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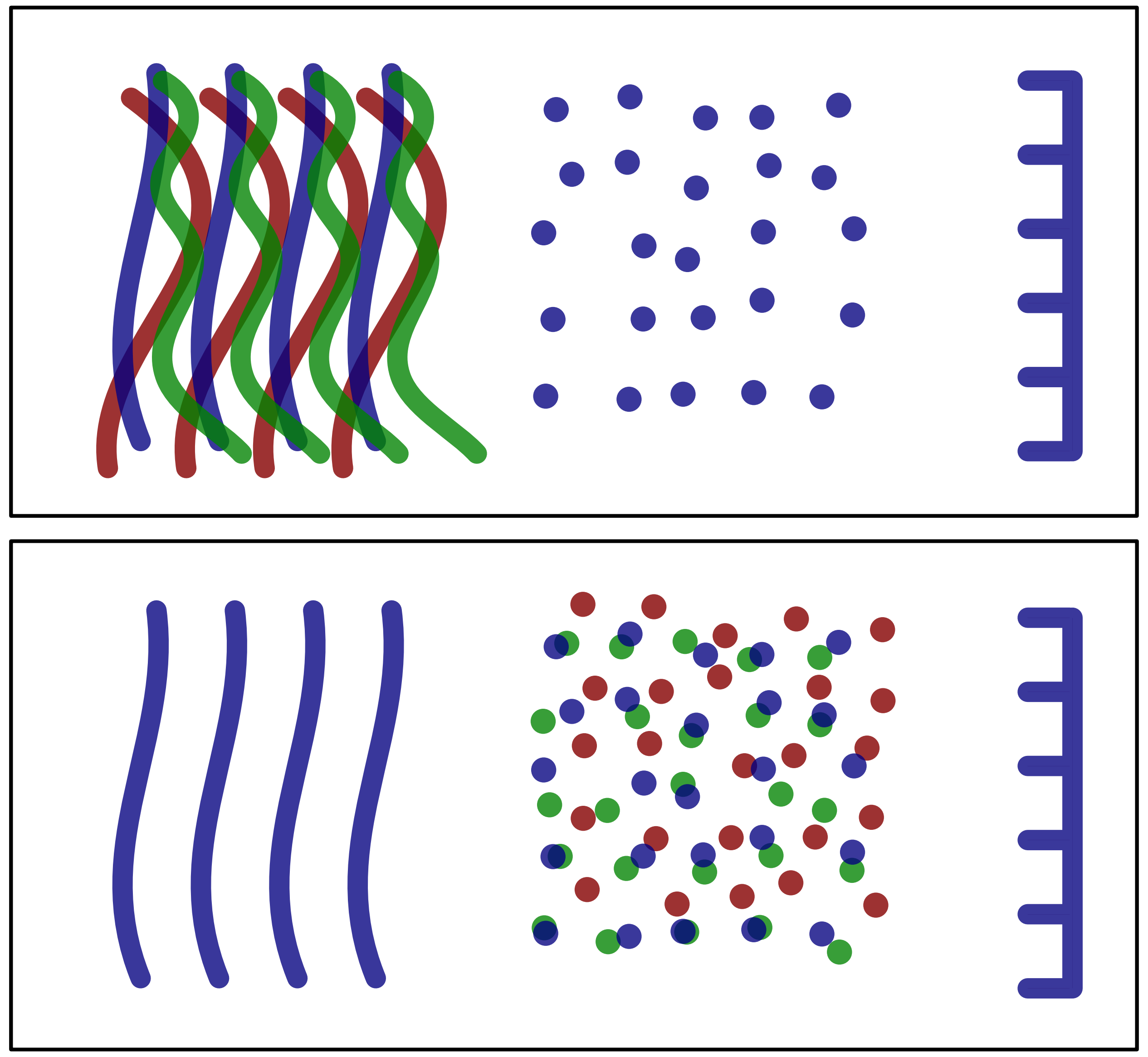
Andreas Menzel on behalf of the **Coherent X-Ray Scattering Group**

cSAXS @ SLS-2

SLS-2 Beamline Proposal Workshop, PSI, October 23/24, 2018

What we do...

cSAXS is the premier X-ray facility at SLS
to make direct use of coherence properties at ~ 5–20 keV.



We used to look at ordered samples having messy beams.
Now we have clean beams to look at messy samples.

(attributed to H. Dosch)

What we do…

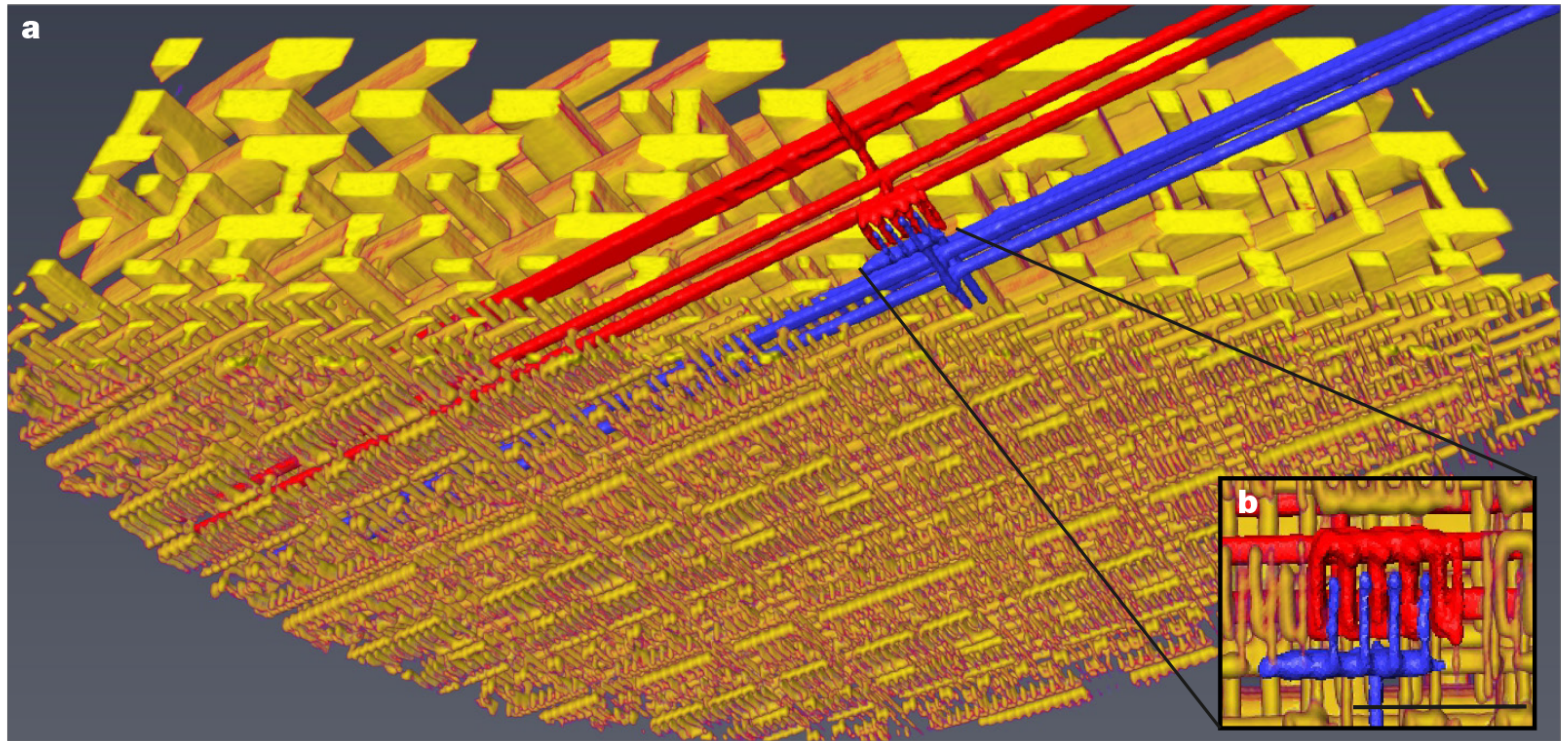
High-Resolution Imaging
Ptychography

LETTER

doi:10.1038/nature21698

High-resolution non-destructive three-dimensional imaging of integrated circuits

Mirko Holler[1], Manuel Guizar-Sicairos[1], Esther H. R. Tsai[1], Roberto Dinapoli[1], Elisabeth Müller[1], Oliver Bunk[1], Jörg Raabe[1] & Gabriel Aeppli[1,2,3]



Holler *et al.* (2017) *Nature* **543**, 402

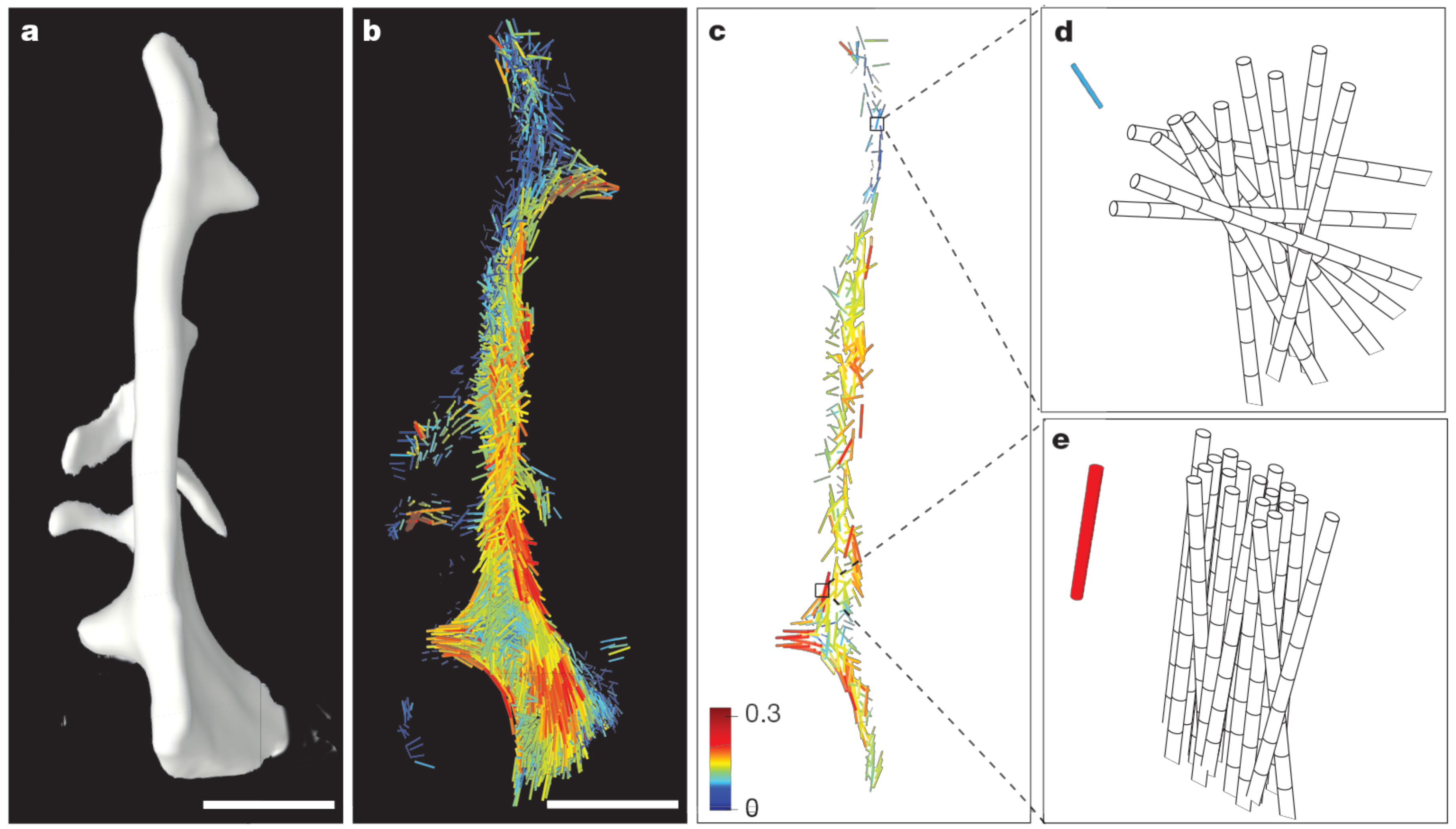
SAXS Imaging, Tomography,
and other High-Brilliance Applications

LETTER

doi:10.1038/nature16056

Nanostructure surveys of macroscopic specimens by small-angle scattering tensor tomography

Marianne Liebi[1], Marios Georgiadis[2], Andreas Menzel[1], Philipp Schneider[3], Joachim Kohlbrecher[1], Oliver Bunk[1] & Manuel Guizar-Sicairos[1]

