sup> PATRIK VAGOVIĆ,<sup>4,5</sup> TAMME WOLLWEBER,<sup>1,2,3</sup> LENA WORBS,<sup>4,11</sup> OLEKSANDR YEFANOV,<sup>4</sup> YULONG ZHUANG,<sup>1,2</sup> FILIPE R. N. C. MAIA,<sup>7,13</sup> DANIEL A. HORKE,<sup>3,4,14</sup> JOCHEN KÜPPER,<sup>3,4,11,15</sup> N. DUANE LOH,<sup>6,16</sup> ADRIAN P. MANCUSO,<sup>5,17</sup> AND HENRY N. CHAPMAN<sup>3,4,11</sup> ✉

Single particle imaging at x-ray free electron lasers (XFELs) has the potential to determine the structure and dynamics of single biomolecules at room temperature. Two major hurdles have prevented this potential from being reached, namely, the collection of sufficient high-quality diffraction patterns and robust computational purification to overcome structural heterogeneity. We report the breaking of both of these barriers using gold nanoparticle test samples, recording around 10 million diffraction patterns at the European XFEL and structurally and orientationally sorting the patterns to obtain better than 5-nm-resolution 3D reconstructions for each of four samples. With these new developments, integrating advancements in x-ray sources, fast-framing detectors, efficient sample delivery, and data analysis algorithms, we illuminate the path towards sub-nanometer biomolecular imaging.



## scientific data

OPEN

DATA DESCRIPTOR

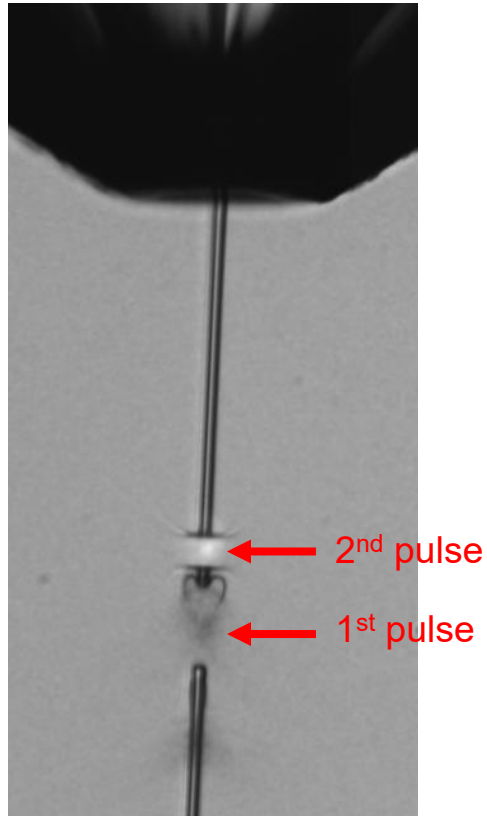
### A multi-million image Serial Femtosecond Crystallography dataset collected at the European XFEL

Henry J. Kirkwood<sup>1,4,✉</sup>, Raphael de Wijn<sup>1,4</sup>, Grant Mills<sup>1,4</sup>, Romain Letrun<sup>1</sup>, Marco Kloos<sup>1</sup>, Mohammad Vakili<sup>1</sup>, Mikhail Karnevskiy<sup>1</sup>, Karim Ahmed<sup>1</sup>, Richard J. Bean<sup>1</sup>, Johan Bielecki<sup>1</sup>, Fabio Dall'Antonia<sup>1</sup>, Yoonhee Kim<sup>1</sup>, Chan Kim<sup>1</sup>, Jayanath Kolyadu<sup>1</sup>, Adam Round<sup>1,2</sup>, Tokushi Sato<sup>1</sup>, Marcin Sikorski<sup>1</sup>, Patrik Vagovic<sup>1</sup>, Jolanta Sztuk-Dambiet & Adrian P. Mancuso<sup>1,3</sup>

Ayyer *et al.*, *Optica* **8**, 15–23 (2021)  
 Zhuang *et al.*, *IUCrJ* **9** 204–214 (2022)  
 Kirkwood *et al.*, *Sci. Data* **9** 161 (2022)



