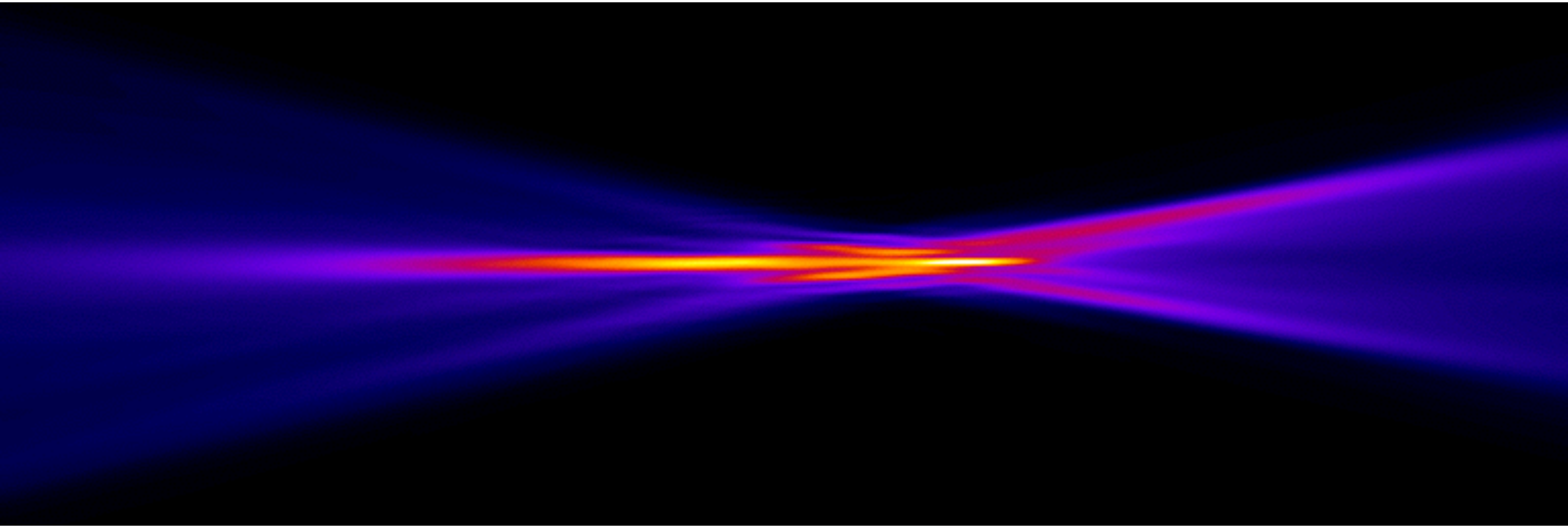
XFEL Science with Nanobeams

Christian G. Schroer
FS-PETRA, DESY & University of Hamburg



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DESY

Collaboration

C. Baumbach, S. Hönig,
R. Hoppe, V. Meier,
J. Patommel, S. Ritter,
D. Samberg, F. Seiboth,
S. Stephan, F. Wittwer,
T. Woike
Inst. f. Strukturphysik,
TU Dresden, Dresden

M. Kahnt, J. Reinhardt,
M. Seyrich, M. Scholz,
A. Schropp
FS-PETRA, DESY

B. Lengeler
RXOptics, Jülich

R. Collins, Y. Ping
LLNL, Livermore, USA

D. Nilsson, F. Uhlén,
U. Vogt, H. M. Hertz
KTH, Stockholm, Sweden

A. Madsen, K. Appel, T. Tschentscher,
European XFEL

H.J. Lee, R. Nagler,
E. C. Galtier, U. Zastrau,
J. B. Hastings, P. Heimann,
B. Arnold
LCLS, Menlo Park, USA

VolkswagenStiftung

Federal Ministry of Education and Research

DESY

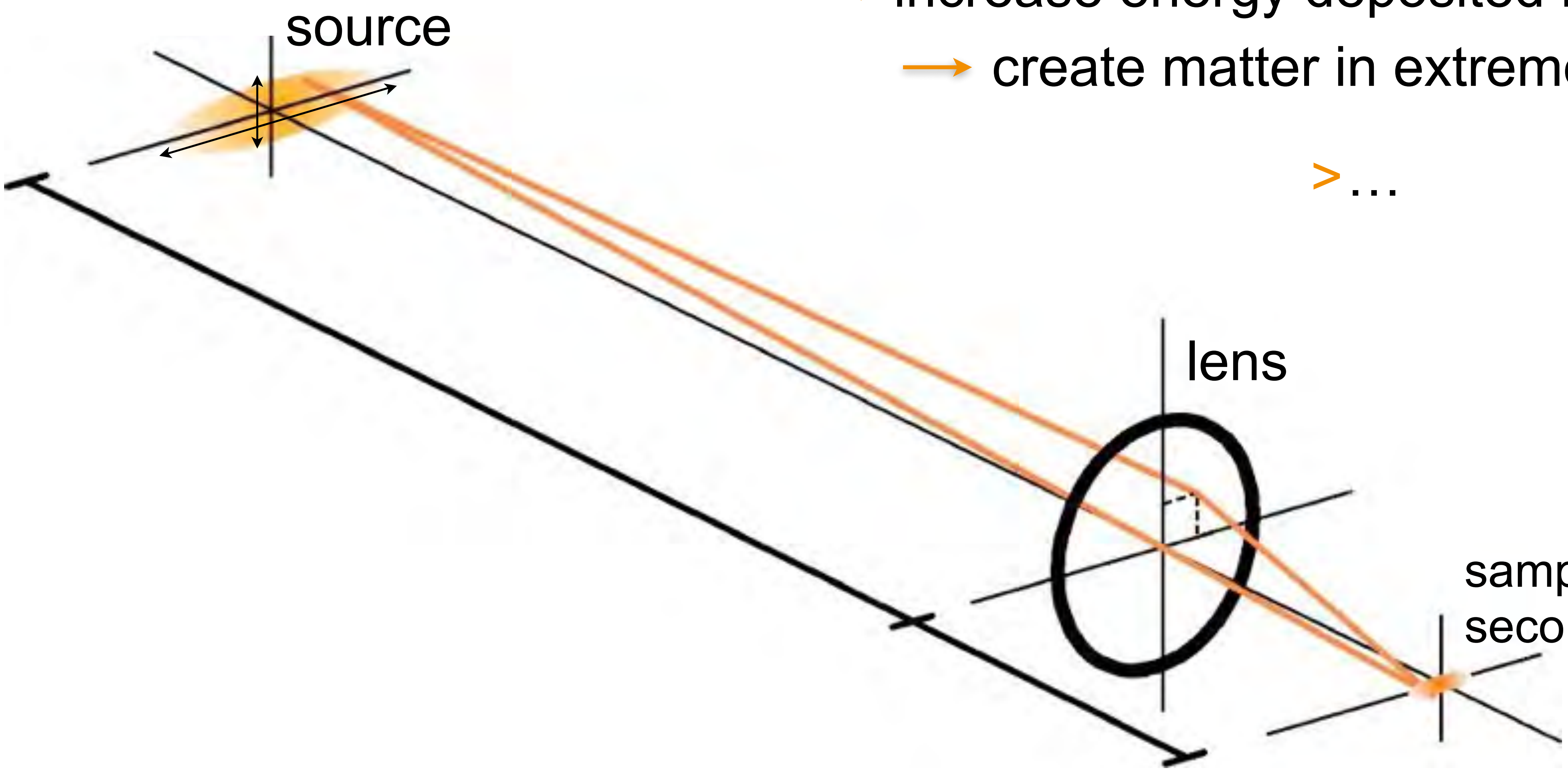
Focusing Hard X-Ray FEL Pulses

> increase fluence for imaging
  → resolution determined by fluence on sample

> increase intensity on sample
  → induce non-linear optical effects

> increase energy deposited in sample
  → create matter in extreme conditions

> …

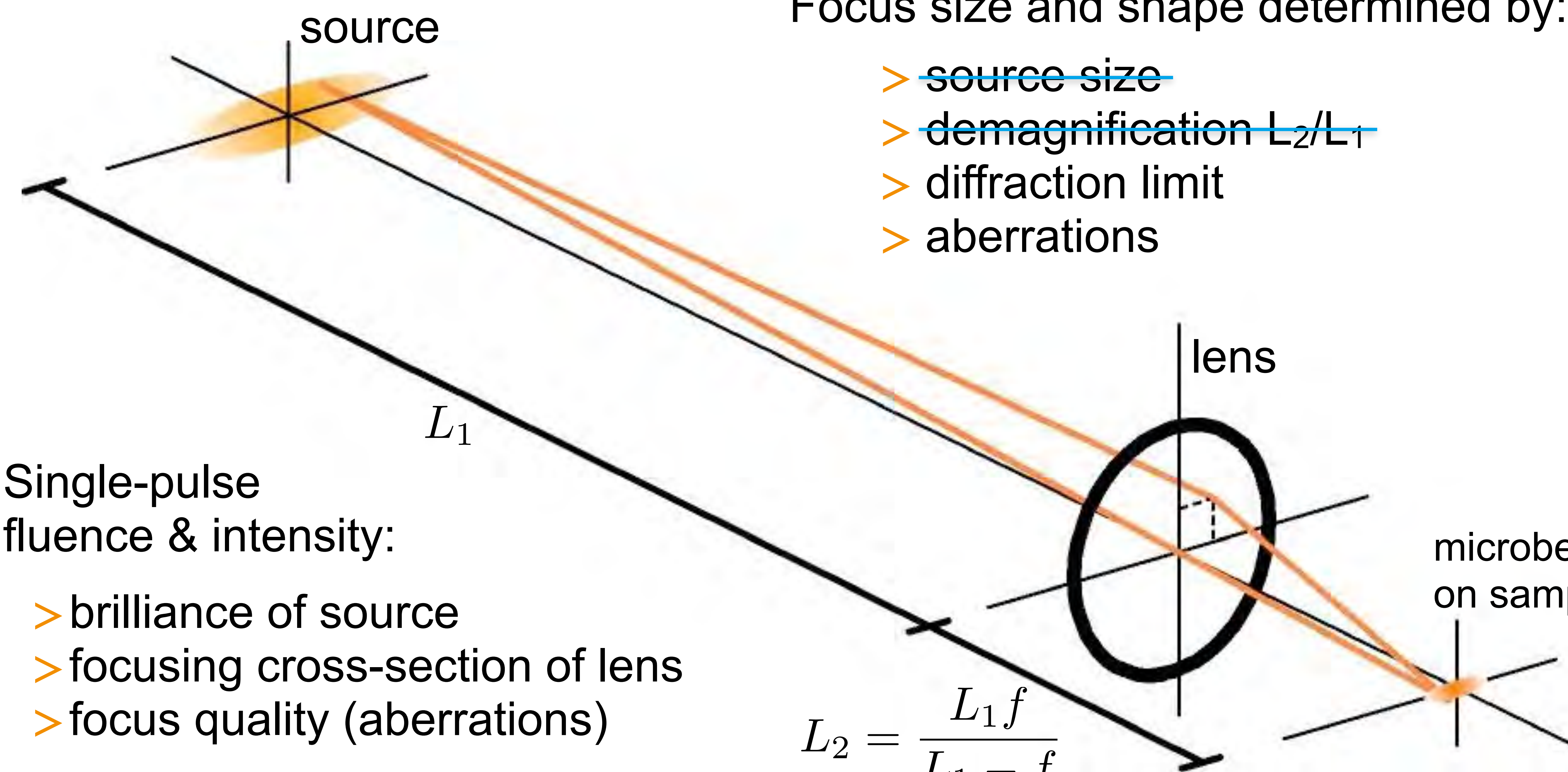


Diffraction-Limited Focusing at XFEL Source

XFEL beam: High degree of transverse coherence

Focus size and shape determined by:

- ~~source size~~
- ~~demagnification L_2/L_1~~
- diffraction limit
- aberrations



$$L_2 = \frac{L_1 f}{L_1 - f}$$

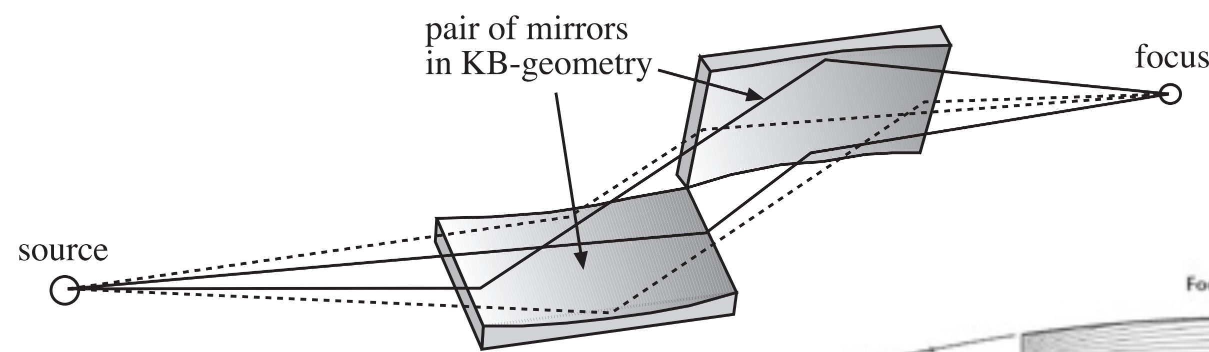
Single-pulse
fluence & intensity:

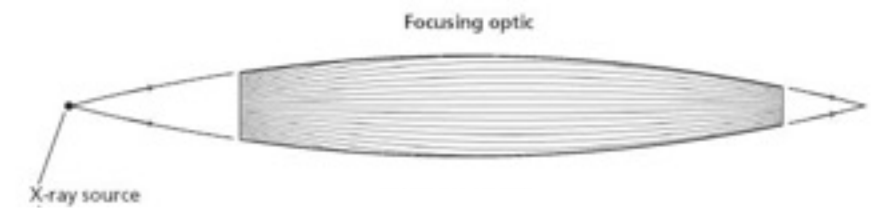
- brilliance of source
- focusing cross-section of lens
- focus quality (aberrations)

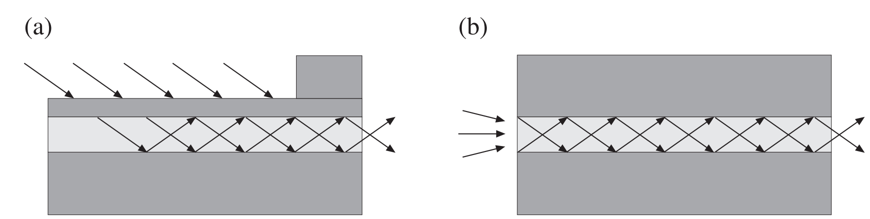
Nanofocusing Optics

reflection:

- mirrors (25 nm)
- capillaries
- wave guides (~10 nm)

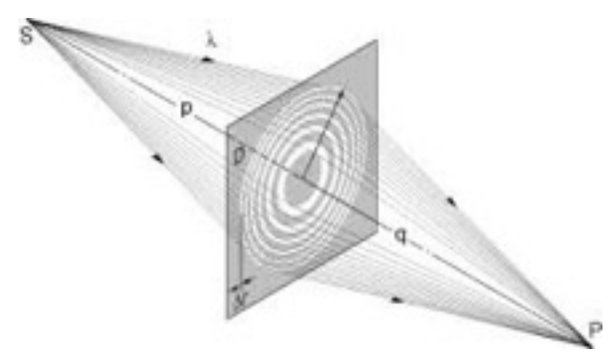


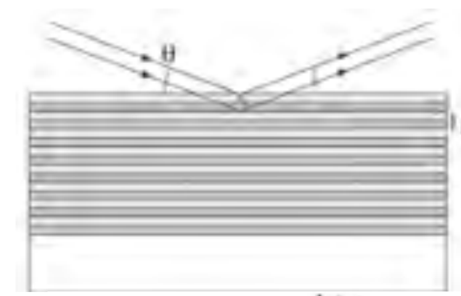


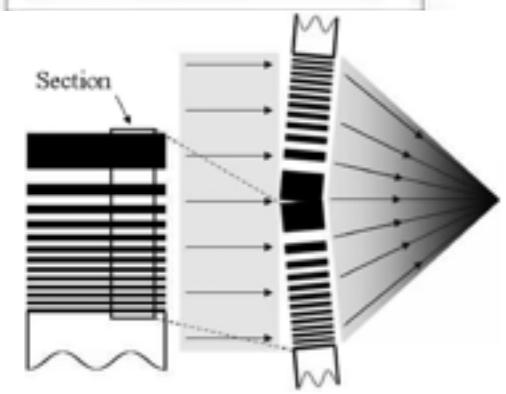


diffraction:

- Fresnel zone plates (~20 nm)
- multilayer mirrors (7 nm)
- multilayer Laue lenses (16 nm)
- bent crystals

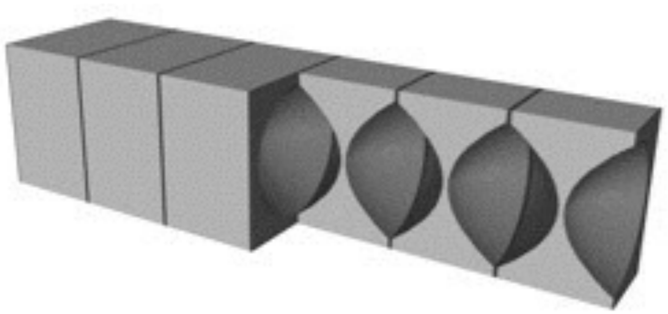






refraction:

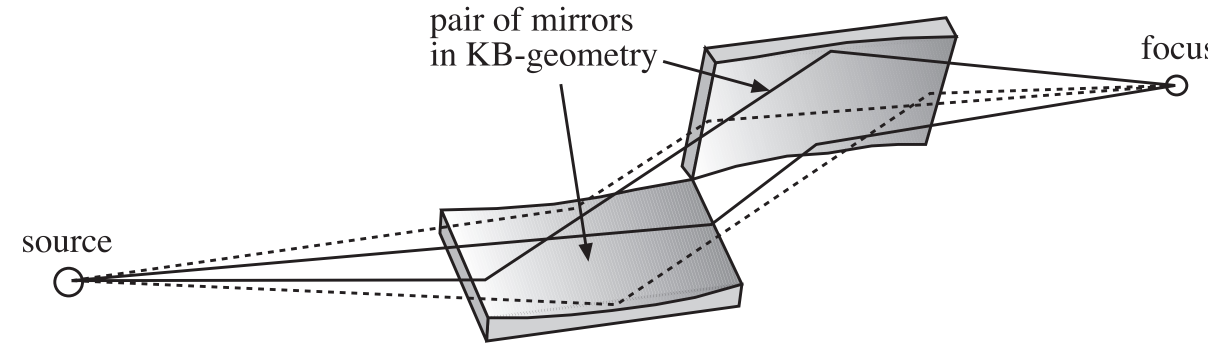
- lenses (43 nm, 18 nm)



Nanofocusing Optics at XFEL

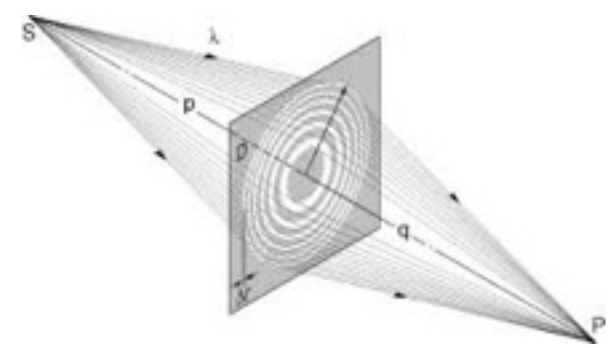
reflection:

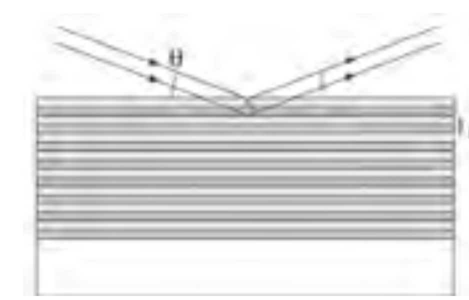
- mirrors (50 nm)
- ~~capillaries~~
- ~~wave guides~~



diffraction:

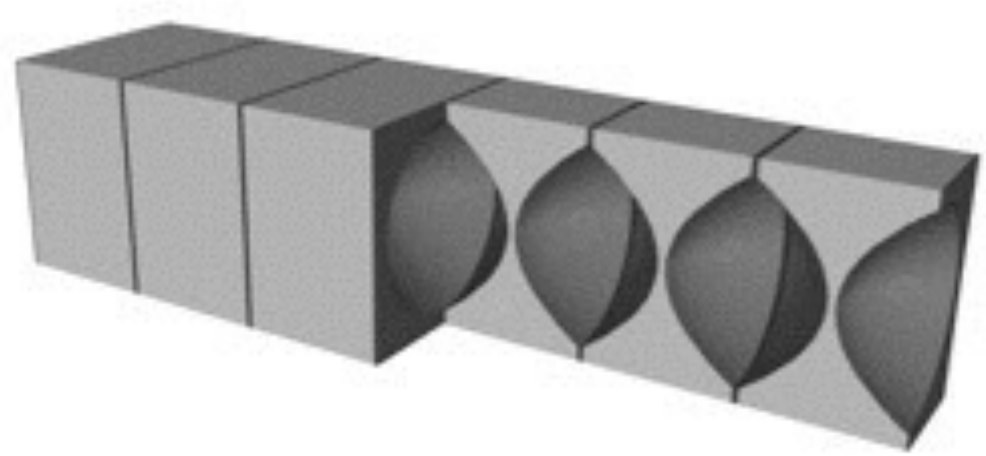
- Fresnel zone plates (~200 nm)
- multilayer mirrors
- ~~multilayer Laue lenses~~
- ~~bent crystals~~





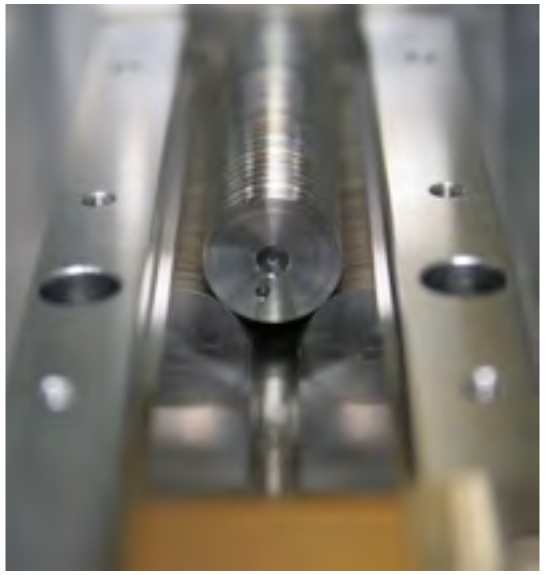
refraction:

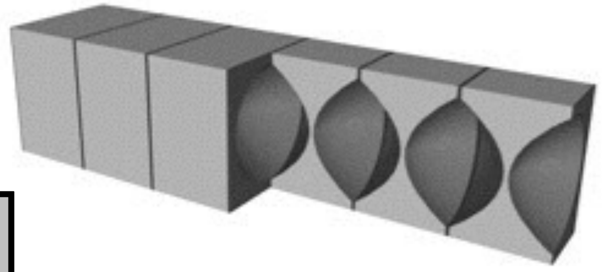
- lenses (125 nm)

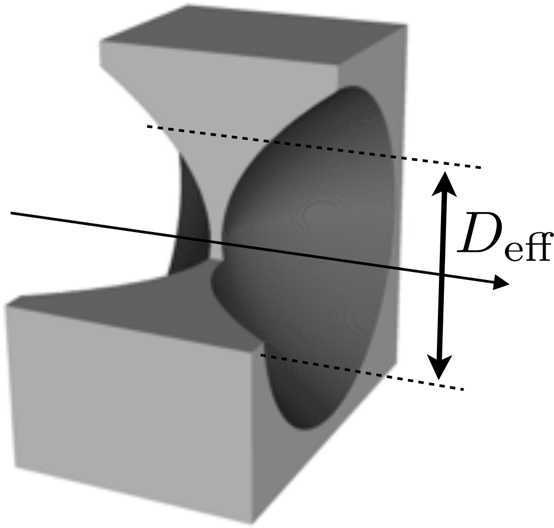


Beryllium Compound Refractive Lenses

- first realized in 1996 (Snigirev et al.)
- a variety of refractive lenses have been developed since
- applied in full-field imaging and scanning microscopy
- Beryllium: withstands single XFEL pulses
- Disadvantage: chromaticity