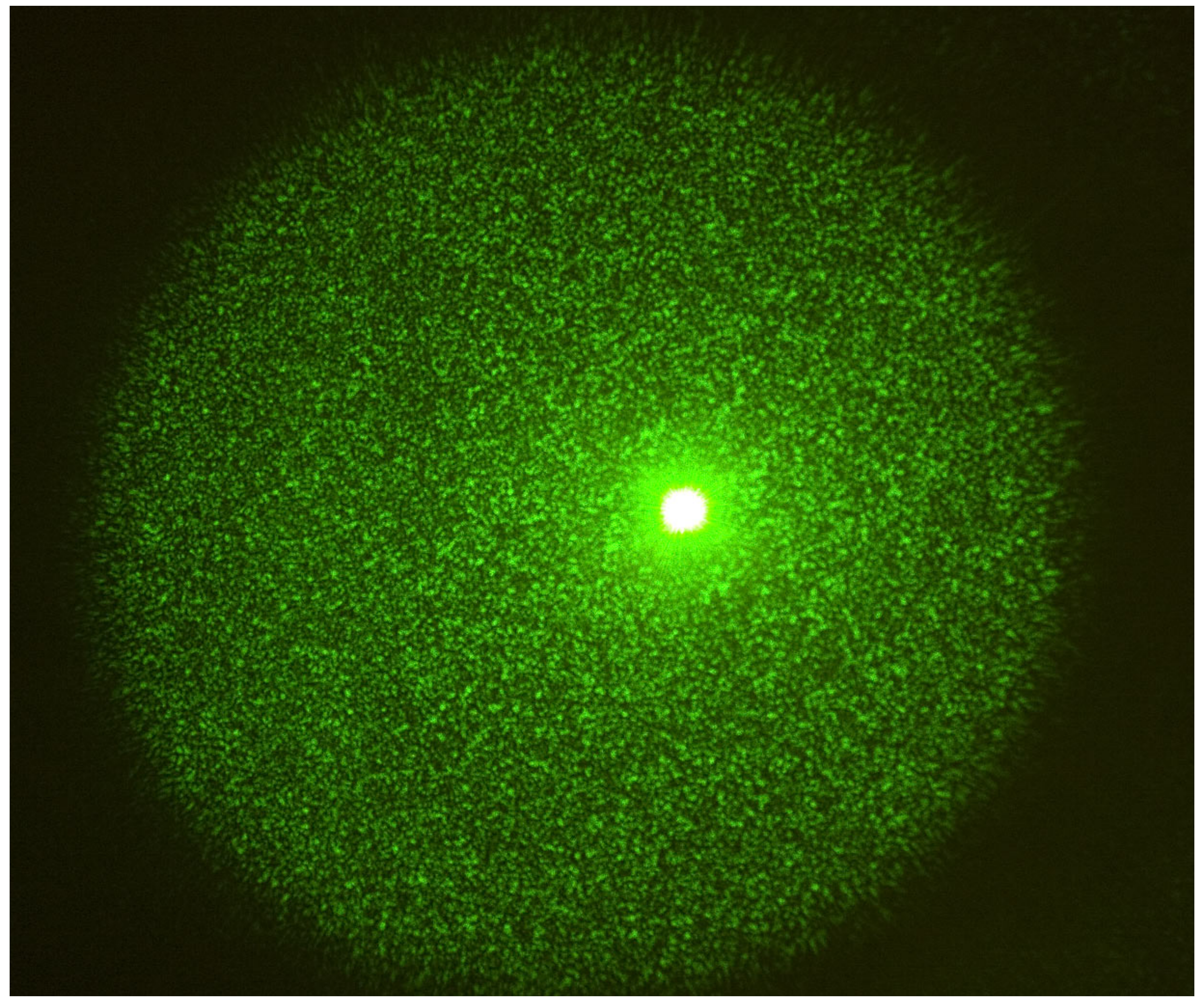


Liebi *et al.* (2015) *Nature* **527**, 349

Coherence

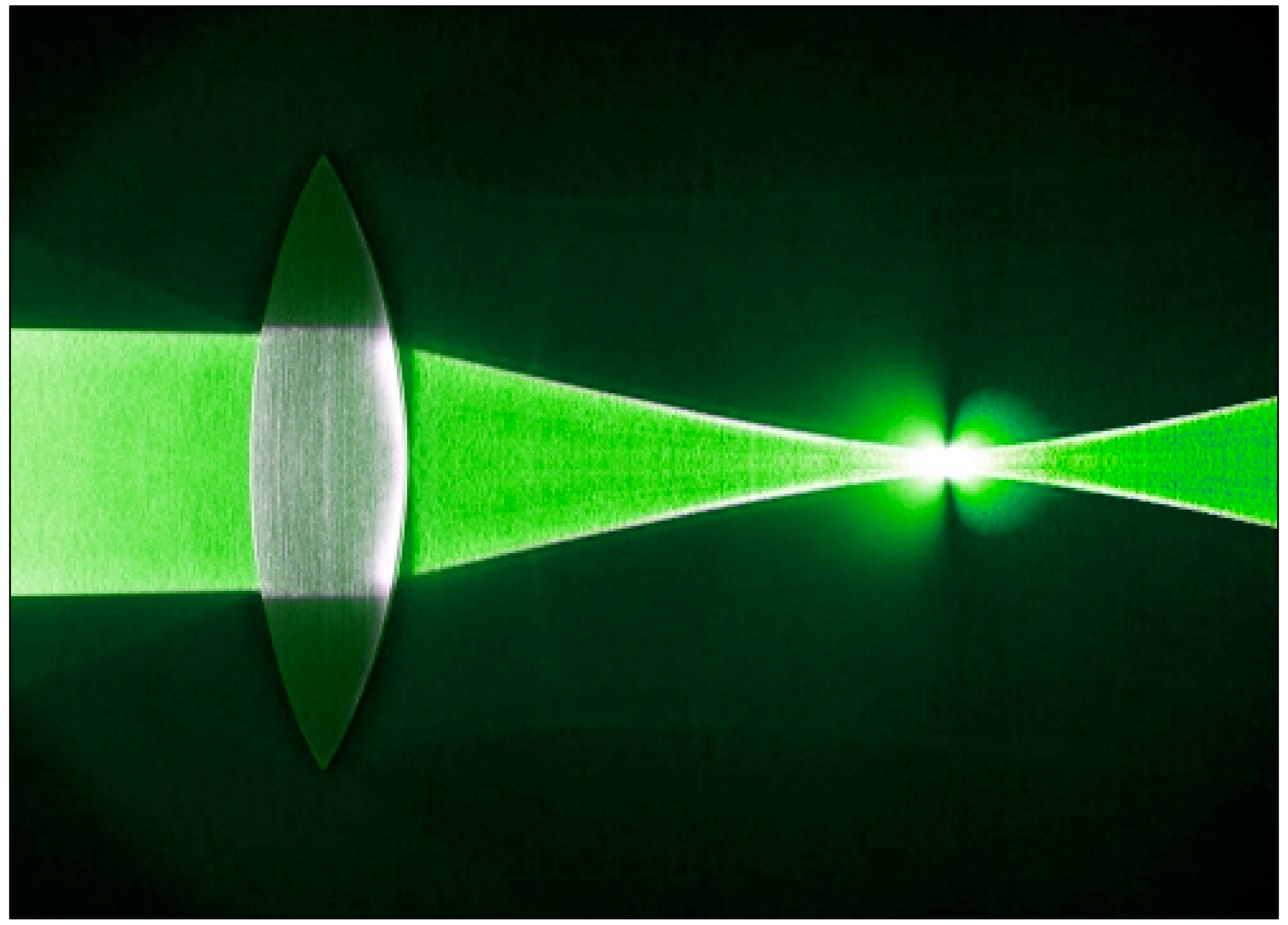
High-Resolution Imaging
Ptychography

- High demands on sample environment/control
- Uses essentially *only* coherent flux
- Computationally very demanding



SAXS Imaging, Tomography, and other High-Brilliance Applications

- High demands on beam conditioning/control
- Uses essentially all flux
- Routinely produces large data volumes



What we can gain from SLS-2

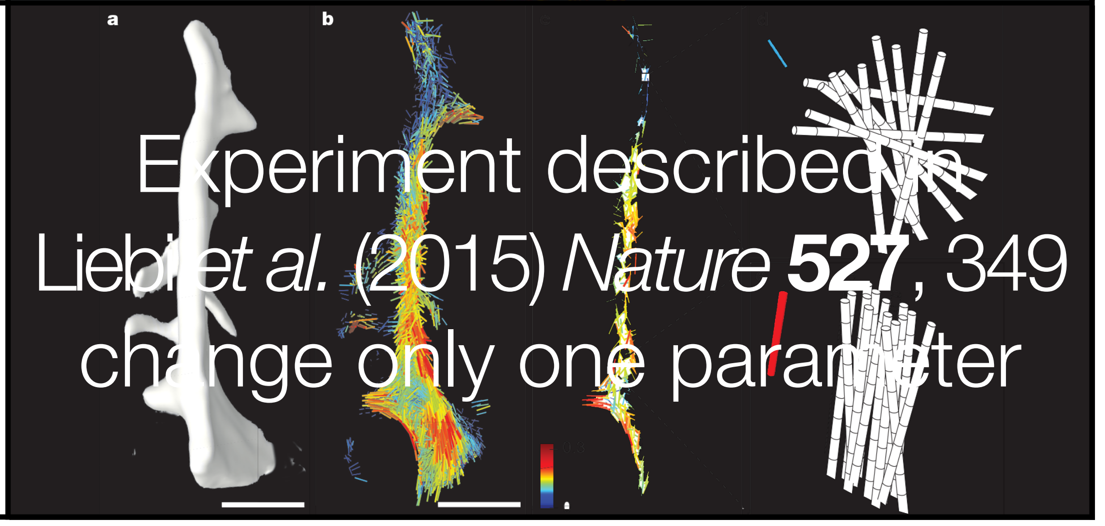
Expt/Source	Figure of merit	Factor improvement SLS-2/SLS	Comment
Ptychographic tomography, 6.2 keV	Resolution [nm] Probed volume [μm^3] Time	10: 14 → 1.4 ($I \propto Q^{-4}$) 10^4: 1800 → 18 × 106 10^4: 22 h → 8 s	 Experiment described in Holler *et al.* (2017) *Nature* **543**, 402 change only one parameter
Scanning SAXS tomography, 12.4 keV	Size sensitivity [nm] probed volume [μm^3] Time	$10^{3/4}$: 56 → 10 10^3: 2.5 → 2500 10^3: 22 h → 80 s	 Experiment described in Liebi *et al.* (2015) *Nature* **527**, 349 change only one parameter

Table II from the *Science Case*

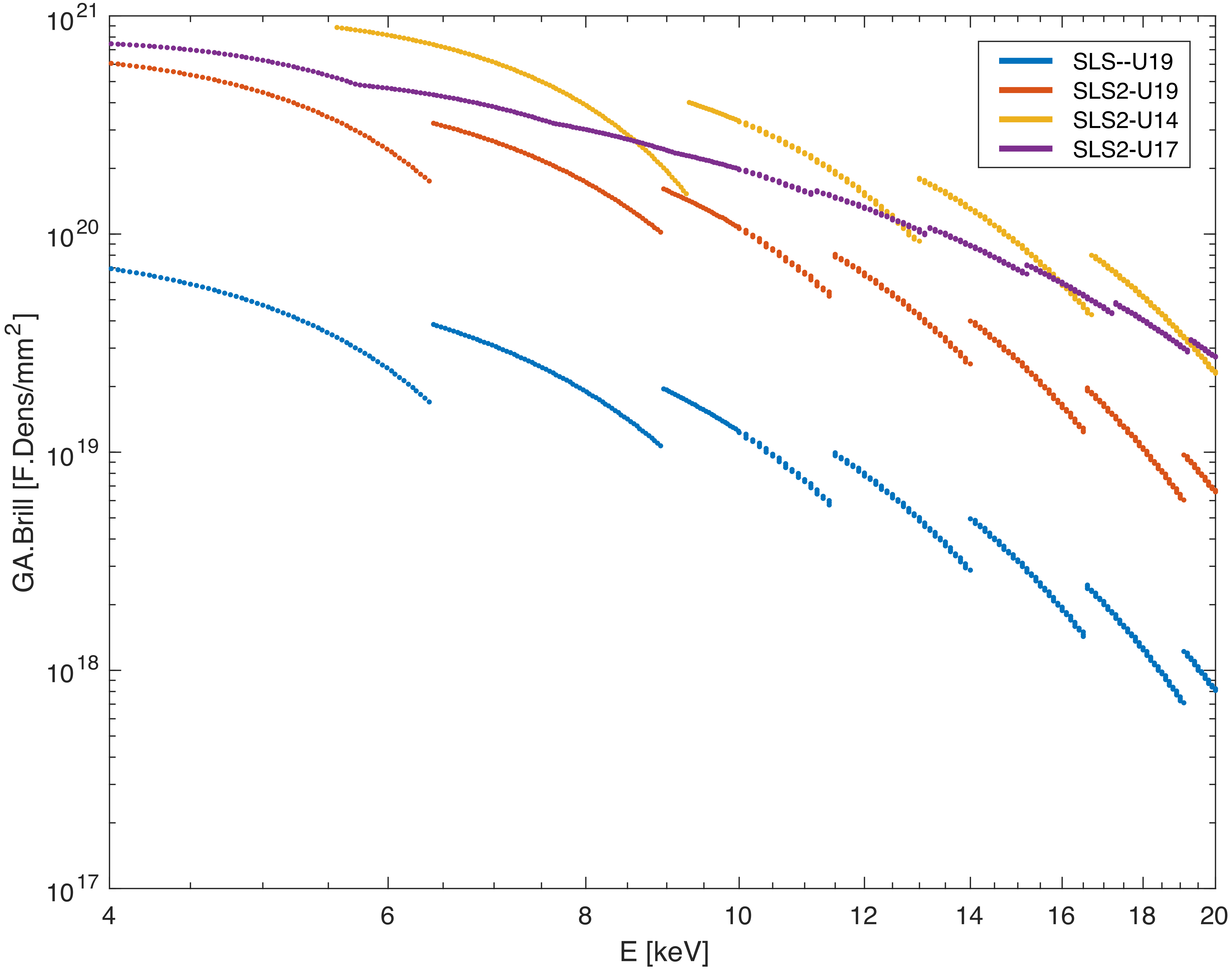
…from the "QUO Vadis?" 2015…

Redesign of various beamline components,
while retaining the current science case, incl. emphasis on flexibility.