## Sample delivery for high repetition rate XFELs

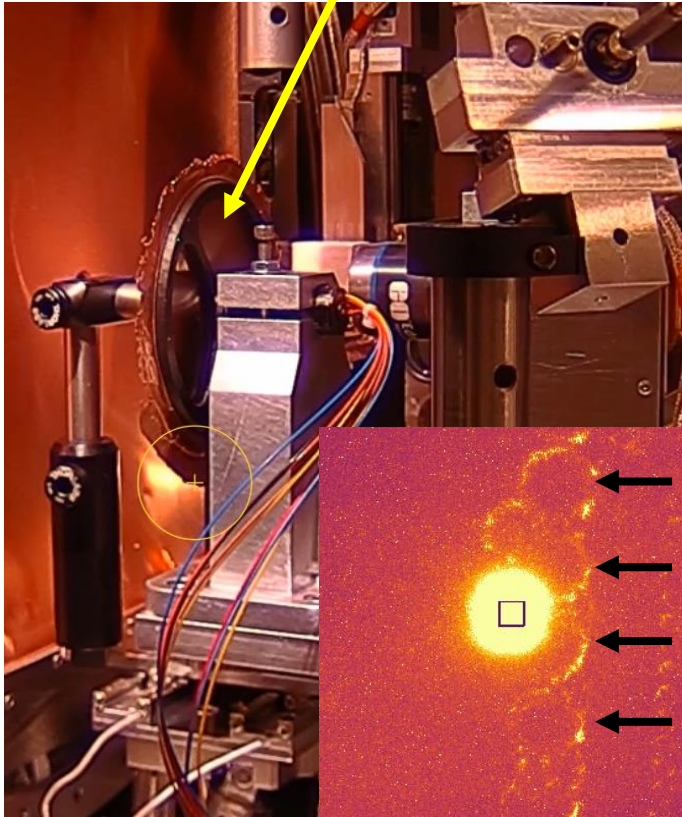


### Liquid/aerosol/gas phase samples

- High jet velocity ( $\geq 50$  m/s for 1.1 MHz)
- very high sample consumption
- velocity limited for thick or viscous jets

## Sample delivery for high repetition rate XFELs

Rotating disk



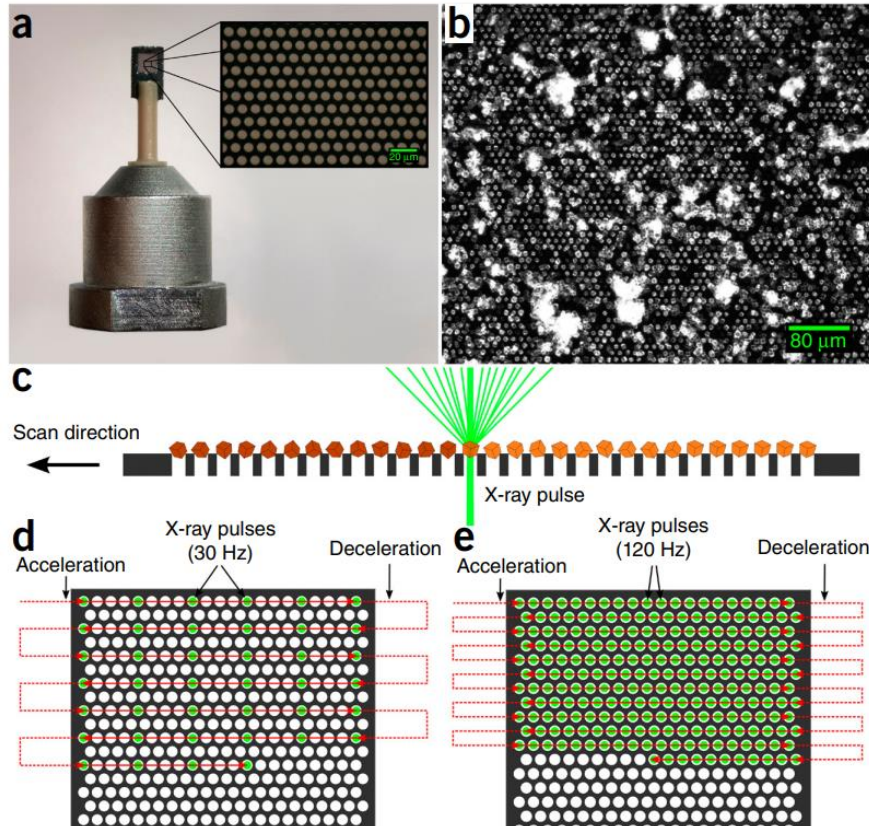
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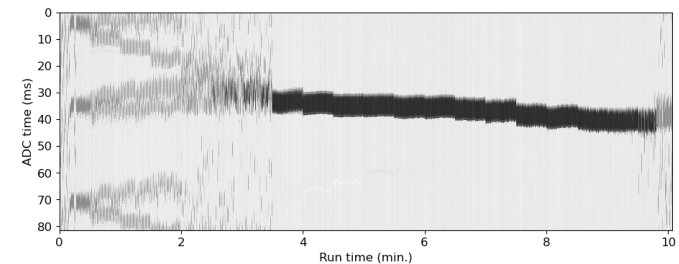
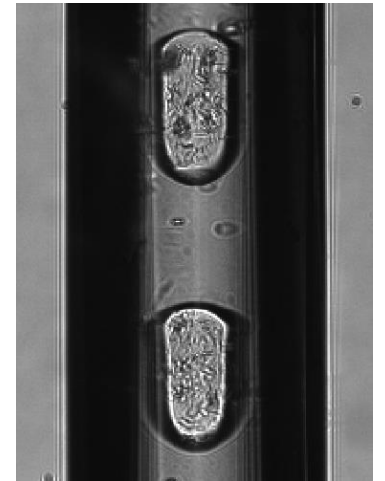
Already complex at low repetition rate