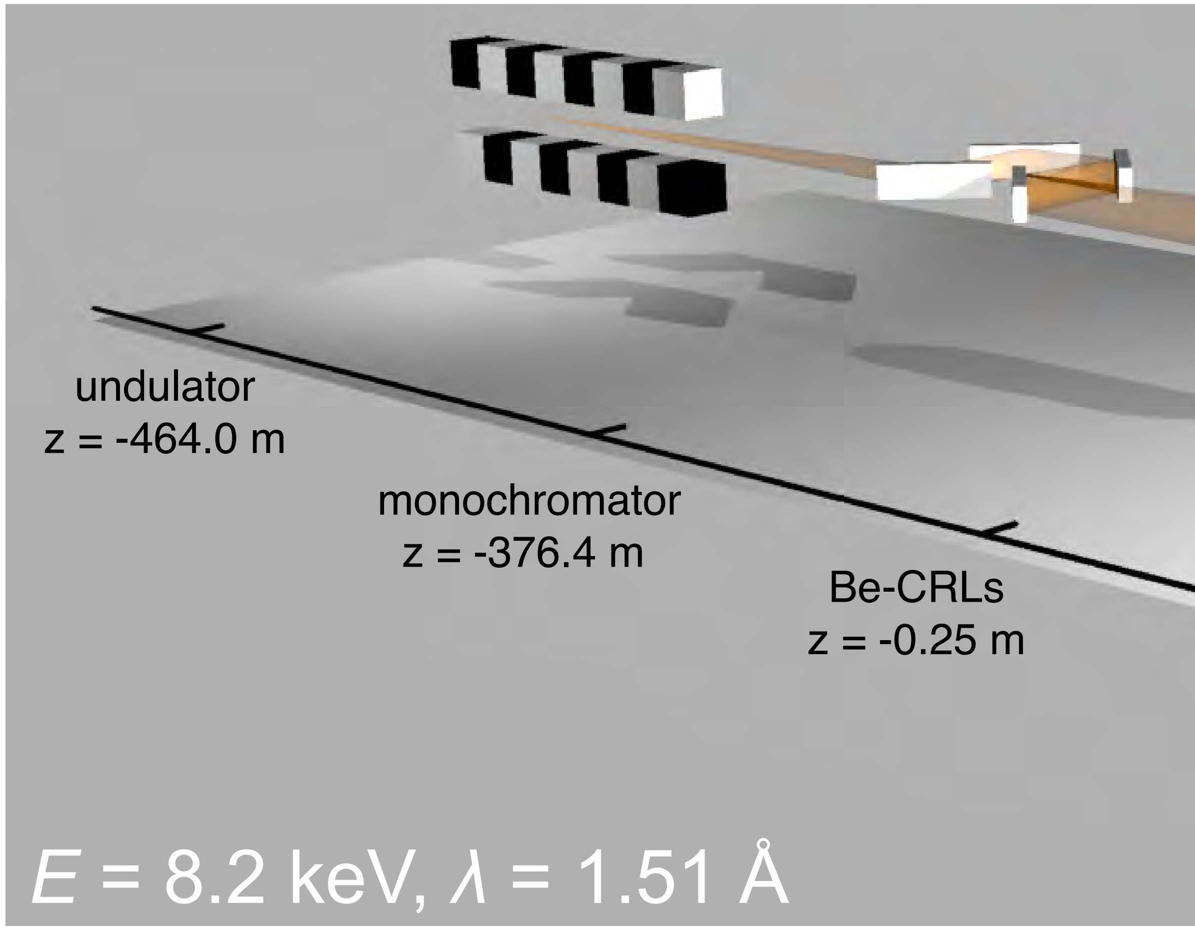


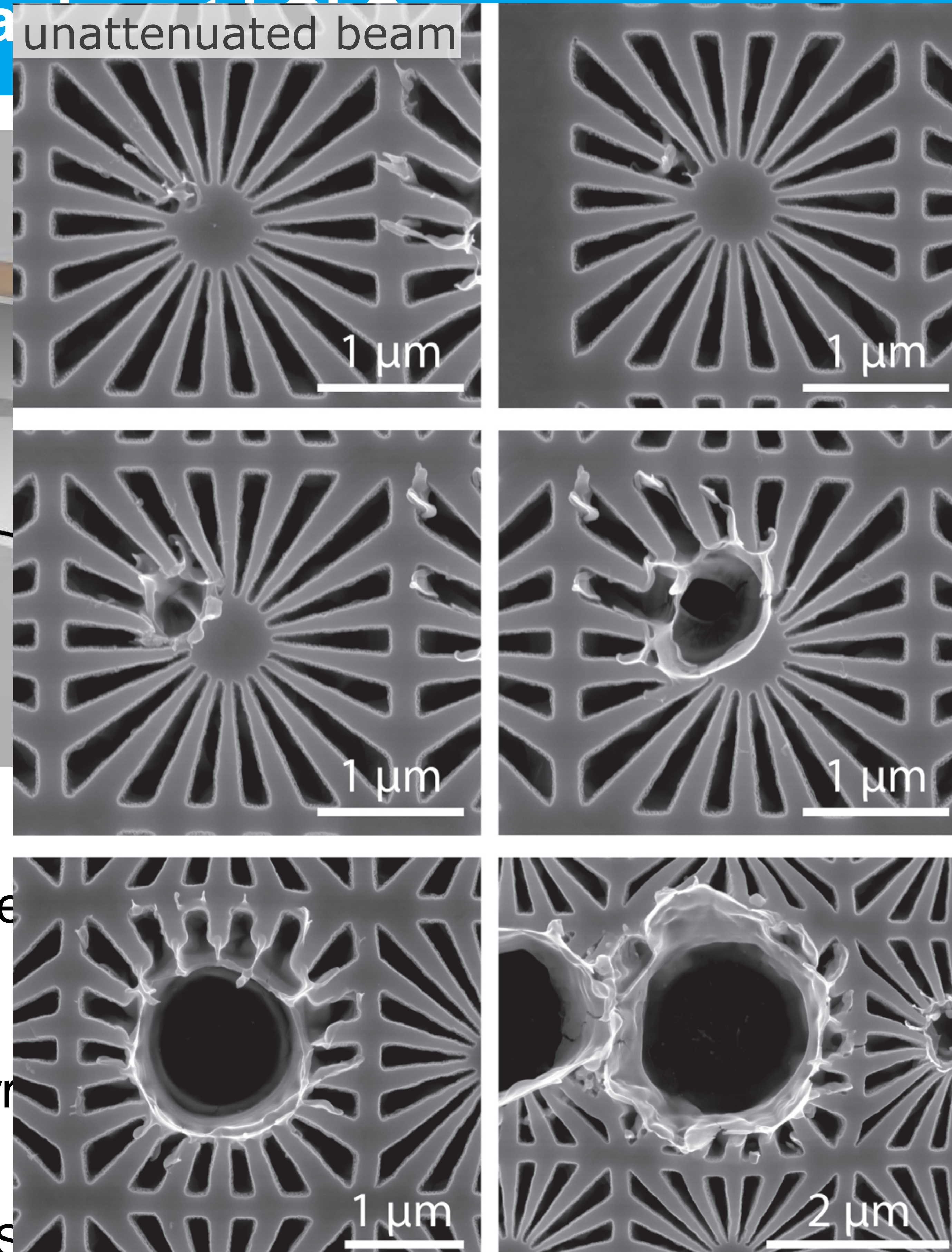
Example parameters for LCLS MEC:

E [keV]	f [mm]	N	NA [mrad]	d_t [nm]	flux [ph/pulse]	power density [W/cm²]	gain
8	200	24	0.70	82	$3.3 \cdot 10^{10}$	$1.33 \cdot 10^{19}$	$7.1 \cdot 10^{6}$
	300	16	0.54	108	$4.7 \cdot 10^{10}$	$1.09 \cdot 10^{19}$	$6.6 \cdot 10^{6}$
	400	12	0.43	133	$6.0 \cdot 10^{10}$	$9.17 \cdot 10^{18}$	$6.0 \cdot 10^{6}$
9	200	31	0.73	71	$3.5 \cdot 10^{10}$	$2.12 \cdot 10^{19}$	$1.0 \cdot 10^{7}$
	300	20	0.54	95	$5.1 \cdot 10^{10}$	$1.73 \cdot 10^{19}$	$9.3 \cdot 10^{6}$
	400	15	0.44	118	$6.3 \cdot 10^{10}$	$1.38 \cdot 10^{19}$	$8.4 \cdot 10^{6}$