Plan: Keeping the flexibility that helped making cSAXS a success.

New source	→ gain in coherent flux:	$10^{1.5}$
New undulator	→ gain in (coherent) flux:	$10^{0.5}$
Broadband option	→ gain in (sufficiently) coherent flux:	10^{1}
Optimized optics	→ gain in (coherent) flux:	10^{1}
total gain in coherent flux		in the order of 10^{4}!
total gain in flux		close to 10^{3}

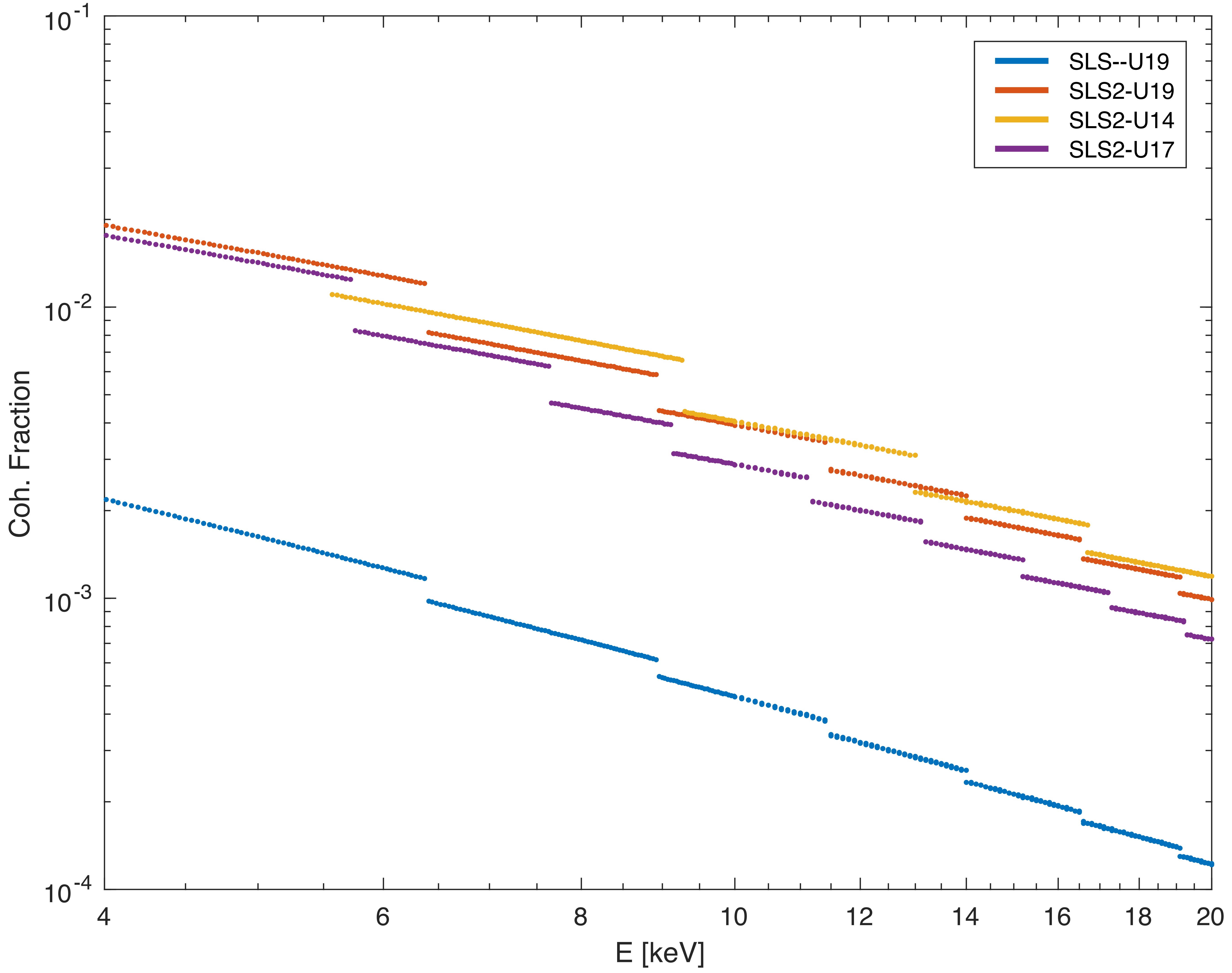
Brightness
courtesy T. Schmidt



Photons in coherence volume scales with Brightness · λ^3

Coherent Fraction

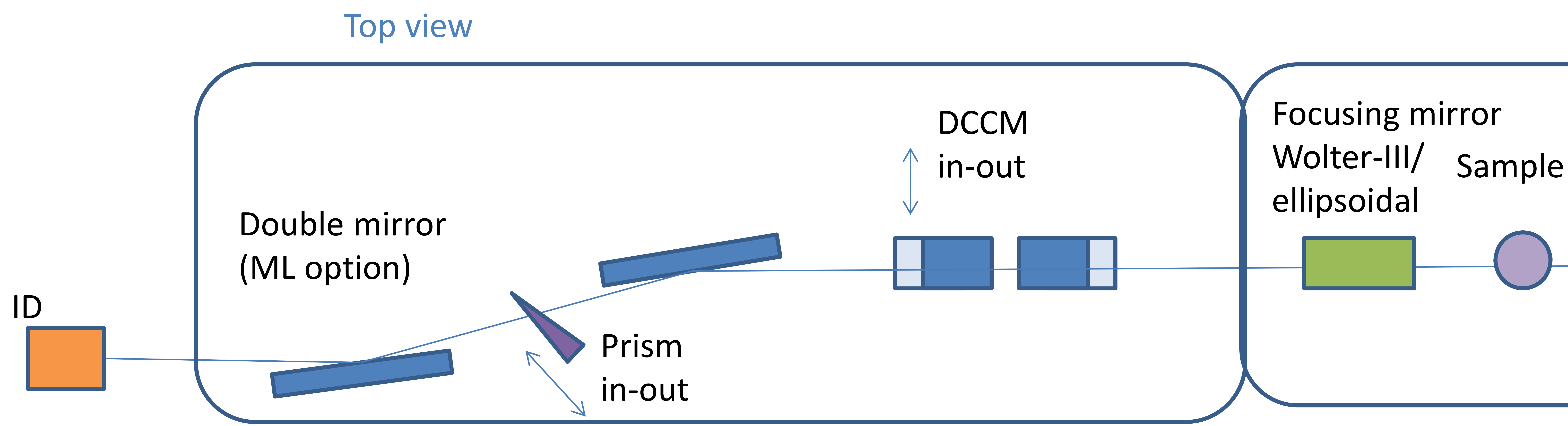
courtesy T. Schmidt



Photons in coherence volume scales with Brightness · λ^3

"Prototypical Design" for Spring-8 Upgrade

Curtosy Makina Yabashi



Difference compared to ideas for "cSAXS-2":
The means of high-order suppression.

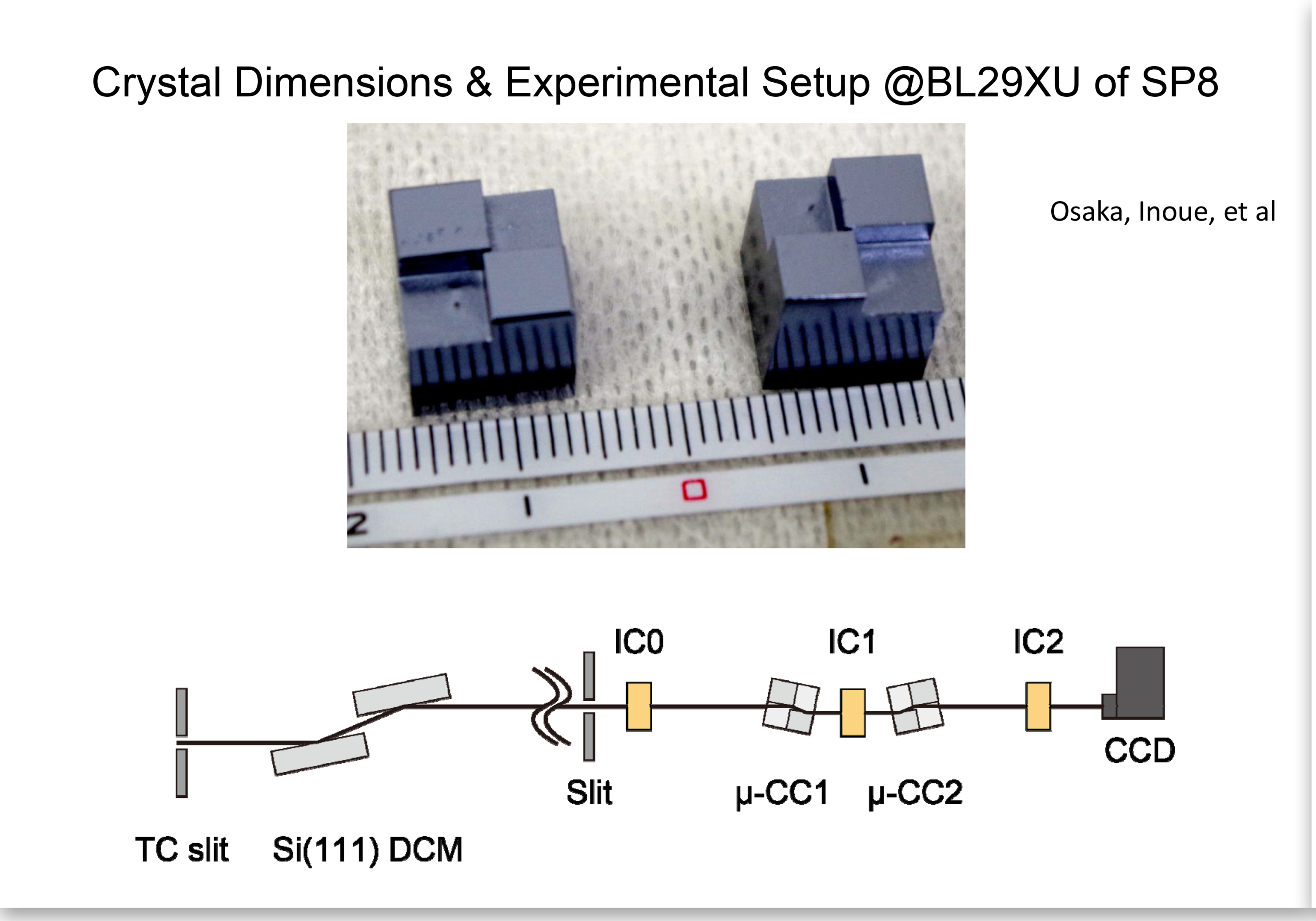
Switching between pink and mono beam
while keeping fixed-exit geometry