## MHz burst mode operation at EuXFEL – A blessing and a curse

- High sample wastage (>99.4% at EuXFEL) for liquid/aerosol jet experiments where sample cannot be recirculated. Those experiments also have an inherently low hit rate (0.1% - ~10%)
  - New sample delivery methods under development, but not yet routine
- Undesirable effects with solid state samples, e.g., heating/cooling strain
- Present 2D area detector technology is trade-off between on-chip memory and pixel size
  - Development ongoing along with better use of existing detectors, e.g. event vetoing
- User data storage
  - Data reduction effort in progress, need to change mindset of users

Aqueous sample droplets in oil at 10Hz

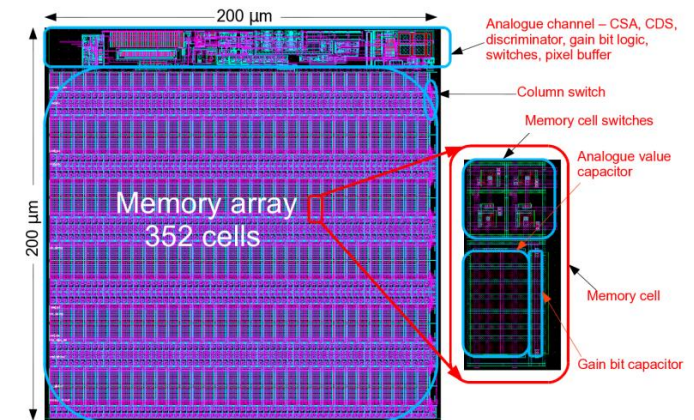


Courtesy of A. Ros, ASU

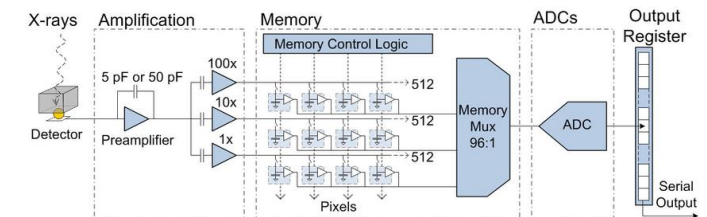
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**AGIPD detector**, 200  $\mu\text{m}$  pixels  
352 memory cells up to 4.5 MHz