parameters without prefocusing, pulse length: 60 fs

Nanofocusing and Nanoima

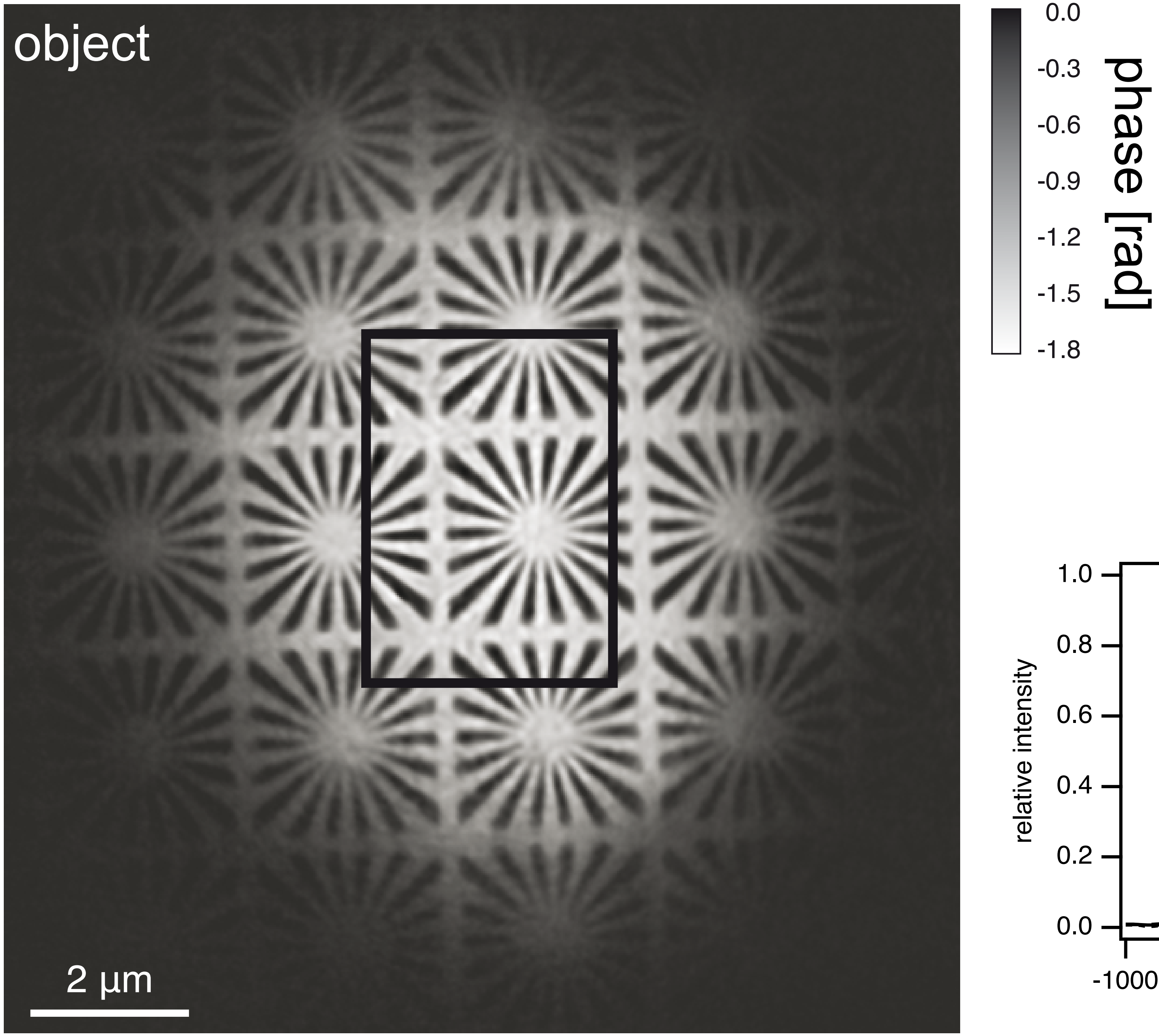


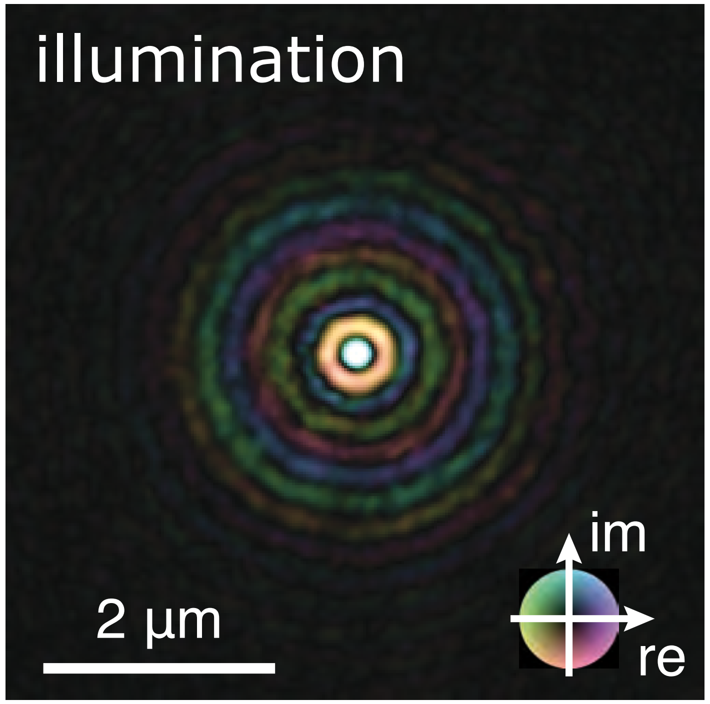


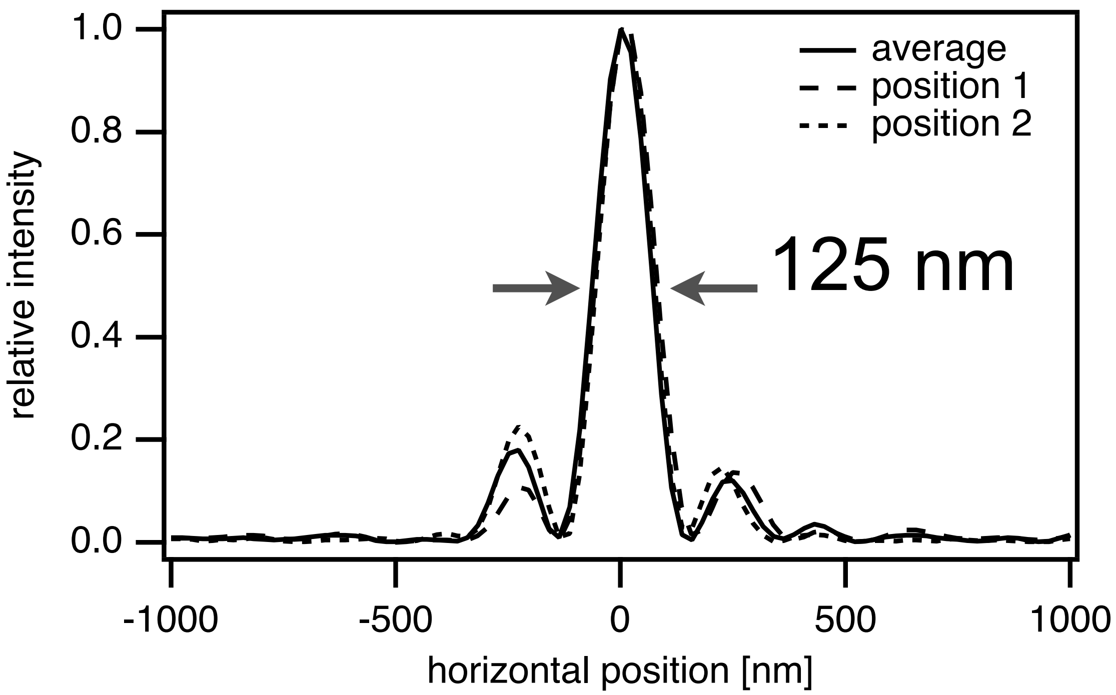
- Nanofocusing by Be CRLs
  - → generate nanobeam for near-fie
- Characterization by ptychography
  - → determine full caustic and aberr

A. Schropp, et al., S

Ptychographic Reconstruction

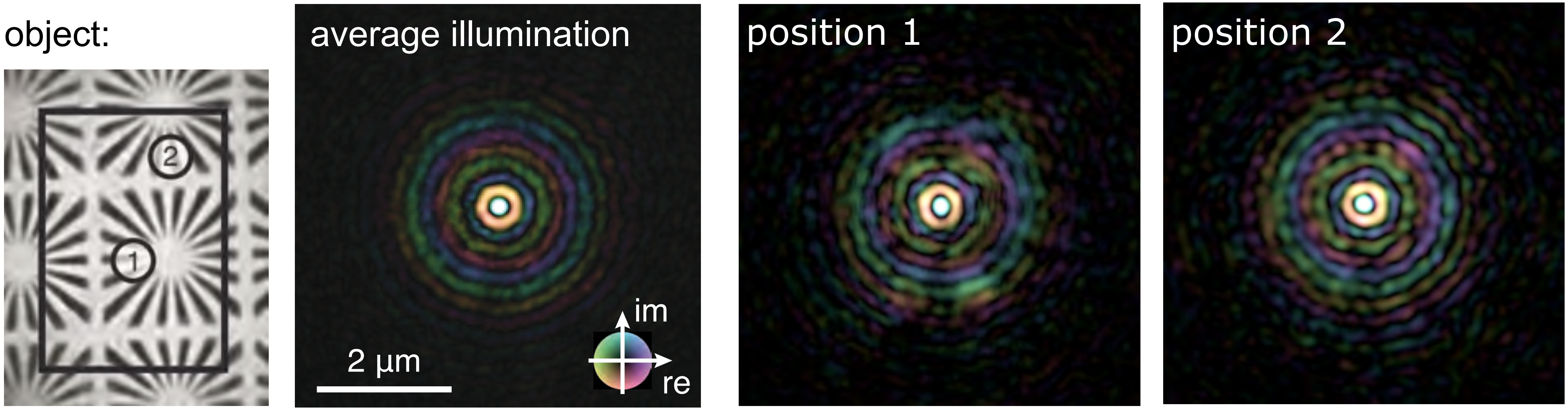


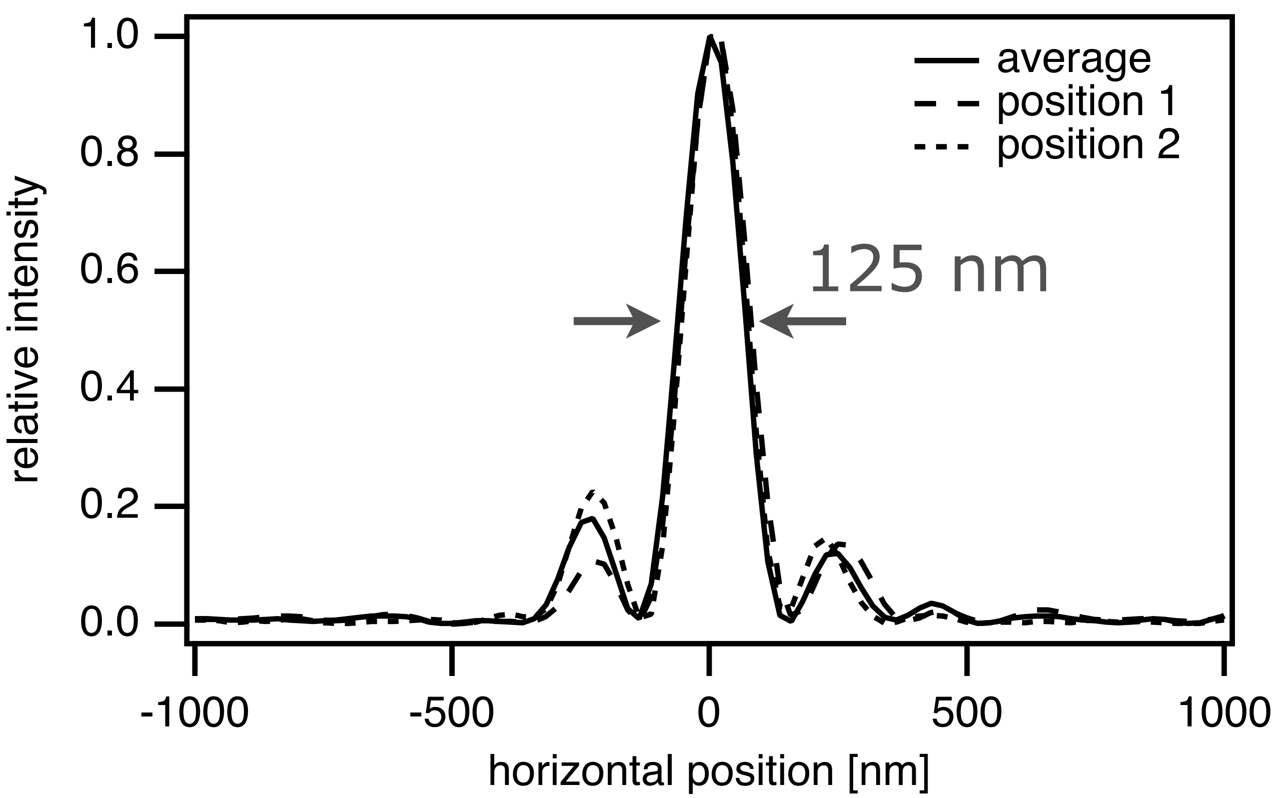




A. Schropp, et al., Sci. Rep. **3**, 1633 (2013).

Illumination: Single-Shot Refinement





Refine single shot illumination:

- fixed, reconstructed object
- individual diffraction pattern

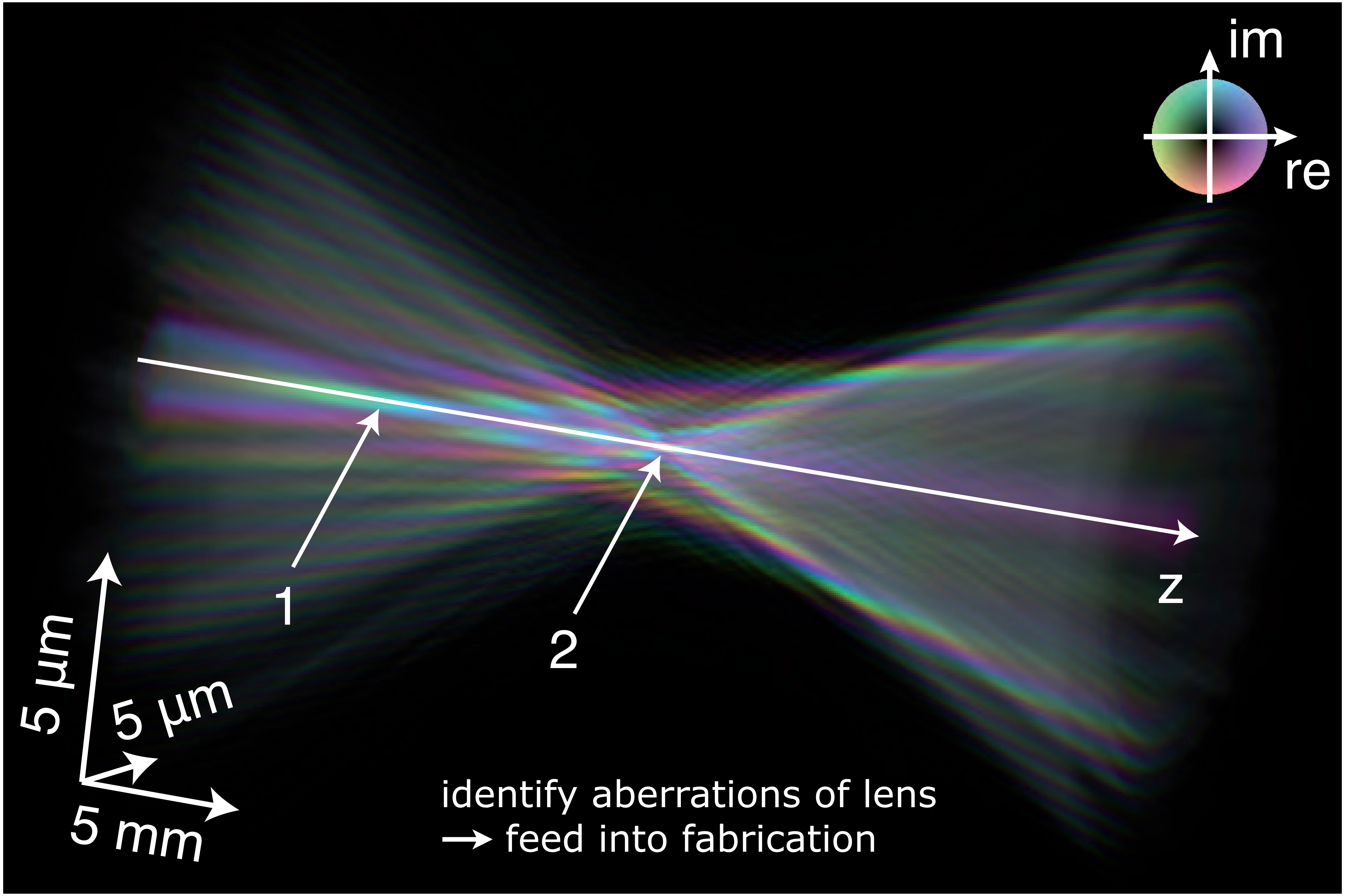
→ *a-posteriori* reconstruction of illumination!