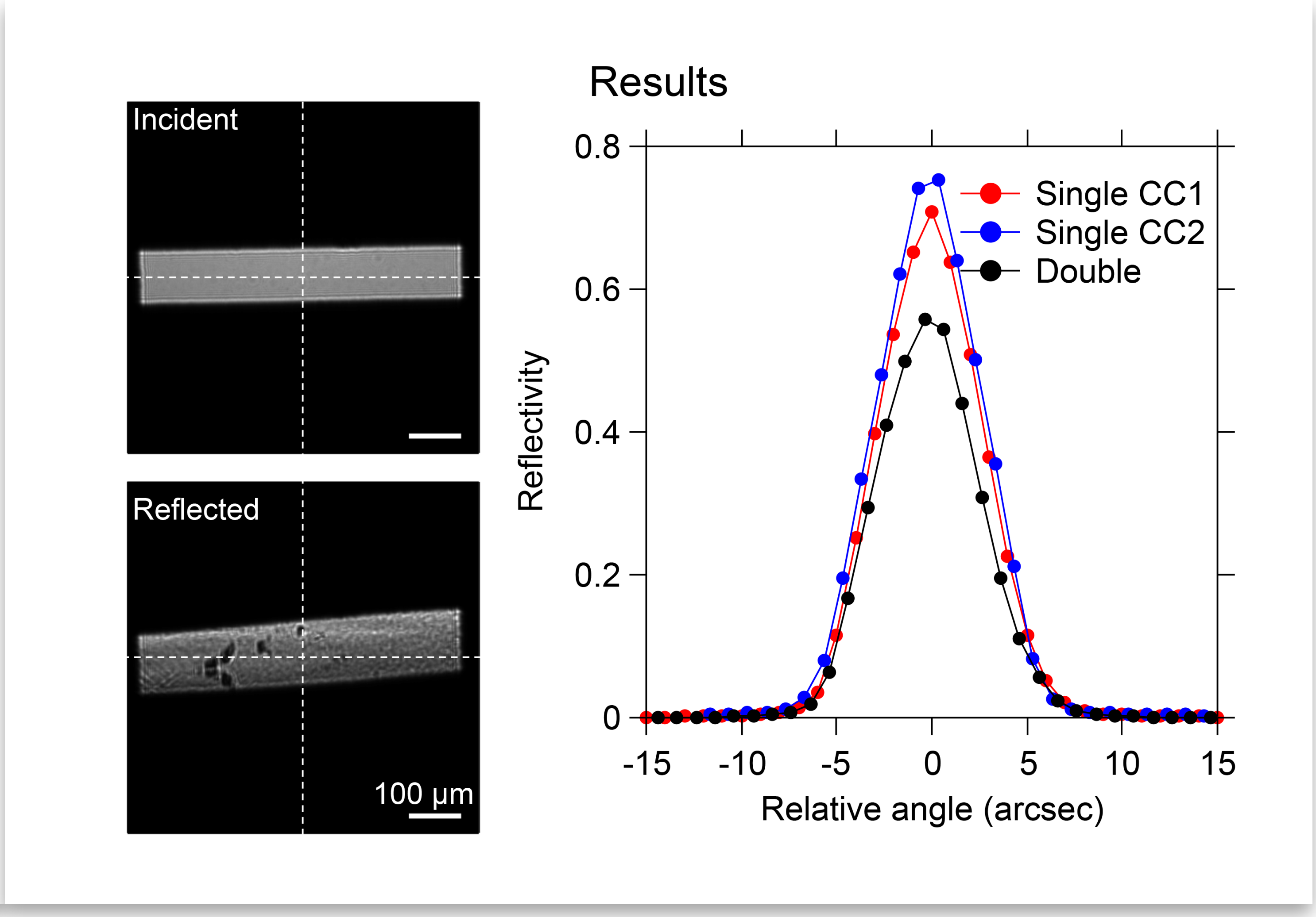
Channel-Cut Quality

REVIEW OF SCIENTIFIC INSTRUMENTS **87**, 063118 (2016)

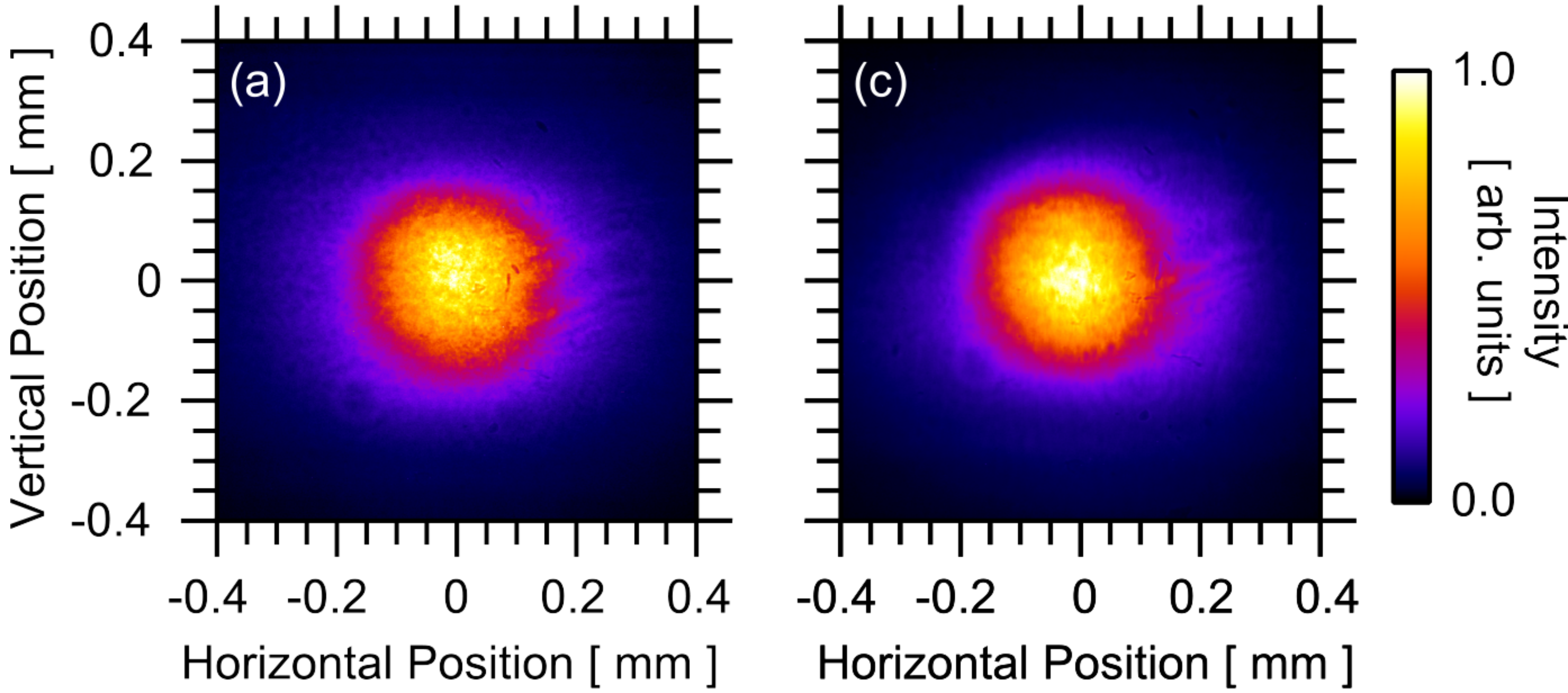
Development of speckle-free channel-cut crystal optics using plasma chemical vaporization machining for coherent x-ray applications

Takashi Hirano,[1,a)] Taito Osaka,[1] Yasuhisa Sano,[1] Yuichi Inubushi,[2] Satoshi Matsuyama,[1] Kensuke Tono,[2,3] Tetsuya Ishikawa,[3] Makina Yabashi,[3] and Kazuto Yamauchi[1]





Slides courtesy of Makina Yabashi



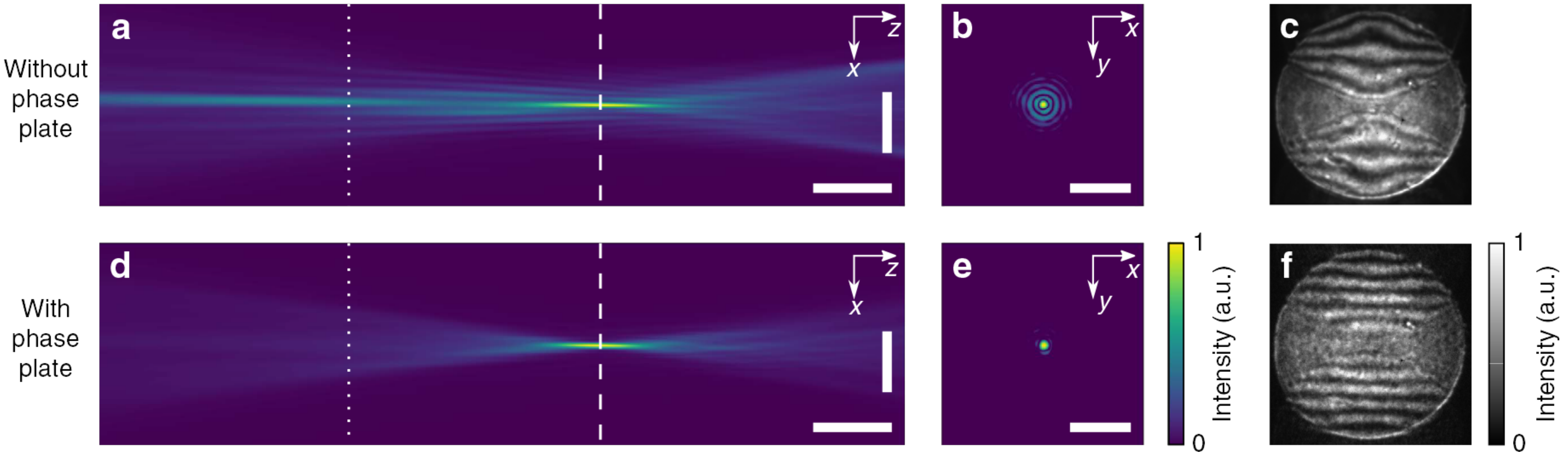
beam before and after passing a channel-cut crystal

Corrective Optics after Multilayers, CRLs, ...

(requiring phase sensing capabilities)

Perfect X-ray focusing via fitting corrective glasses to aberrated optics

Frank Seiboth[1,†], Andreas Schropp[2], Maria Scholz[2], Felix Wittwer[1,2], Christian Rödel[3,4], Martin Wünsche[3], Tobias Ullsperger[5], Stefan Nolte[5], Jussi Rahomäki[6], Karolis Parfeniukas[6], Stylianos Giakoumidis[6], Ulrich Vogt[6], Ulrich Wagner[7], Christoph Rau[7], Ulrike Boesenberg[2], Jan Garrevoet[2], Gerald Falkenberg[2], Eric C. Galtier[4], Hae Ja Lee[4], Bob Nagler[4] & Christian G. Schroer[2,8]