**LPD detector**, 500  $\mu\text{m}$  pixels  
512 memory cells up to 4.5 MHz

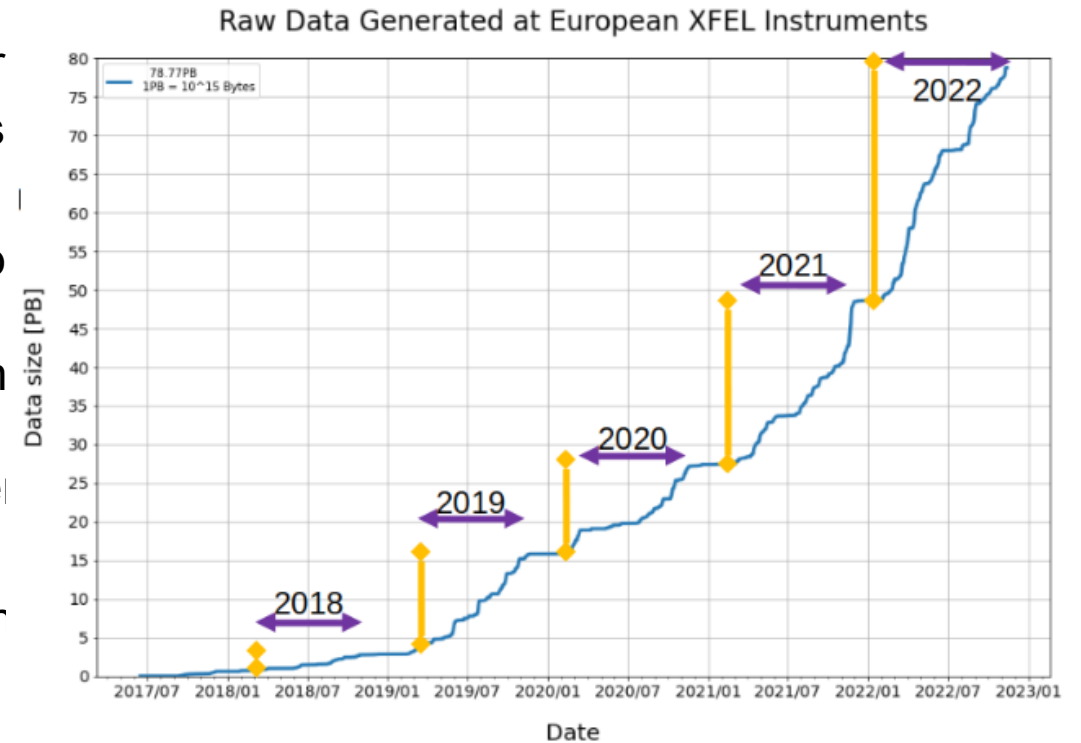


Allahgholi *et al.*, *JINST* **10** C01023 (2015)

Koch *et al.*, *JINST* **8** C11001 (2013)

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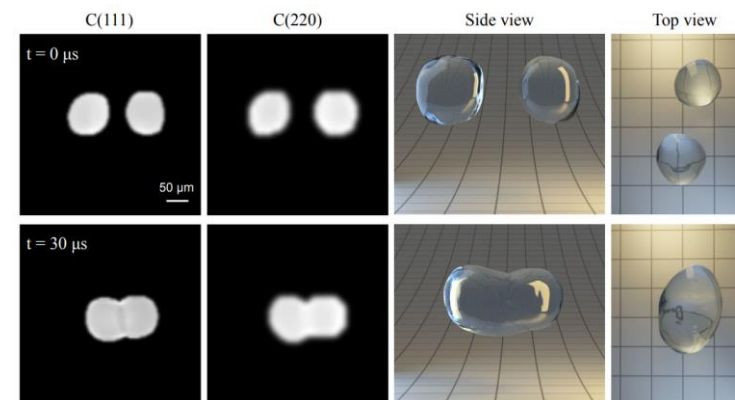
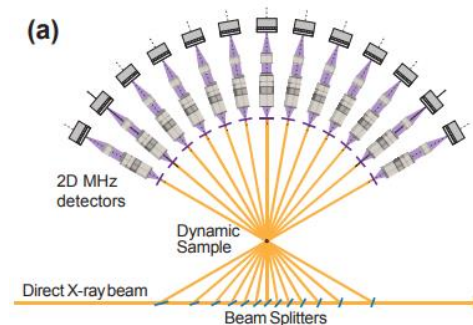
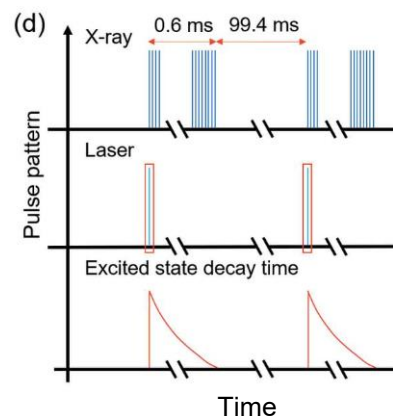
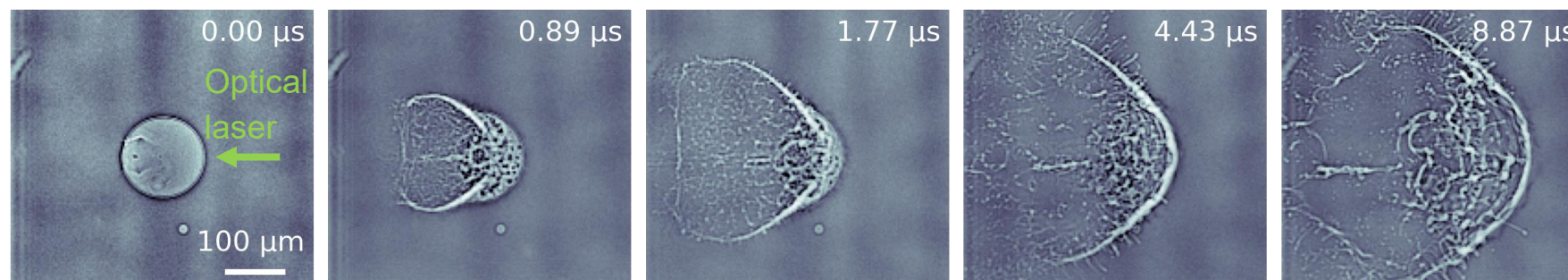
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## MHz burst mode applications