In future:

→ derive non-invasive single-shot diagnostics

A. Schropp, et al., Sci. Rep. **3**, 1633 (2013).

Nanofocused LCLS Beam Profile

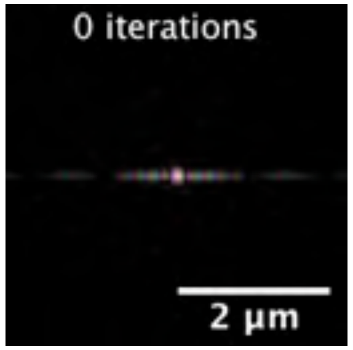


A. Schropp, et al., Sci. Rep. **3**, 1633 (2013).

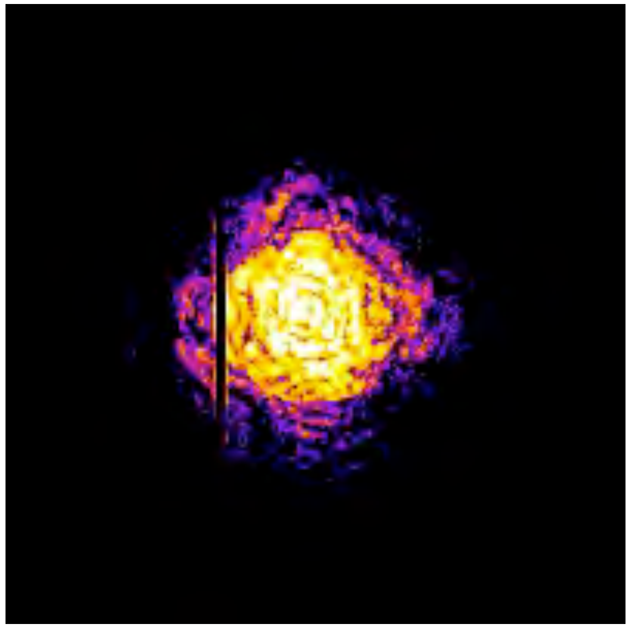
Fast XFEL-Nanobeam Characterization

Example: Ptychography at 120 Hz (LCLS)

nanostructured sample (SEM image)

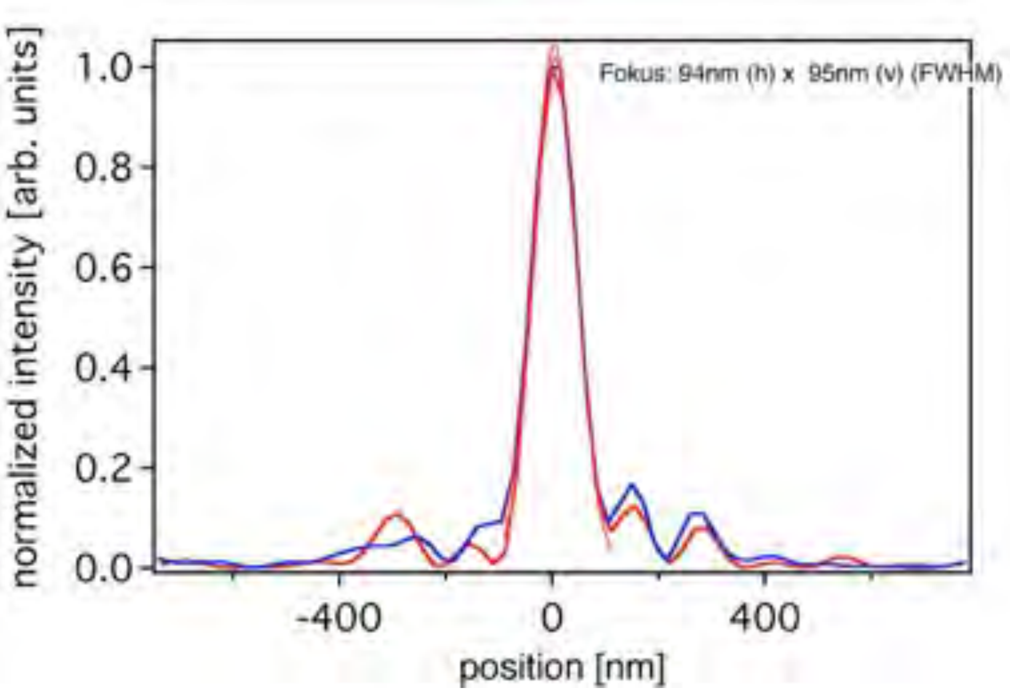


- stack of 30 Be-CRLs, f = 170mm
- 2D-scan: 50 x 50 steps with a step size of 100 nm
- theoretical focus size: 85nm (FWHM)
- measured focus size: 95nm (FWHM)



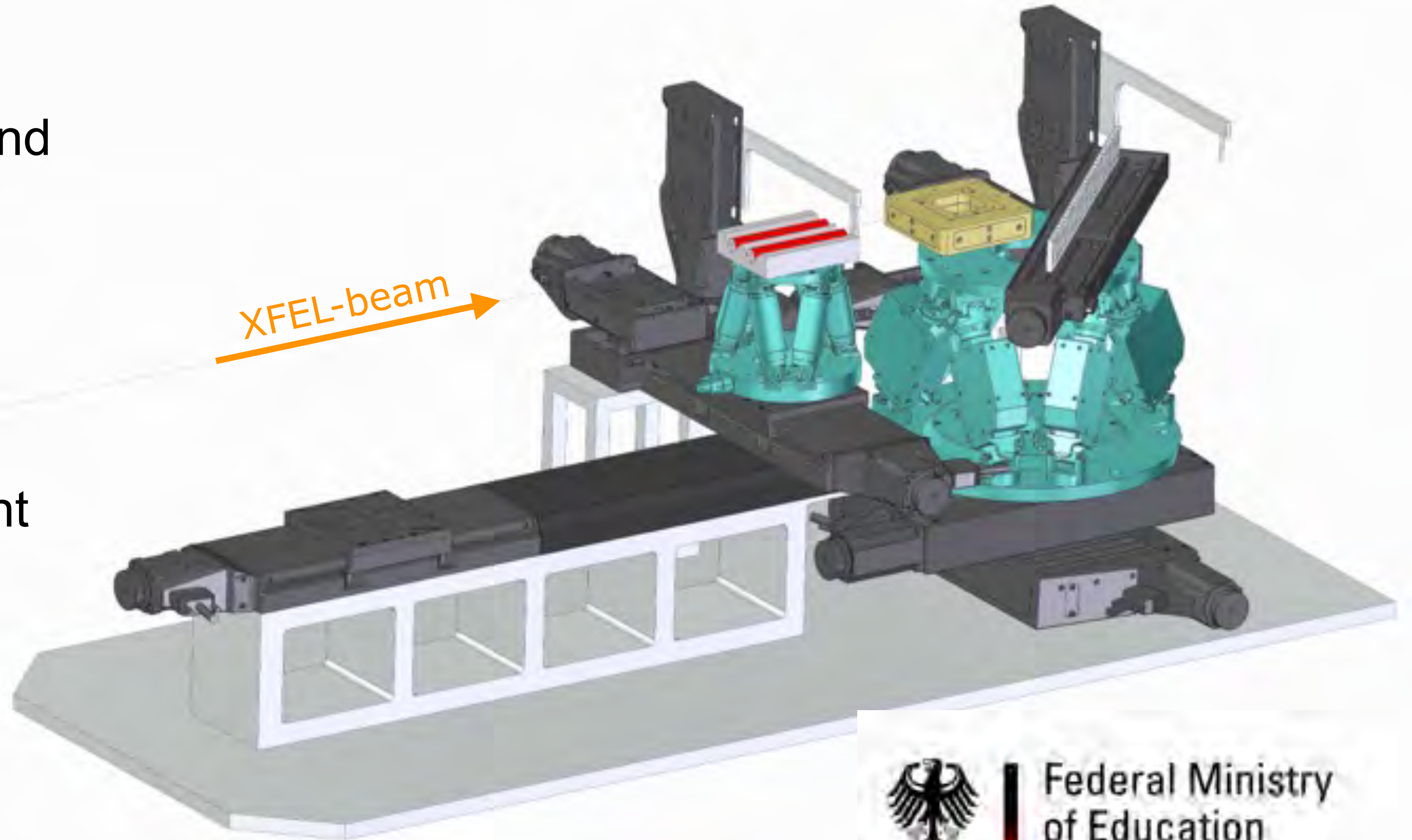
diffraction patterns

object reconstruction



Dedicated Nanofocusing Setup for LCLS/MEC and MID

- combines ptychography and near-field phase-contrast imaging
- high stability
- high positioning accuracy
- hexapods for the alignment of Be-CRLs and sample
- long travel range for the alignment of Be CRLs (FOV)
- cleaning aperture after lens
- beam stop
- compact design in order to enable a fast experimental setup



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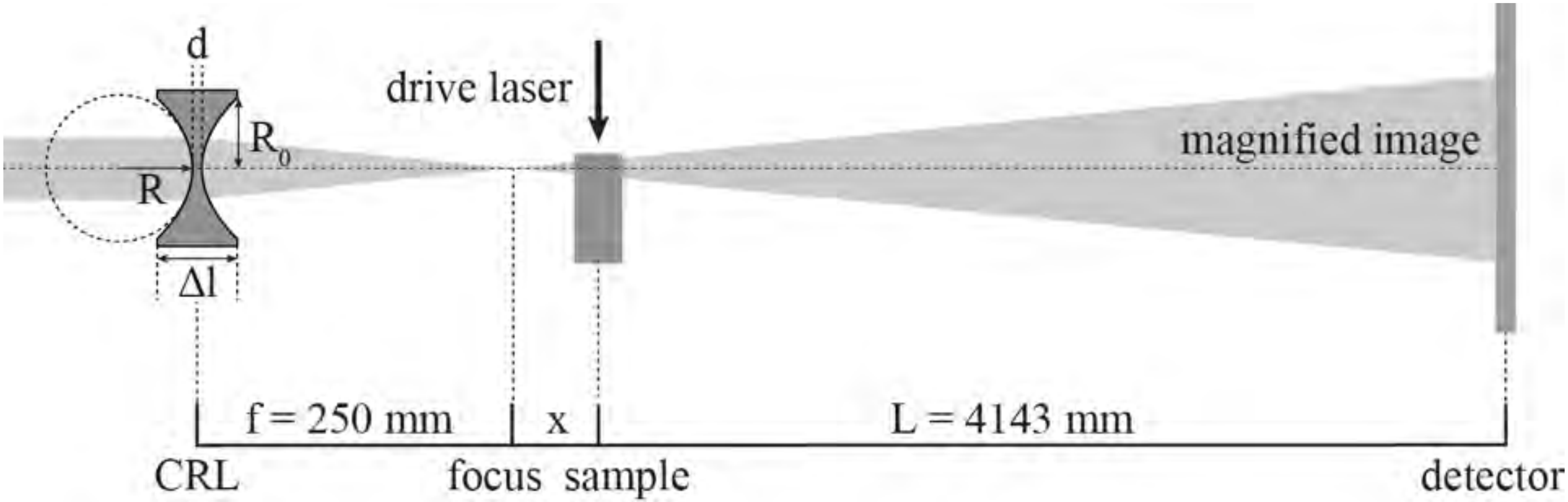
Integration in MID at XFEL:

- redesign lens stage to fit vacuum vessel
- make use of sample stage

Example: High Resolution X-Ray Imaging at LCLS

Method: magnifying phase contrast imaging



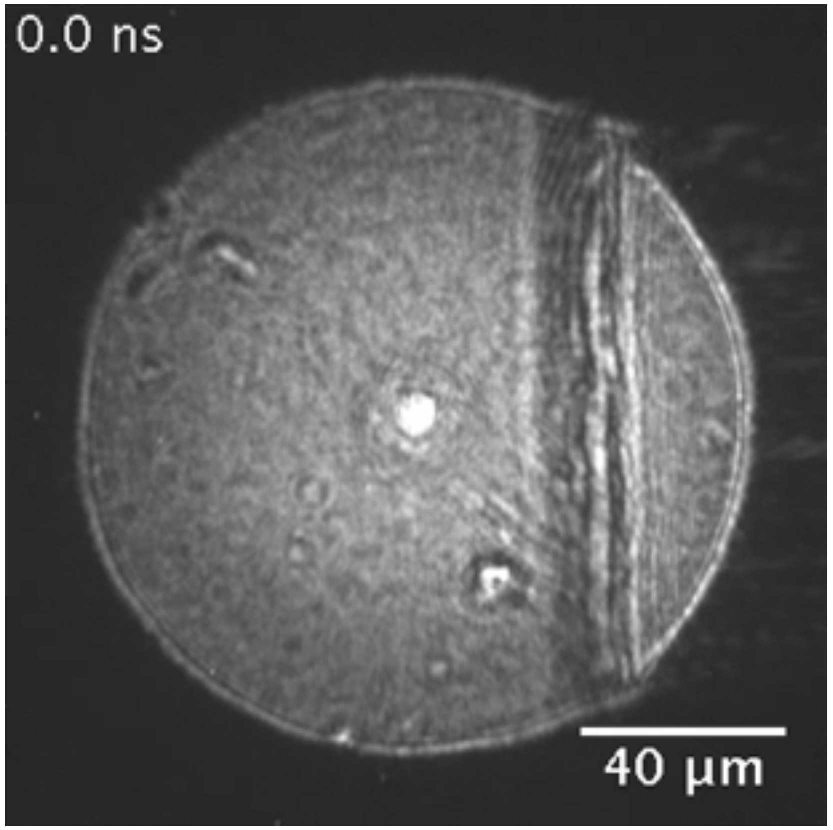
- imaging with secondary point source: efficient use of fluence
- phase contrast: for quantitative results, phase retrieval required