Seiboth *et al.* (2017) *Nat. Comm.* **8** 14623

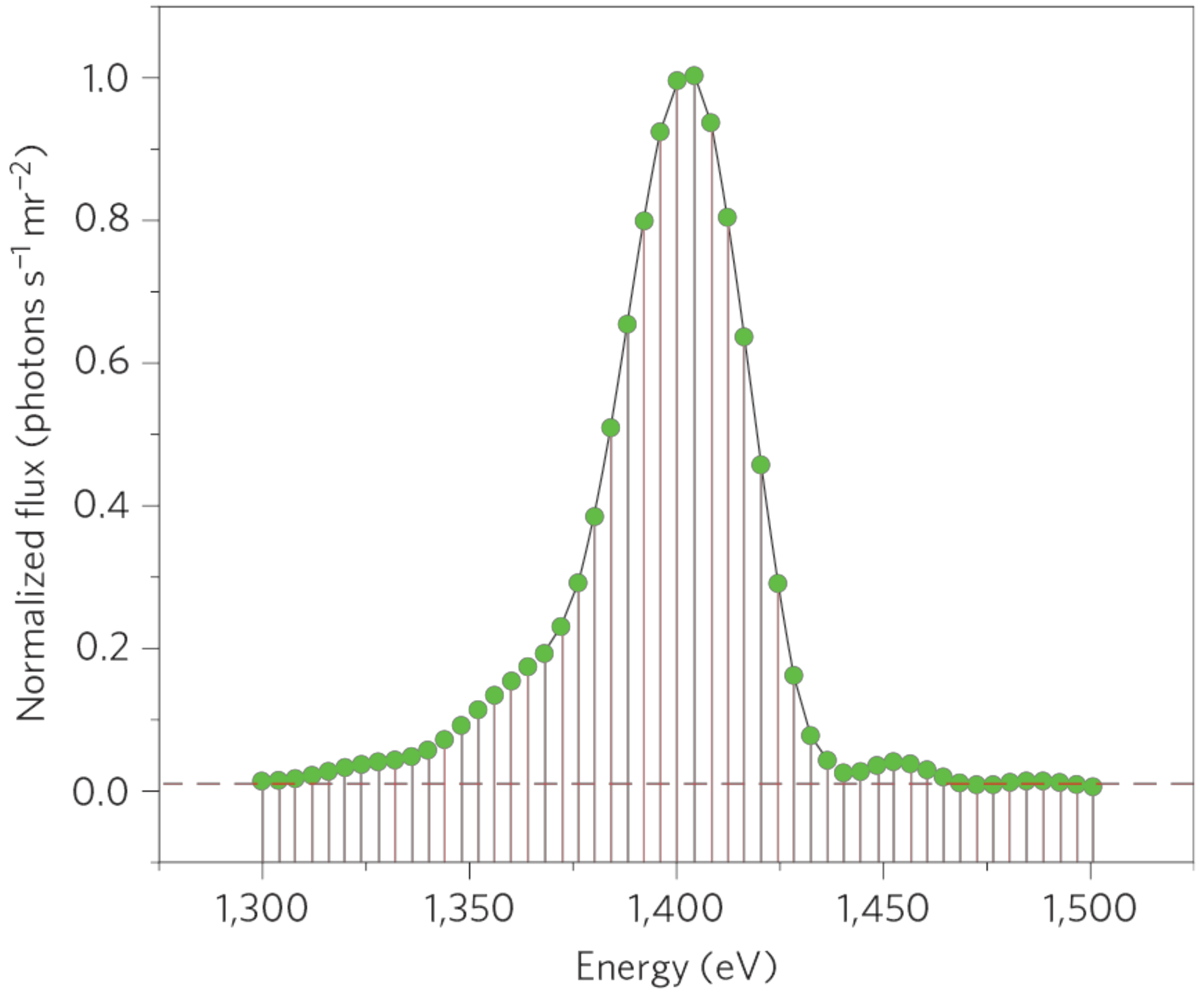
Broadband Illumination

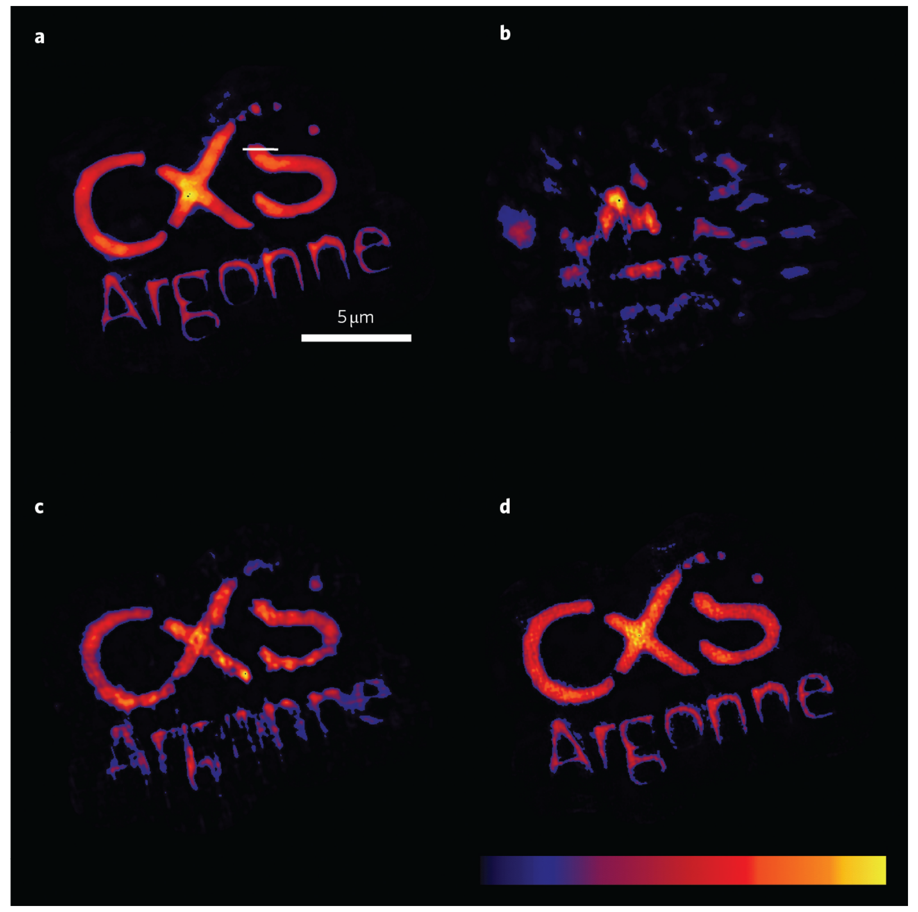
Usage of broadband illumination for coherent diffractive imaging, incl. ptychography, has been demonstrated with particular success for non dispersive samples.

LETTERS
PUBLISHED ONLINE: 26 JUNE 2011 | DOI: 10.1038/NPHOTON.2011.125
nature photonics

Lensless imaging using broadband X-ray sources

Brian Abbey[1], Lachlan W. Whitehead[1], Harry M. Quiney[1], David J. Vine[1], Guido A. Cadenazzi[1], Clare A. Henderson[1], Keith A. Nugent[1]*, Eugeniu Balaur[2], Corey T. Putkunz[2], Andrew G. Peele[2], G. J. Williams[3] and I. McNulty[4]

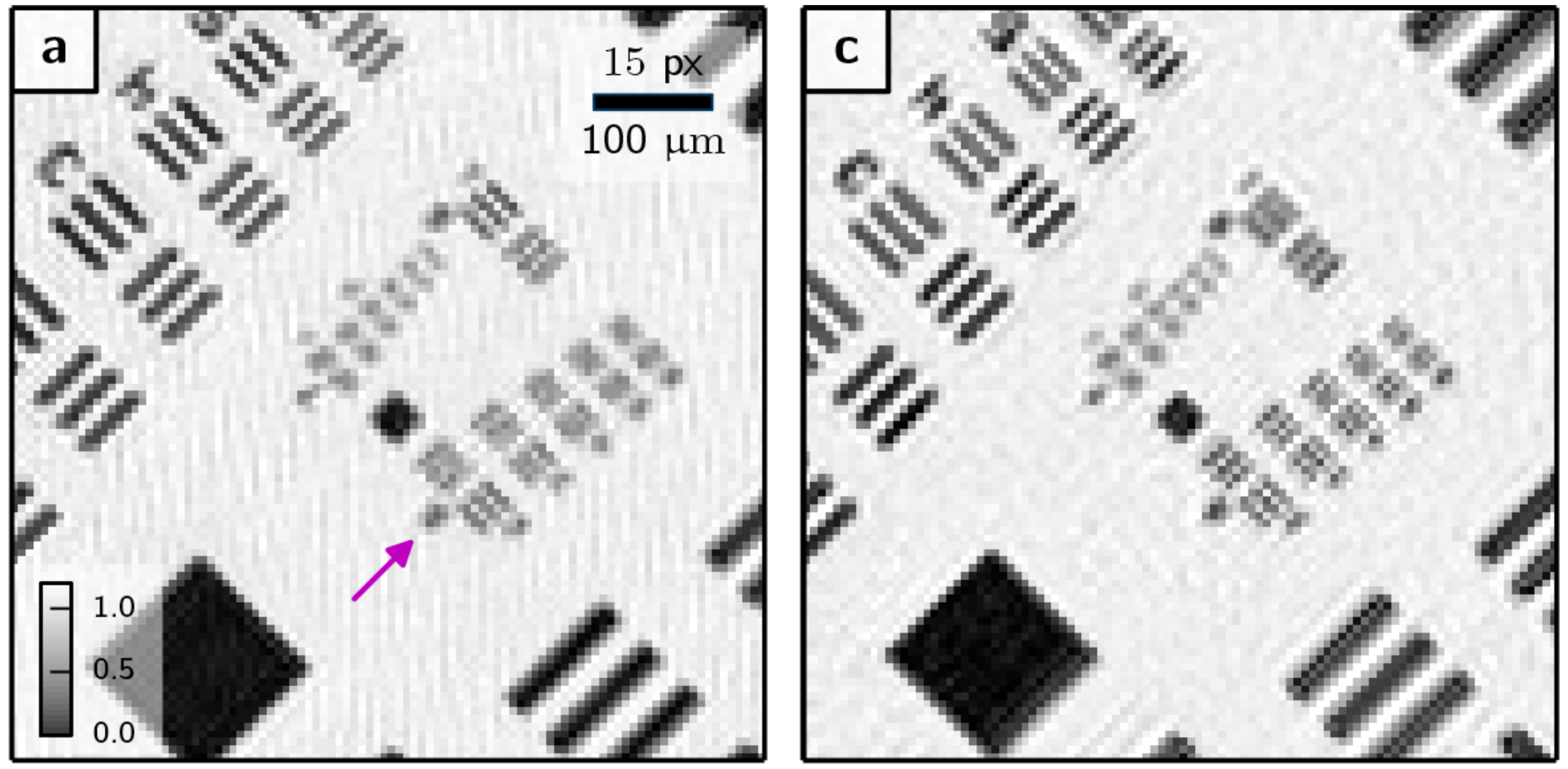




Abbey *et al.* (2011) *Nat. Photonics* **5** 420

Development and Application of Decoherence Models in Ptychographic Diffraction Imaging

Björn Enders



Enders *et al.* (2014) *Appl. Phys. Lett.* **104** 171104
Enders (2016) *PhD Thesis*, TU Munich

Broadband Illumination

Usage of broadband illumination for SAXS is advantageous, *inter alia*, in measurements requiring high spatial and/or temporal resolution.

LETTER

doi:10.1038/nature16056

Nanostructure surveys of macroscopic specimens by small-angle scattering tensor tomography

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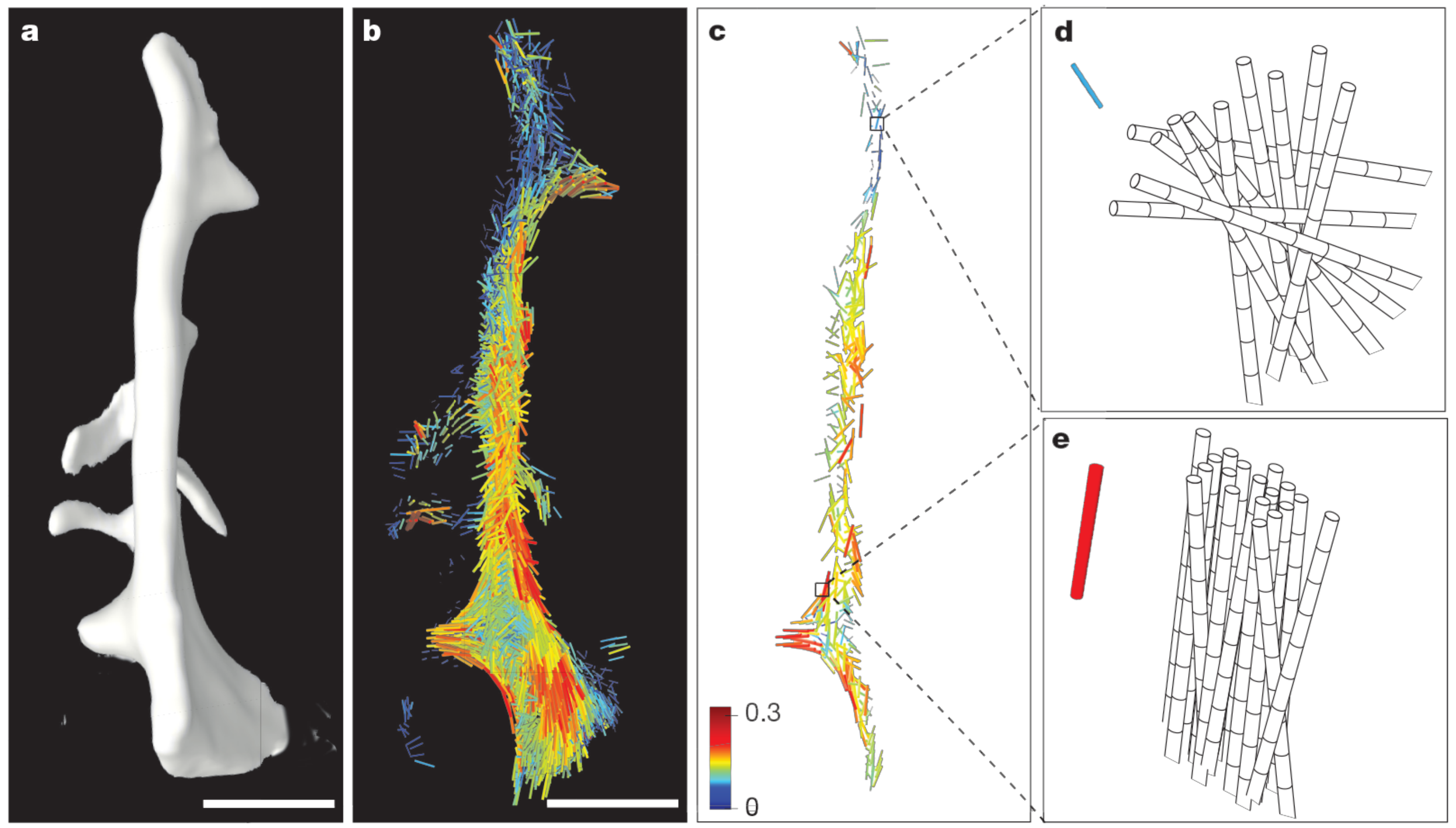