Dynamics on microsecond timescale - Time grid defined by pulse period

Time-resolved  
X-ray microscopy

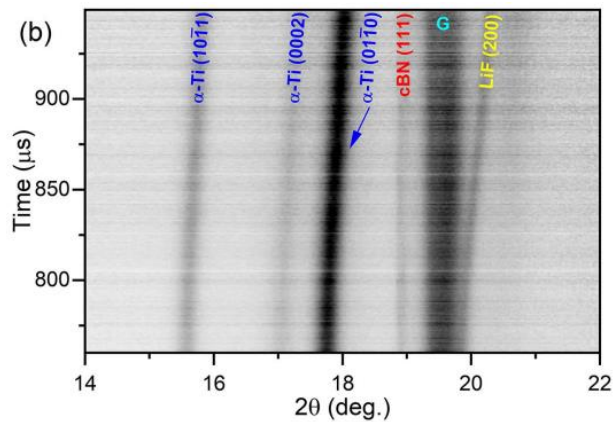


Reuter *et al.*, under review  
Villanueva-Perez *et al.*, under review

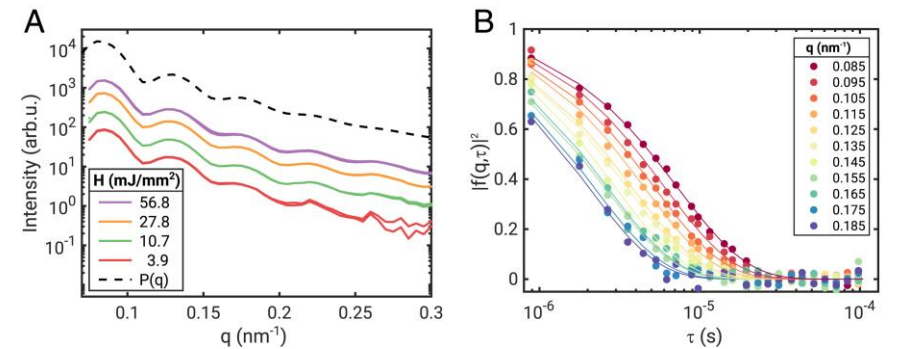
# MHz burst mode applications

Dynamics on microsecond timescale, but also femtosecond timescale

Dynamic compression



X-ray photon correlation spectroscopy



Husband *et al.*, *J. Synchrotron Rad.* **30** 671-685 (2023)  
 Lehmkuhler *et al.*, *PNAS* **117** 24110-24116 (2020)



## Towards higher duty cycle operation

### 10s to 100s kHz CW or long burst operation

- Would support many classes of experiment
  - Relaxed sample delivery requirements, reduction of sample wastage
- Longer burst: easier to accommodate independent RF regions for each beamline → increased flexibility

### MHz CW or burst operation

- Leveraged by a limited number of experimental techniques at the moment, but has opened up new opportunities
- Applications specific to MHz burst mode

**Not a one-size-fits-all!**

## Acknowledgements

DESY accelerator team

EuXFEL instruments and technical groups

EuXFEL users community