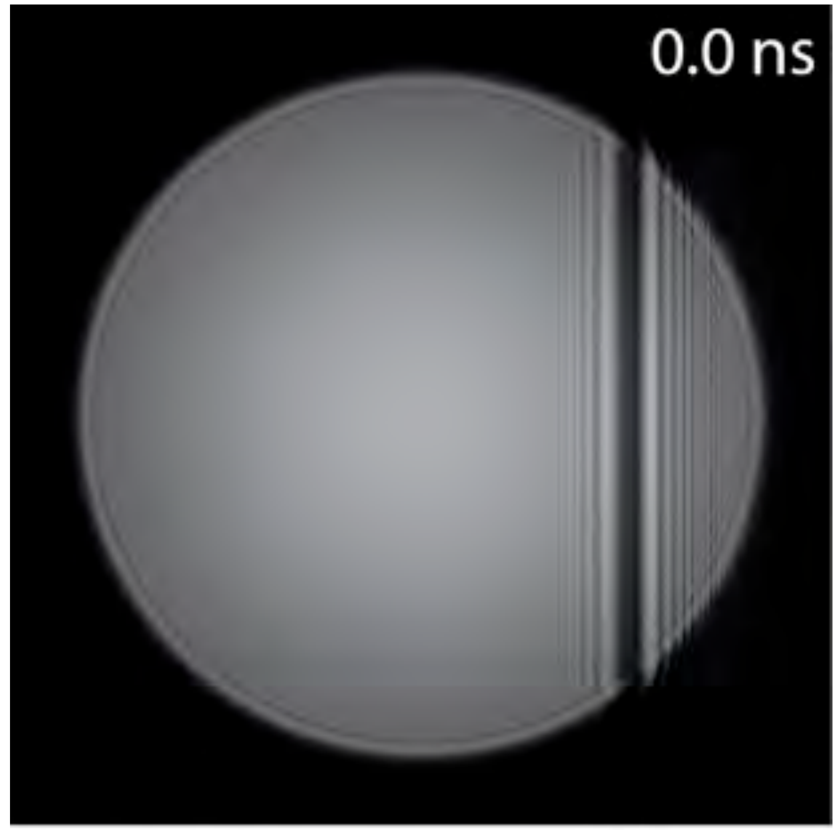
Alternatively:

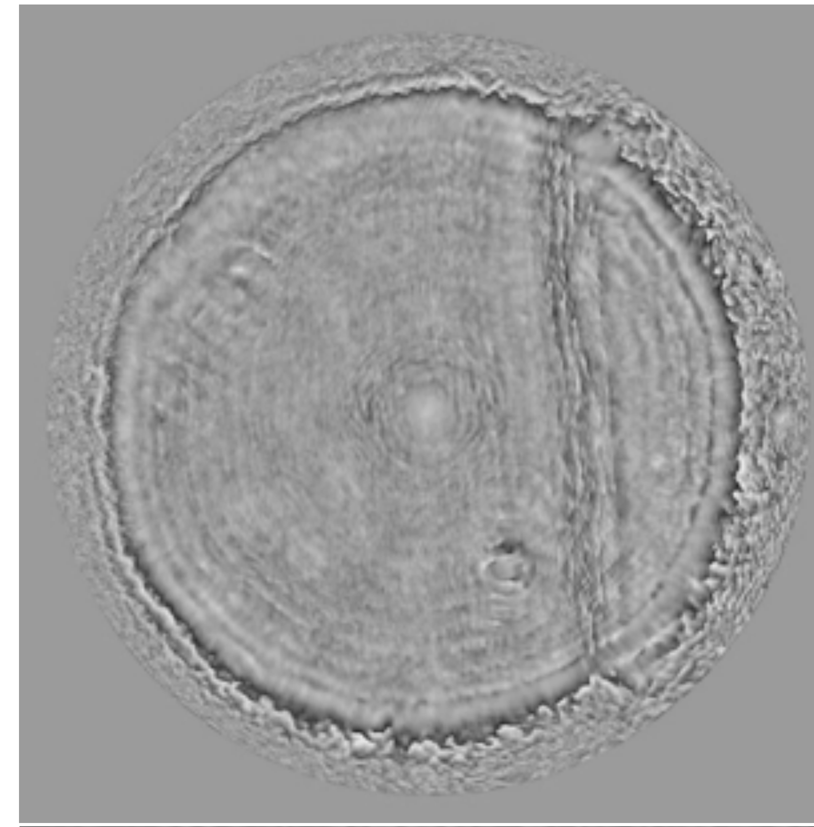
Time-resolved diffraction in focus of nanobeam