Liebi *et al.* (2015) *Nature* **527**, 349

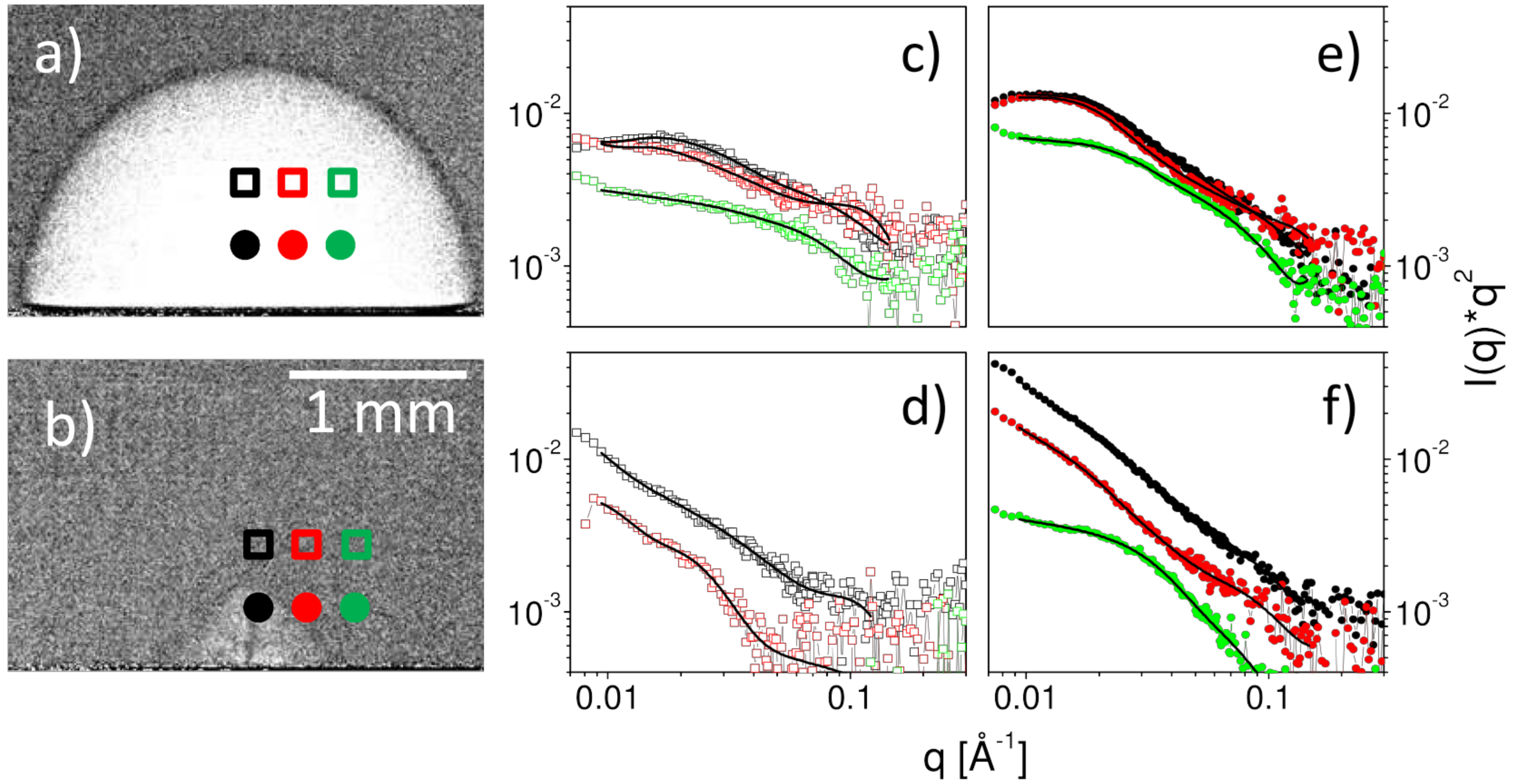
SCIENTIFIC REPORTS

OPEN

A hierarchical view on material formation during pulsed-laser synthesis of nanoparticles in liquid

Received: 21 May 2015
Accepted: 12 October 2015
Published: 09 November 2015

Shyjumon Ibrahimkutty[1,†], Philipp Wagener[2], Tomy dos Santos Rolo[1], Dmitry Karpov[1,†], Andreas Menzel[3], Tilo Baumbach[1,4], Stephan Barcikowski[2] & Anton Plech[1]



Ibrahimkutty *et al.* (2015) *Sci. Rep.* **5**, 16313

A “Minimal” Approach

Just moving today’s cSAXS to SLS-2

Ptychography: faster acquisitions
low-contrast samples
higher energies become more feasible

SAXS: less of a compromise between resolution in real and reciprocal space
access to lower momentum transfer, i.e., longer length scales

…from the QUO Vadis, 2015…

Redesign of various beamline components,
while retaining the current science case, incl. emphasis on flexibility.

Plan: Keeping the flexibility that helped making cSAXS a success.

New source	→ gain in coherent flux:	$10^{1.5}$
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Optimized optics	→ gain in (coherent) flux:	10^{1}
total gain in coherent flux		in the order of 10^{4}!
total gain in flux		close to 10^{3}

Paul Scherrer Institut PSI

S

A "minimal" move,
trying to take profit
from the new source
but little more…

Gain in flux of about ~ 10

→ 3×10^5 CHF

M

**Some upgrades
beyond the bare requirements
to keep on functioning**,
ID, detector, …

The most important upgrade
(i.e., the most limiting element
currently) would be the undulator.

→ 10^6 CHF

L

**Essentially
a redesigned beamline**
incl. optimized optics, …

Gain in usable flux of up to 10^4

→ 4×10^6 CHF

Beamline functionality would be
ensured from "day 1" but would not
immediately rely on novel methods
(e.g. broad-band).

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Budget "L"
Excluding Personnel Costs

Insertion Device	refurbishing existing U19	0.3 MCHF	new ID not necessary on day 1
Electronics/Controls		0.5 MCHF	
Frontend		0.5 MCHF	
Beamline Optics	double-multilayer monochromator DMLM	1 MCHF	determines beam path, rejects higher harmonics
	double-channel-cut monochromator DCCM	1 MCHF	highly beneficial from day 1
	transfocators	0.4 MCHF	either high- or low-energy focusing can possibly be delayed
	diffractive optics	0.1 MCHF	
Beam Diagnostics	BPMs	0.1 MCHF	all but two can be delayed
	wave front sensing	0.2 MCHF	can be delayed
Experiment	sample environment and detector can largely be taken over	0.2 MCHF	
	large-scale detector	2 MCHF	can be delayed
	hutches/infrastructure	0.8 MCHF	
IT		n MCHF	funded by Controls, AIT, …?
Contingency		10 %	

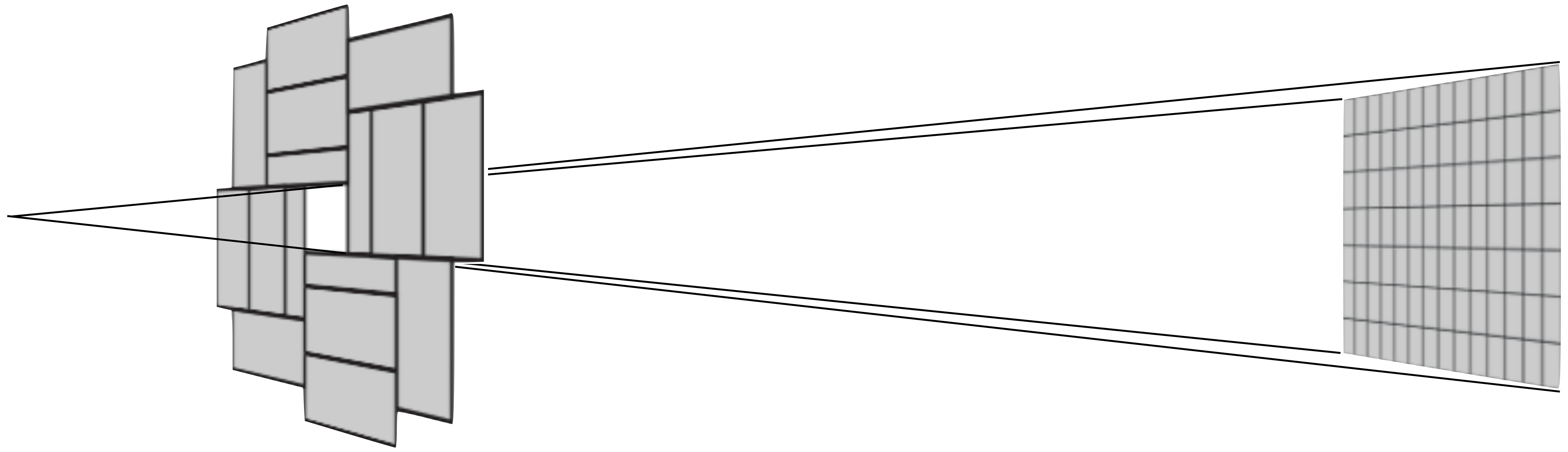
Detector Strategy

From: Bernd Schmitt [mailto:bernd.schmitt@psi.ch]
Sent: Wednesday, July 20, 2011 9:58 AM
To: Bunk Oliver
Subject: 4,16,25,36 oder 49?

Hallo Oliver,

wie sieht das bei cSAXS aus, habt Ihr kein Interesse an einem 16 oder 25M Eiger? Man könnte die Module, welche man ausliest dann frei bestimmen.

Gruss,
Bernd

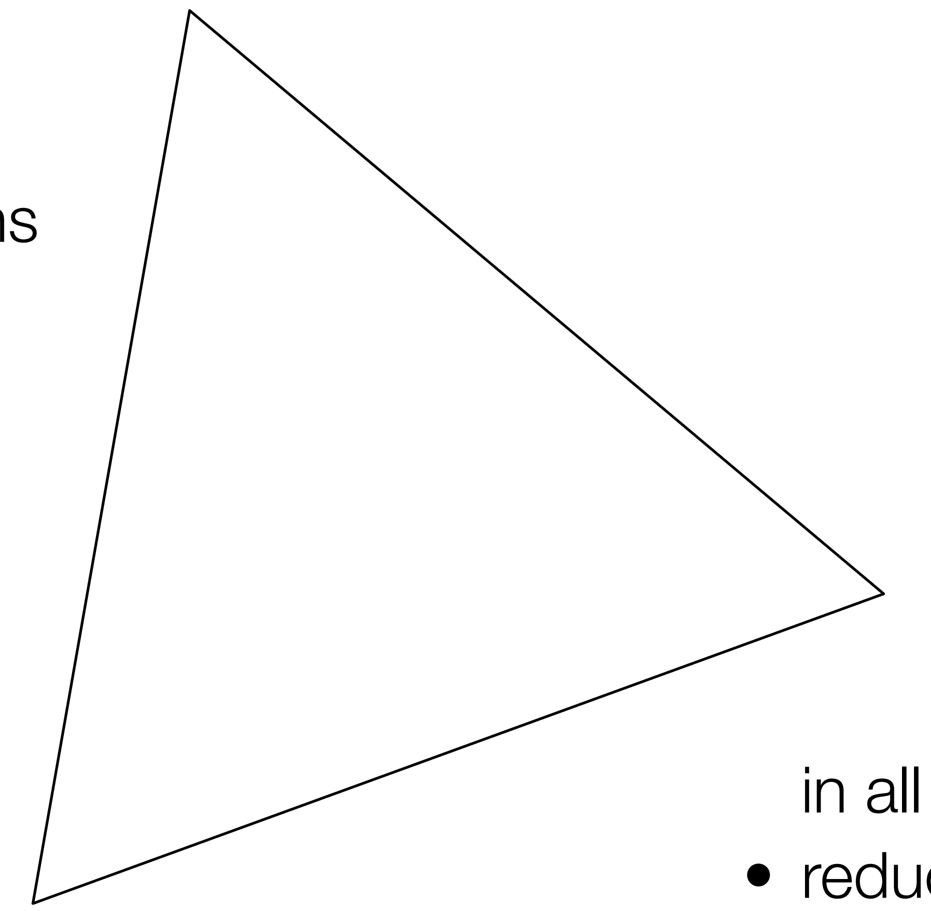


for good measure:
a WAXS detector
to be operated in parallel:
7M

large
in-vacuum detector
at fixed distance:
49M

Detector Strategy

Updating the detector to be operated in vacuum, thus eliminating one of the remaining sources of background