Shockwaves in Diamond

Diamond at high pressure and temperature

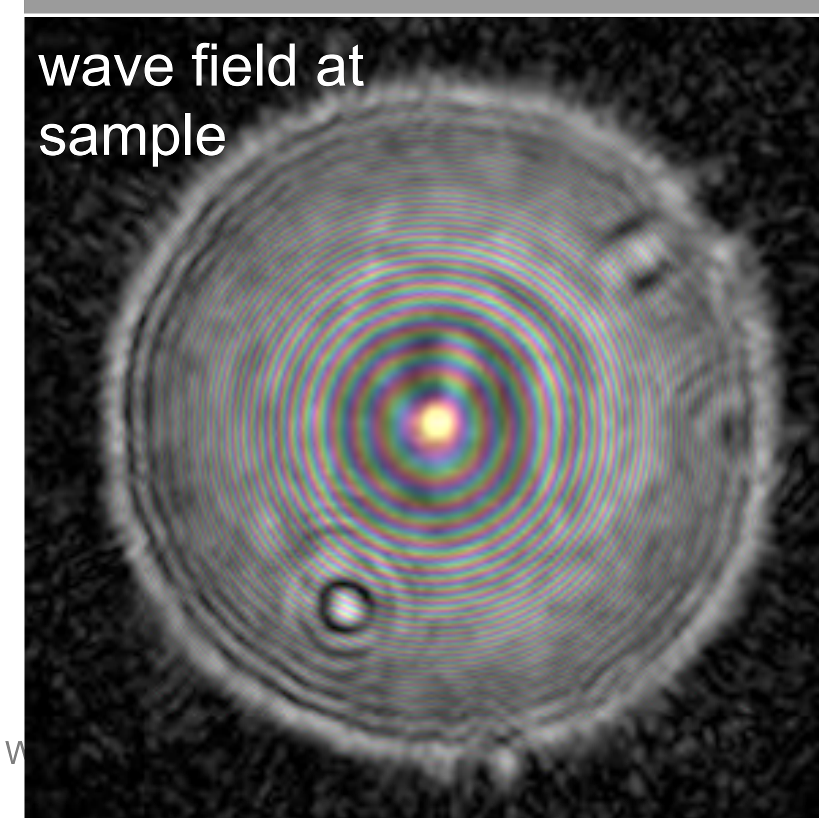






projection images

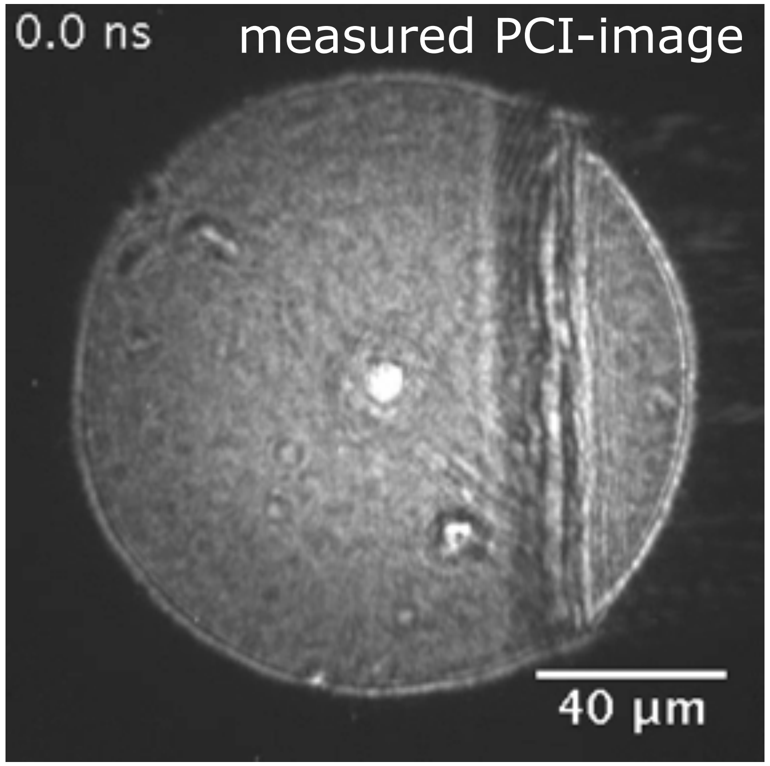
model density

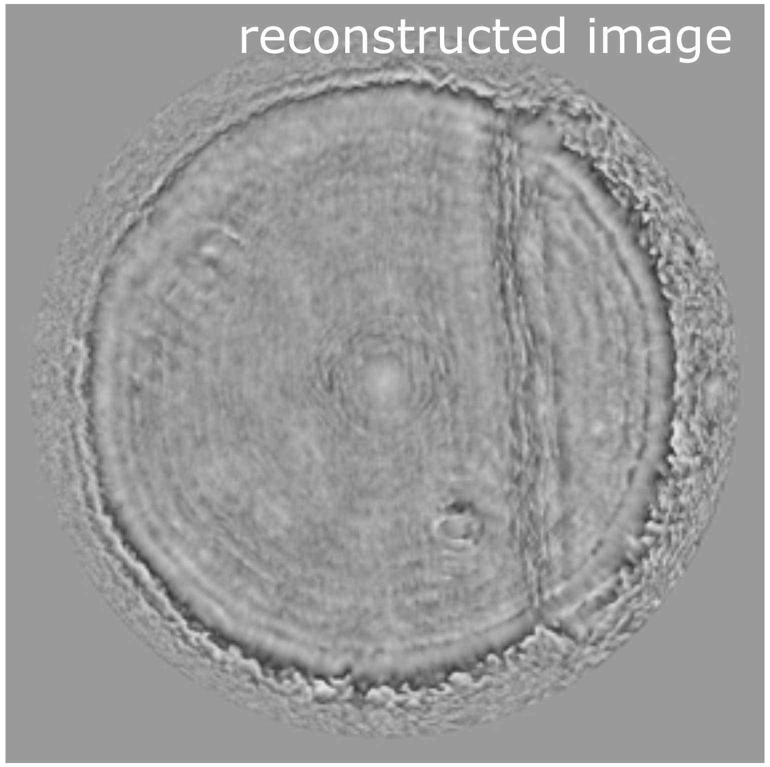


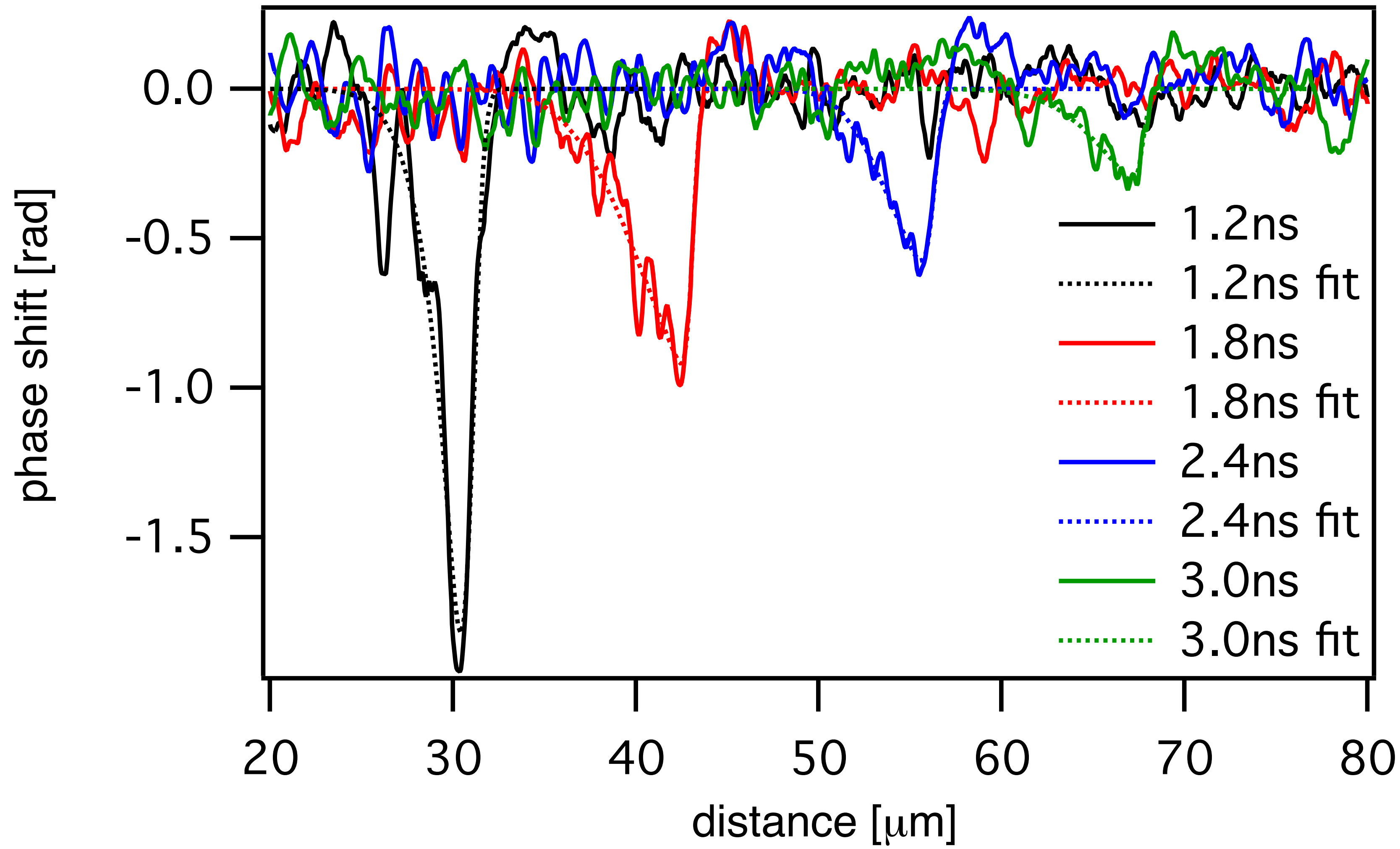
- exposure time 50 fs
- 5 billion images per second (stop-trick movie)

A. Schropp, et al., unpublished.

Elastic Wave in Diamond





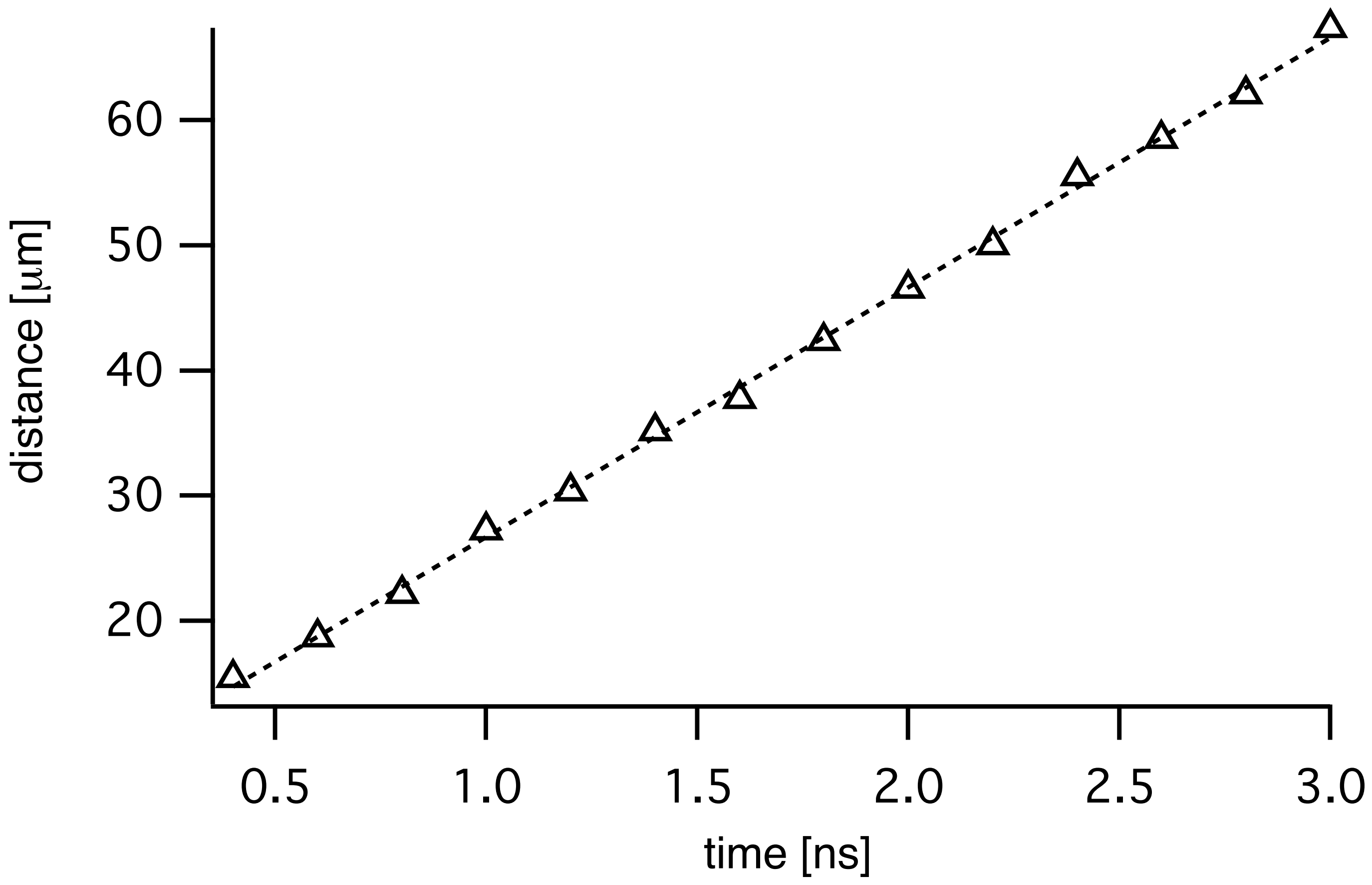


- shock velocity
- density distribution with both high spatial and temporal resolution

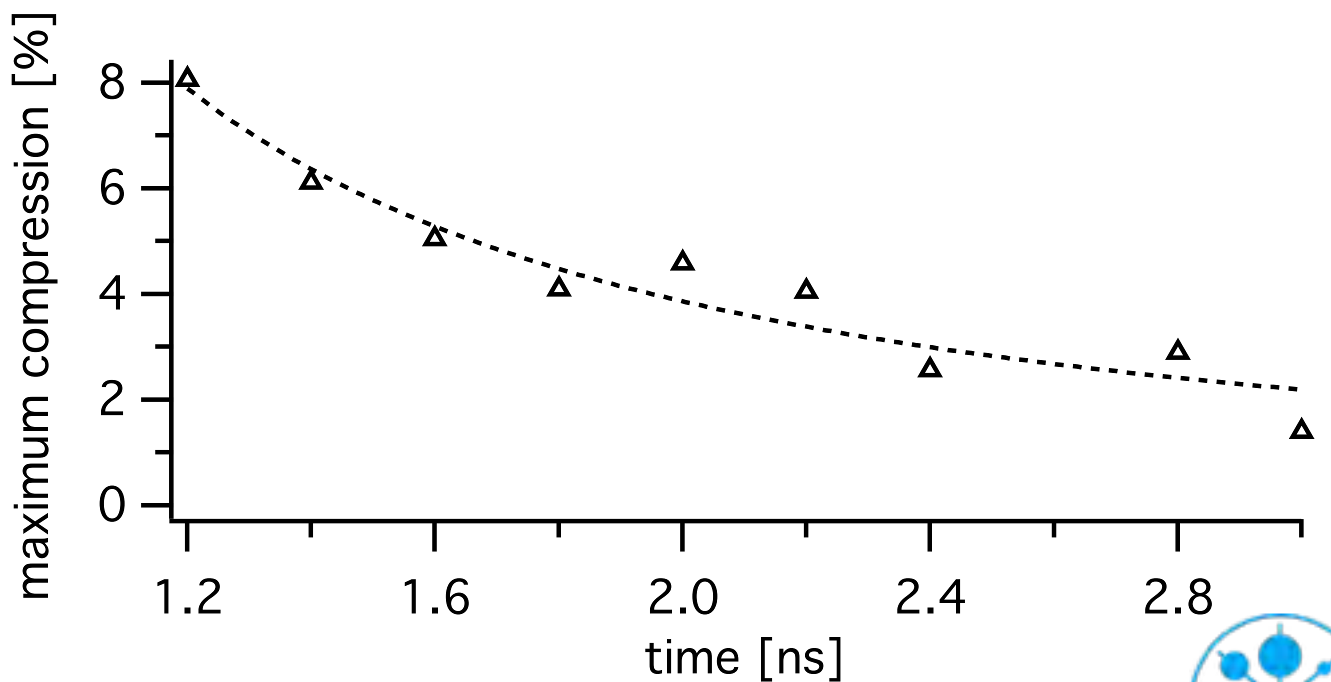
Elastic Wave in Diamond

Quantitative information on

- shock velocity
- compression values
- characteristic time scale of shock decay

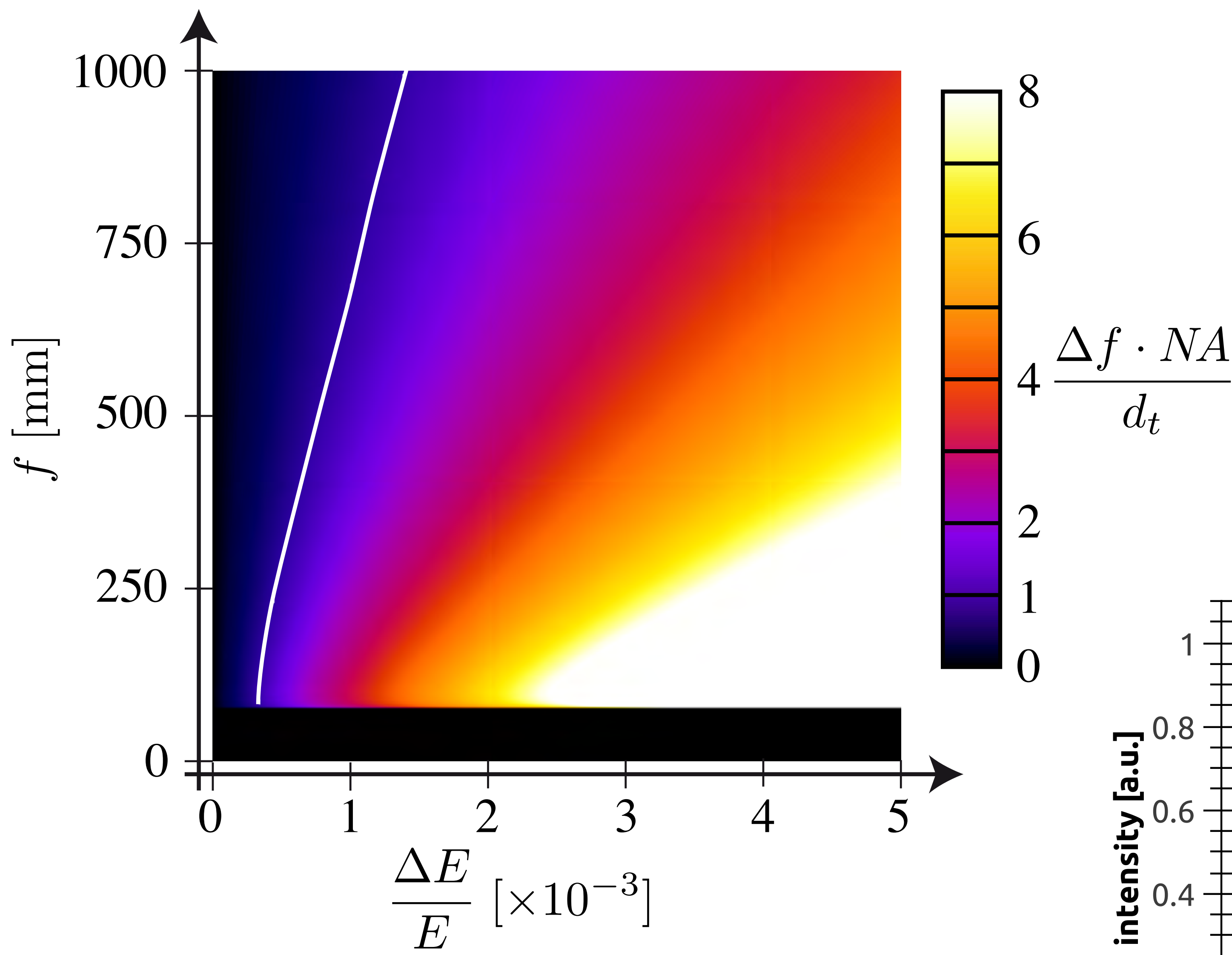


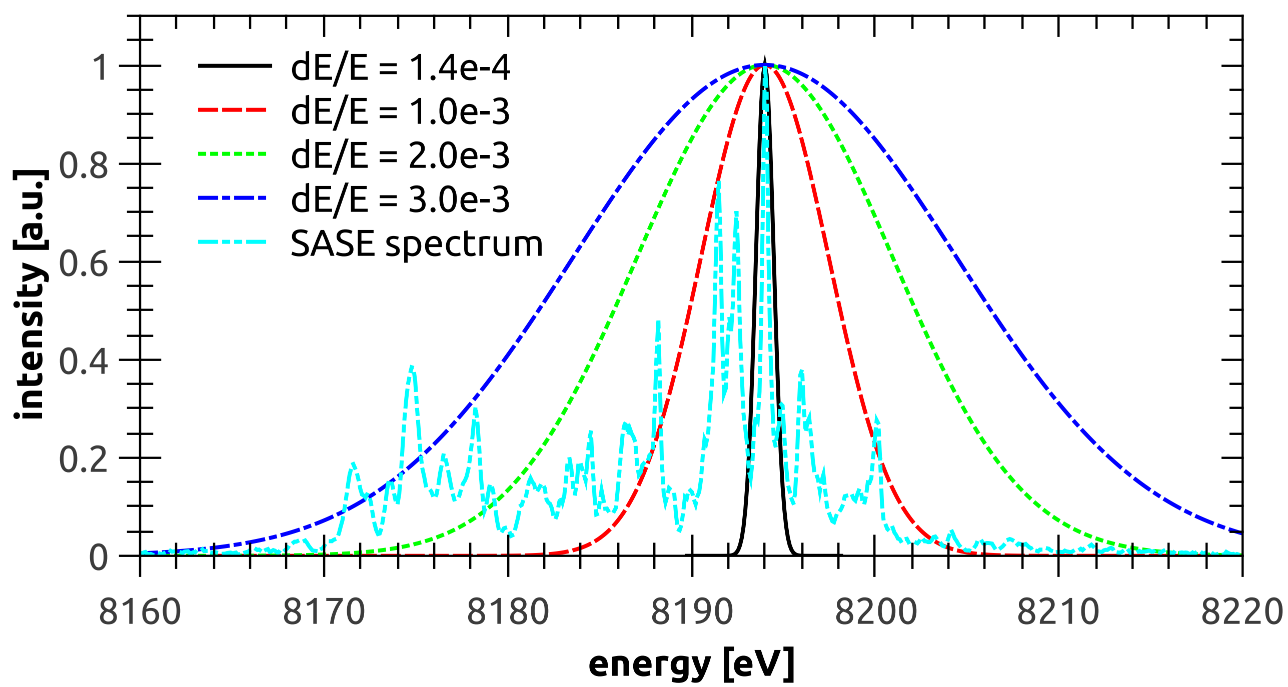
- spatial resolution of about 300nm (SASE)
- PCI: high sensitivity of about 1% lattice compression (not visible in absorption!)



Chromaticity

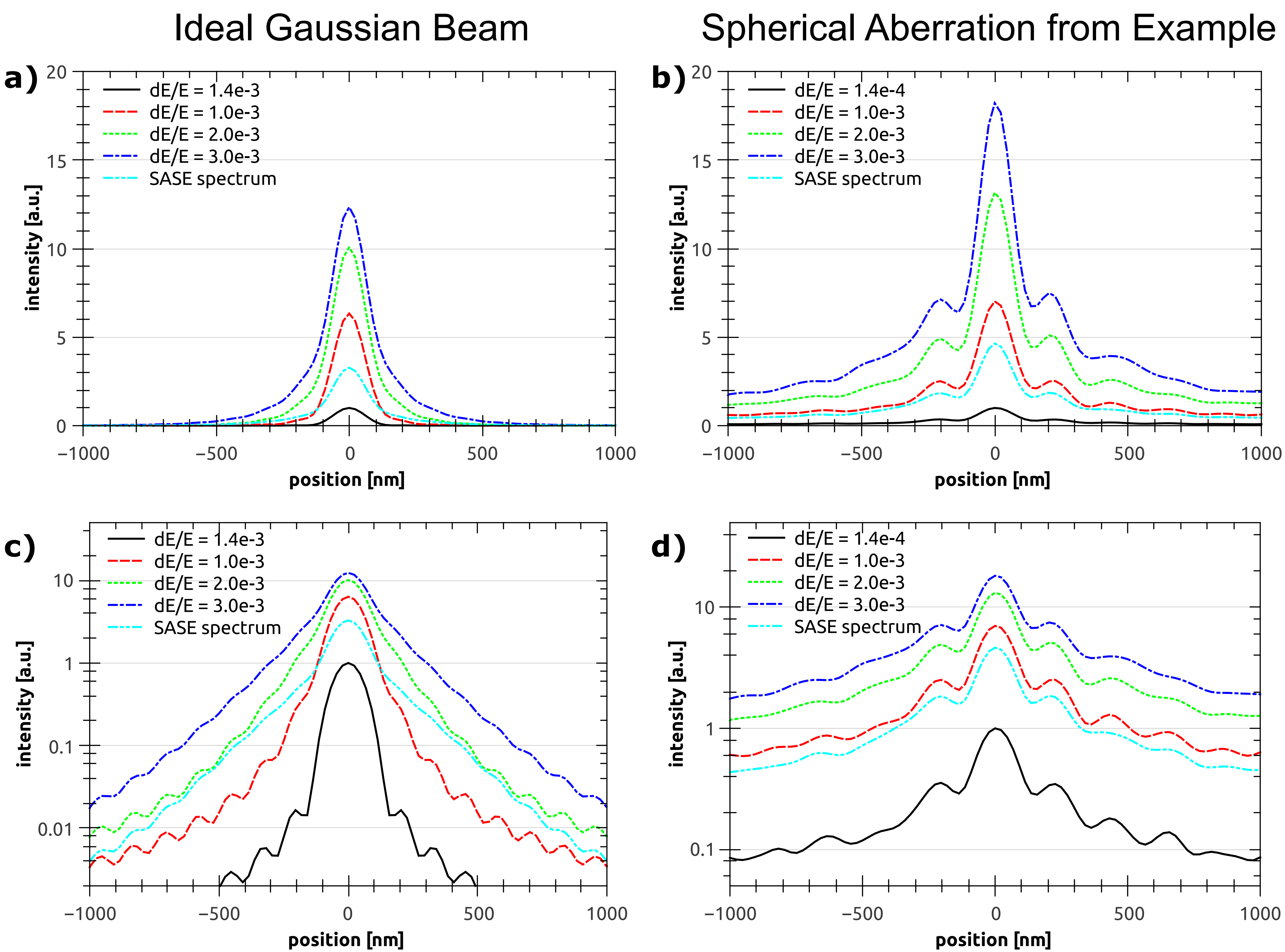
Broadening of beam relative to diffraction limit:





F. Seiboth, et al., J. Phys: Conf. Ser. **499**, 012004 (2014).

Chromaticity and Spherical Aberration



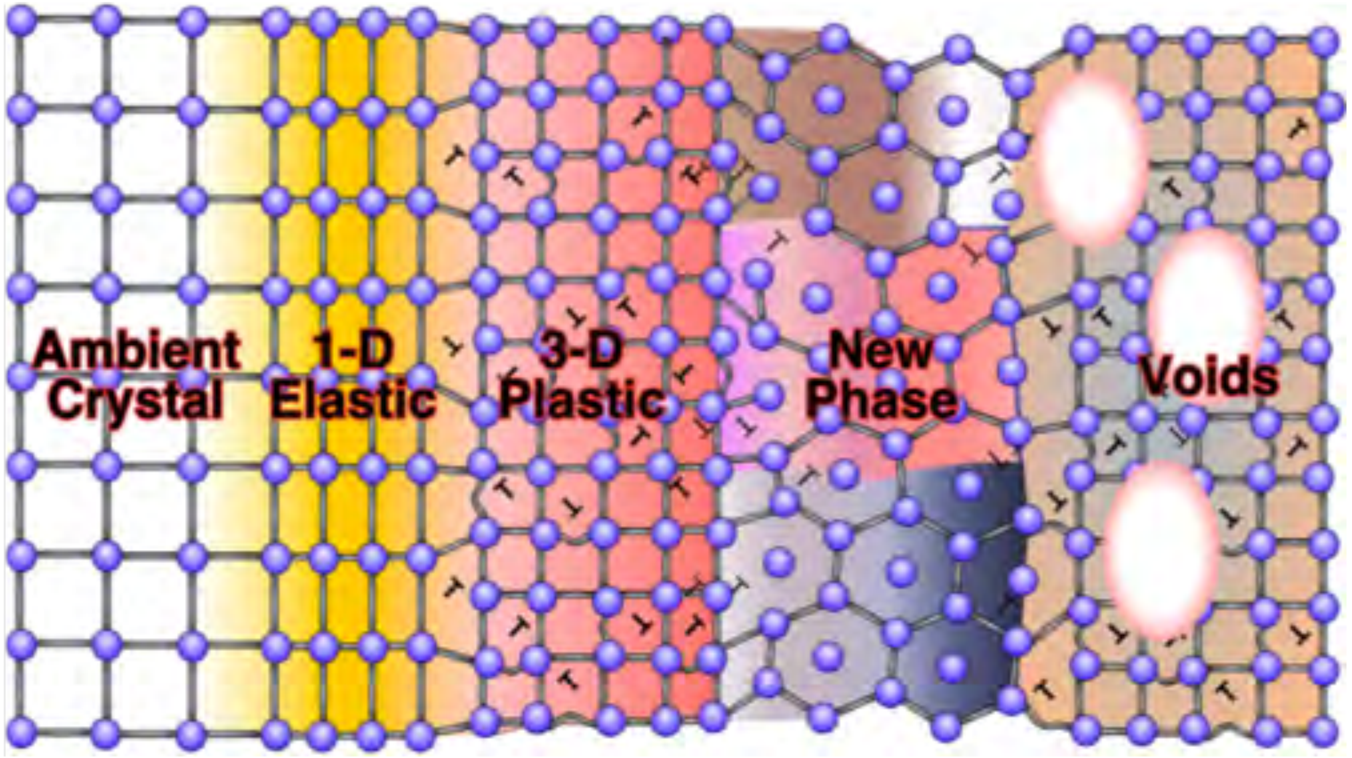
F. Seiboth, et al., J. Phys: Conf. Ser. **499**, 012004 (2014).

Phase Contrast Imaging & Diffraction

Improvements:

- Seeded FEL: improved contrast and resolution in PCI
- Reduced aberrations: intensive Gaussian-limited beam
- focusing XFEL beam to < 100 nm:
  increase field of view in PCI
  increase spatial (thus temporal) resolution in SAXS/WAXS
- complementary diagnostics: diffraction, spectroscopy, VISAR, …

- structural information on the atomic scale to identify phase transformations
- excitation states
- small angle x-ray scattering for intermediate resolution regime covering length scales between 0.1 - 50 nm



Research Opportunities with Nanobeams

Imaging

- CXDI: highest resolution requires maximal fluence (extreme focusing)
- Near-field phase contrast imaging (with magnification):
  Intermediate resolution (e. g., down to 50 nm) with
  larger field of view (smaller beam → larger FOV)

Time-resolved determination of structure and dynamics

- local structure determination

  SAXS, WAXS, spectroscopies

  to avoid averaging over inhomogeneities

Create matter in extreme conditions

- homogeneous heating with x-rays

Non-linear optics

- highest intensities (multi-photon processes)