small pixels

in **ptychography**:
- facilitating sampling in q-space
- reducing the number of scan positions

in **SAXS**:
- extending the length scale

rapid readout

in all **scanning microscopy**:
- reducing detector overhead
- many low-SNR measurements often preferable to few high-SNR measurements

in **SAXS**:
- extending time resolution
- allowing high-repetition-rate experiments

large area

in **SAXS**:
- necessary for high spatial resolution

in **ptychography**:
- rather limited by module size than total detector size

Address these issues by a single detector at fixed sample-to-detector position,

49 Megapixel detector (or larger...)

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Detector Strategy

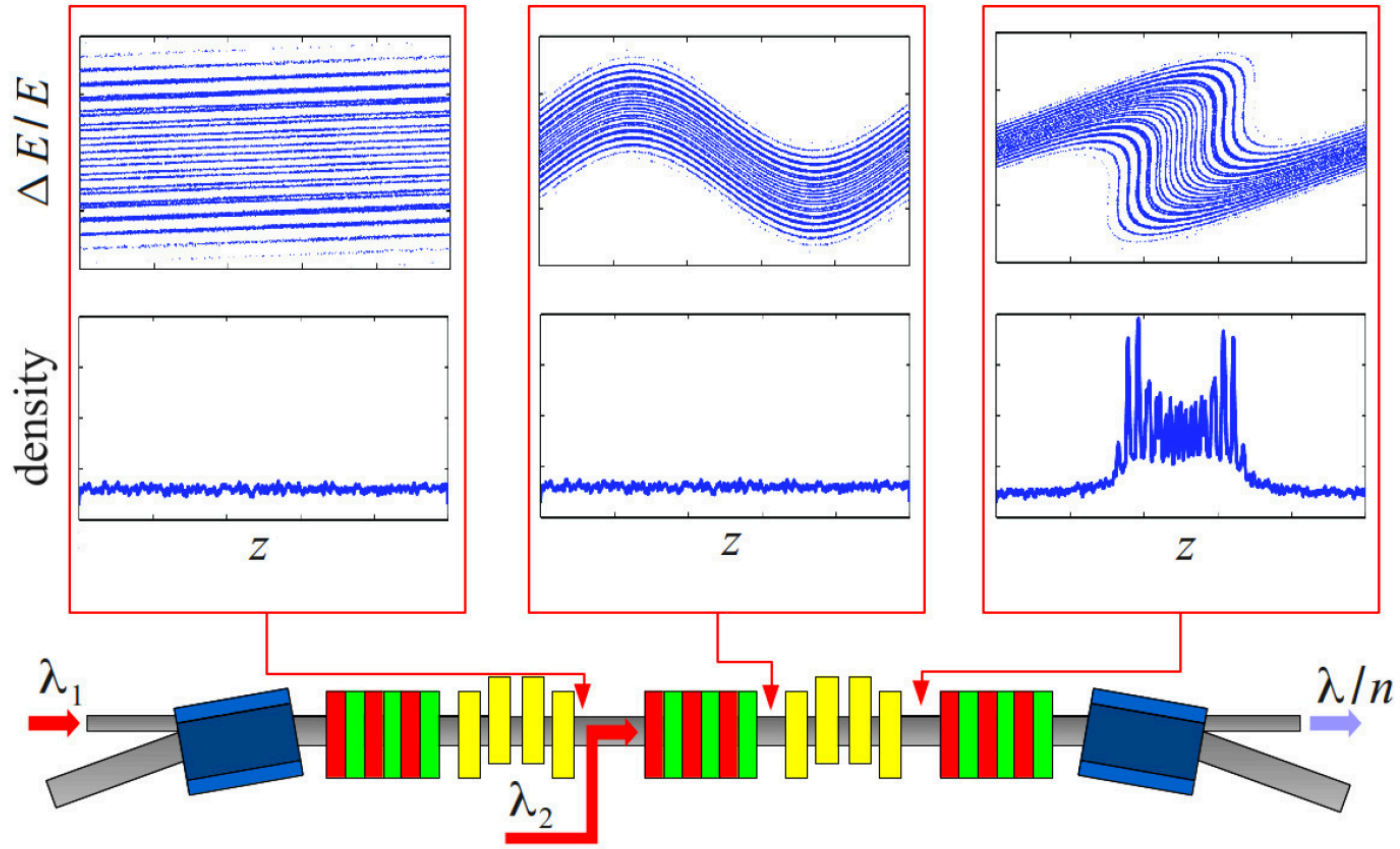
	Eiger	Mönch	Jungfrau
detection mode	photon counting	charge integrating	charge integrating; possibly switchable to photon counting
availability	would require upgrade to Eiger-II, PSI has tons of expertise	the most unknown of the three	in use at SwissFEL, at the beginning of the learning curve for synchrotron applications
pixel size	75μm	25μm sub-pixel resolution possible	75μm
max. count rate	~ 1 MHz	t.b.d.	> 100 MHz
max. read out rate	~ 10 kHz	~ 2 kHz	~ 2 kHz

Echo Enabled Harmonic Generation (EEHG)

(courtesy to T. Schmidt)

EEHG needs 2 modulators, 2 chicanes and high-power Ti:sapphire laser:

1. in a modulator the electron energy is modulated by an external laser
2. in a strong dispersive element (chicane) the phase space is rotated
3. a second laser-induced energy modulation in the second modulator
4. a second magnetic chicane (like a small phase matcher) generates microbunches



microbunch spacing can be adjusted to the undulator wavelength by the laser amplitude

this causes coherent radiation

10^2 – 10^4 × higher flux

In SLS 2, first chicane is replaced by dispersion in the arc between two straights no emittance blow-up.

Molo *et al.*, EEHG and femtoslicing at DELTA, Proc. FEL 2013

IT Requirements
(work in progress)

Experiment	days/y	when?	detector	DCU spec. Req.	Measuremen speed (Hz)	Online+FFB CPU cores	peak bw GB/s	data set size GE	Comment
Ptycho-tomo***	180 days #	2024	Eiger 9M*		160**	**2392**	**0.4**	**1250**	Offline tasks for ptycho are driven by more detailed analysis, or parameter search for a few tomograms, or by method development from our own research projects.
Ptycho-tomo multislice ****		2024	Eiger 9M*		160**	**14352**	**0.4**	**6250 &**	
Scanning SAXS	120 days #	2024	Eiger 9M		2000	**7680**	**5**	**360**	
SASTT		2024	Eiger 9M		2000	**7680**	**5**	**36000 $**	

* Even if a larger detector is available processing effectively 9M pixels should be enough, either by cropping or binning. This is not the case for SAXS, for SAXS more pixels would lead to more data being useful, read, and stored.

** Assumes 6 ms measurement period, from having 3 ms position settling time. There is no indication what technology will need to be developed to reach this increase of a factor of 13x from today posibility. This is a projection more based on the experience that we have improved this technology continuously and consistently in the past 5-10 years.

*** This is PXCT as we process today

**** Increase in flux from SLS 2.0 will allow to image larger volumes at smaller resolution. At some point there is a price to pay in processing due to the need of multislice ptychography. Factor of 5x is a very rough estimate.

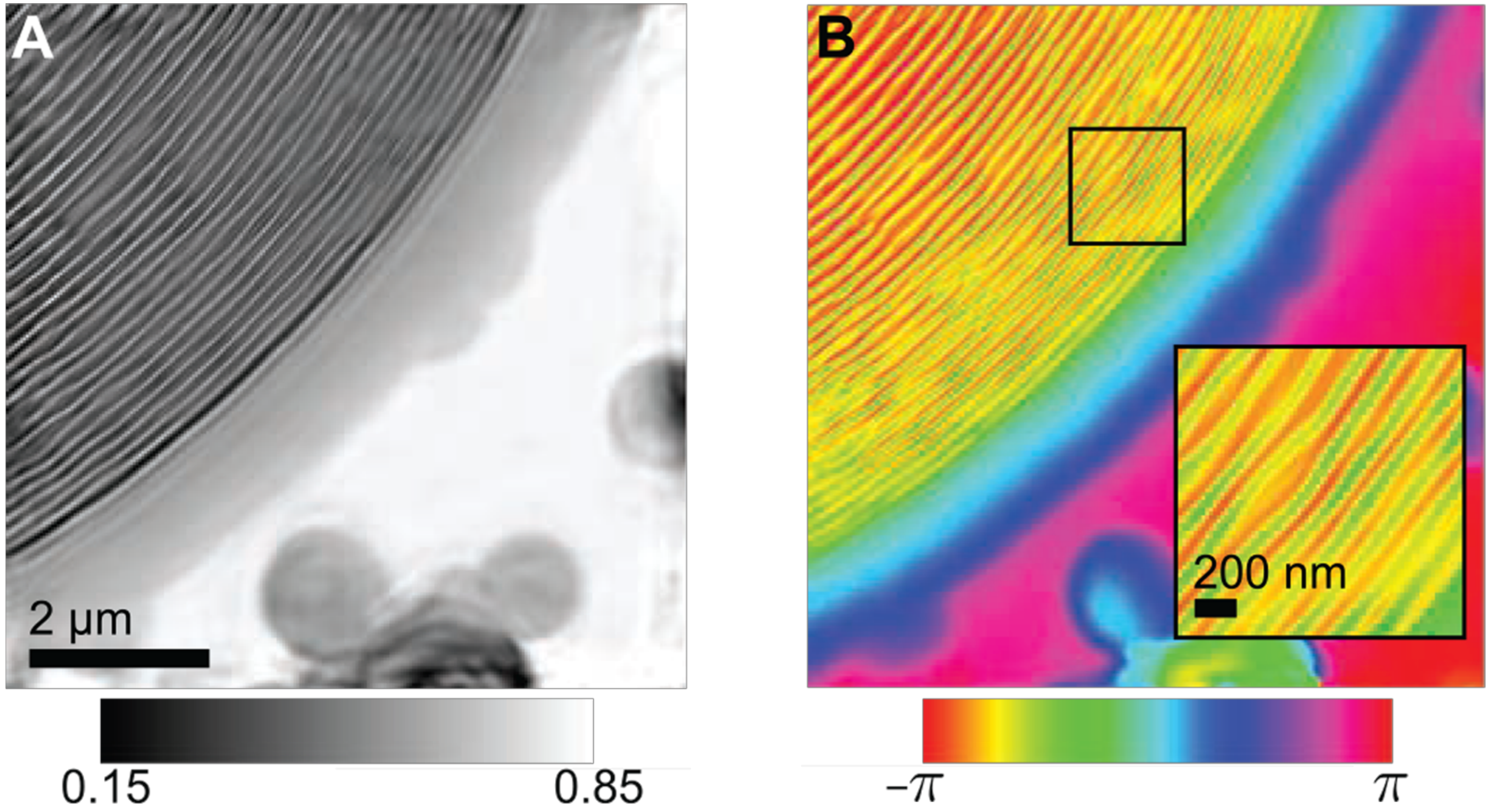
Based on a very rough estimate that 50% of beamtime will be ptycho tomo and 30% on imaging SAXS either in 2D or 3D. Ultimately impossible to predict because it depends on the PRC. The 180 days are somehow split between normal ptycho-tomo and ptycho-tomo multislice, it is not possible to predict how much each because it depends on the specific needs of the user, the needed resolution vs representative volume. The 120 days are split between Scanning SAXS and SASTT, these have the same requirements for online processing and data flow, but they have different needs in terms of datasize, I keep separate here but could easily be conceptually bonded together if wanted.

& x5 from above because I expect a growth in the data as we have larger volume at higher resolution. Simple but also naively I estimate the factor of 5 from the multislice.

$ This data does not need to be loaded at once in RAM for processing, only smaller chunks are needed at a time maybe 1%. I think for SASTT we will be dealing with samples that will take a few hours to measure, the faster we go the larger the volumes of interest will become. I put here 2 hours at 2 kHz as a very rough estimate. The real numbers depend completely on the size of the sample and resolution needs of the user.

Calculation of number of cores	Current cores	Increase of speed x13	Increase from 1.5M (ptycho) or 2M (SAXS) to 9M pixels used	Increase of x5 for multislice ptycho
Ptycho tomo	184	2392	14352	71760
Scanning SAXS	96	7680	34560	-

Advanced Processing
(mixed states for decoherence effects, multi-slice for thick objects, ...)



Thibault *et al.*, *Science* **321** (2008) 379

Advanced Processing

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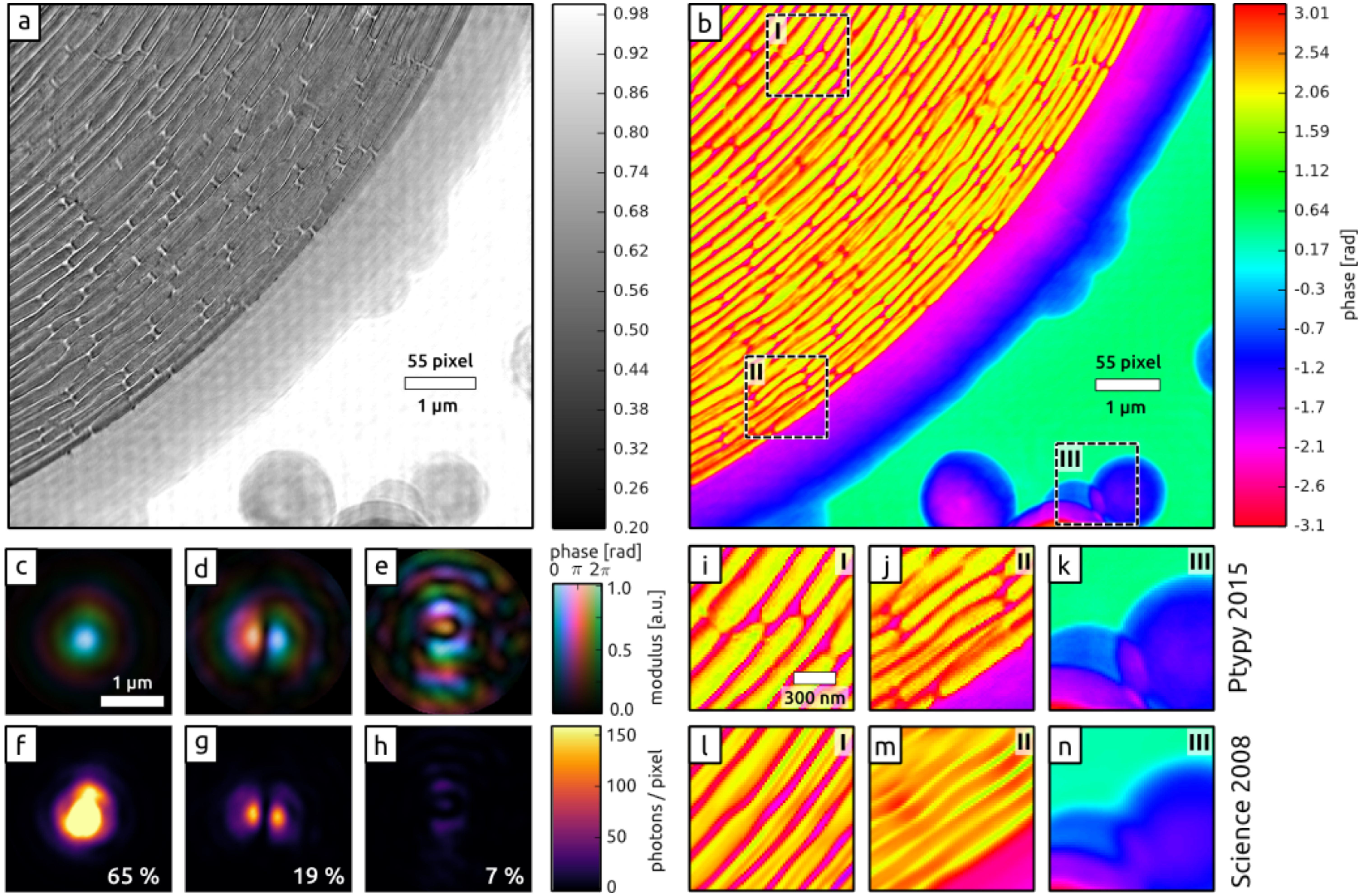

Thibault, Menzel, *Nature* **494** (2013) 68

B. Enders, PhD Thesis, TU Munich 2015

cSAXS ∈ SLS

High-Resolution Imaging
Ptychography

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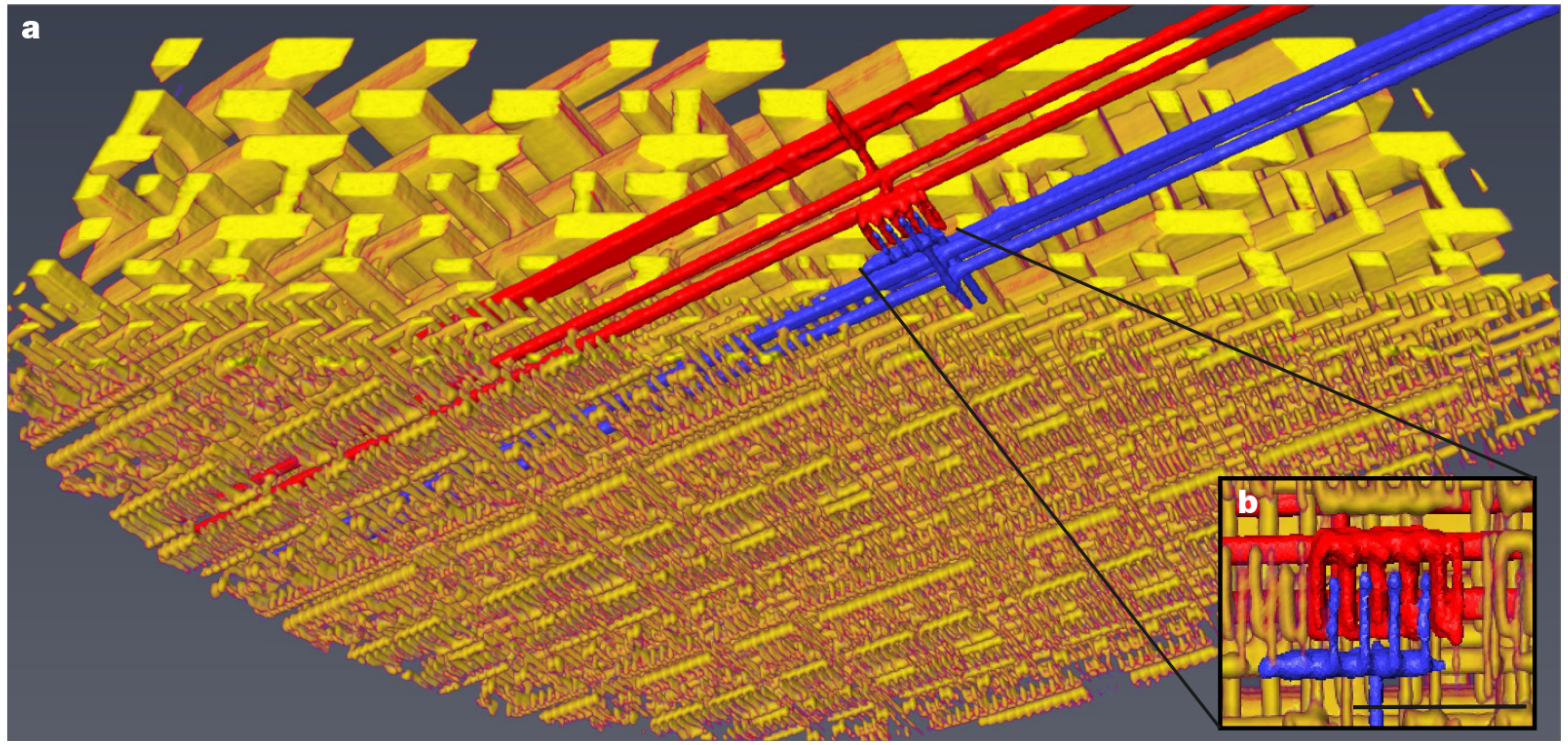
Mirko Holler[1], Manuel Guizar-Sicairos[1], Esther H. R. Tsai[1], Roberto Dinapoli[1], Elisabeth Müller[1], Oliver Bunk[1], Jörg Raabe[1] & Gabriel Aeppli[1,2,3]



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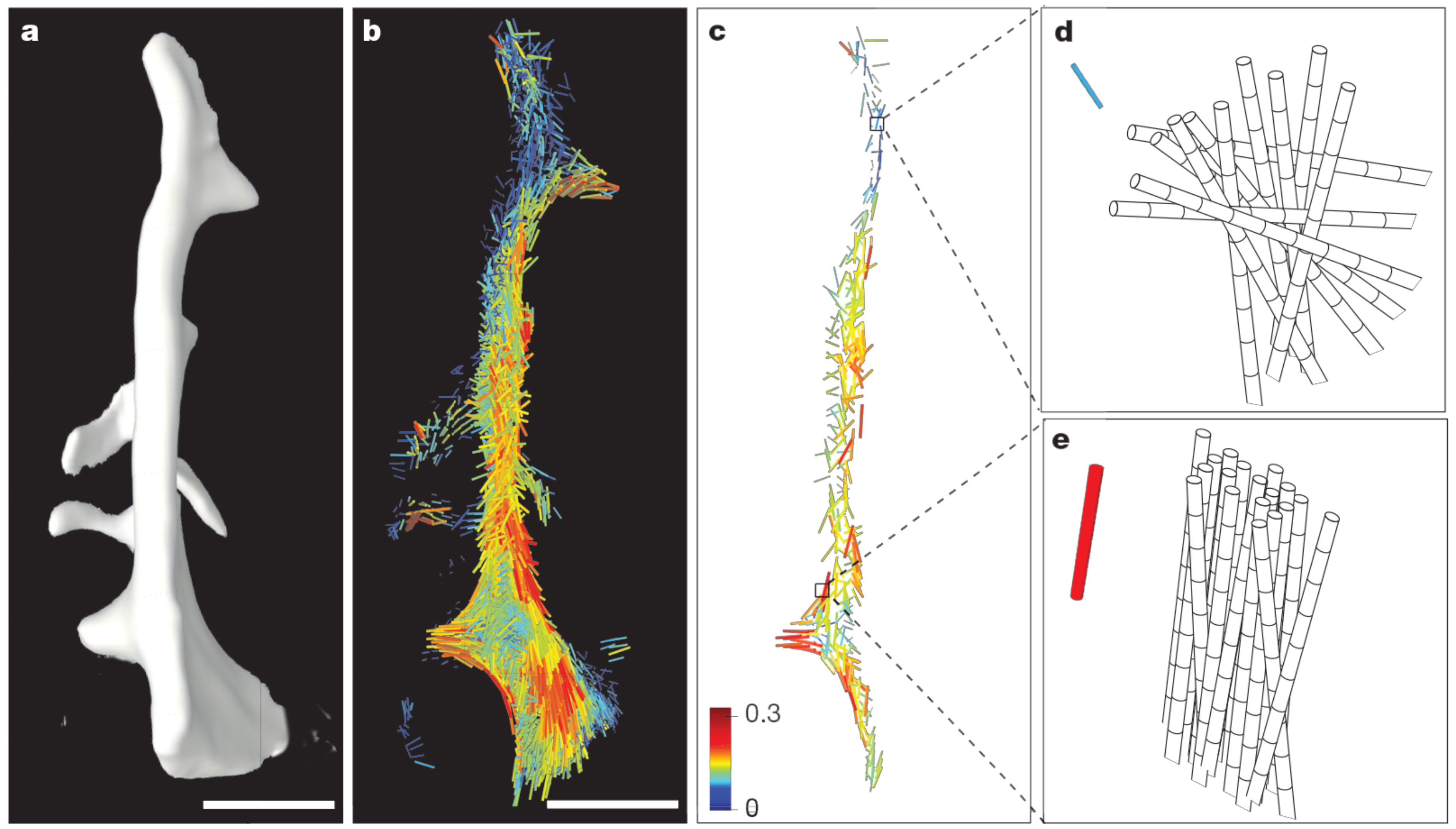

Liebi *et al.* (2015) *Nature* **527**, 349

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cSAXS $\in$ SLS

High-Resolution Imaging
Ptychography

- SLS-2 will help to make the nature of the technique less important: **Ptychography can be just another type of microscopy.**
- SLS can maintain its leading position compared with ESRF, Petra-III, APS, …
- Our focus on high-resolution/ high-specificity imaging will complement imaging offered at TOMCAT
- Ptychography at cSAXS will be complemented by ptychography at lower energies, i.e., at PHOENIX, SIM, … any by other capabilities at TOMCAT, microXAS

SAXS Imaging, Tomography, and other High-Brilliance Applications

- The demand in SAXS imaging has consistently been toward high spatial resolution, i.e., small beams.
- The demand in time-resolved SAXS has consistently been toward high time resolution, i.e., high flux.
- At SLS, demanding SAXS applications shall be addressed at cSAXS, complemented at higher energies by MS and at lower energies by PHOENIX.

cSAXS ∈ SLS

High-Resolution Imaging Ptychography

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Optics Characterization etc. for FEL Applications

- Demands high flexibility and representative beam conditioning and detection capabilities.
- This demand shall remain addressable at SLS-2, and out track record is excellent.

Coherent Applications for Single-Crystal Characterization

- A future upgrade may involve a diffractometer and related detector positioning for Bragg-CDI etc.

Questions?
Comments?

image credit: **Nick Veasey**

andreas.menzel@psi.ch