Ptychographic imaging for the characterization of X-ray free-electron laser beams

S Sala[1,2,3], BJ Daurer[4], MF Hantke[4], T Ekeberg[4], ND Loh[5], FRNC Maia[4] and P Thibault[3]

[1] Department of Physics & Astronomy, University College London, London WC1E 6BT, UK
[2] Diamond Light Source, Harwell Science & Innovation Campus, Didcot OX11 0DE, UK
[3] Department of Physics & Astronomy, University of Southampton, Southampton SO17 1BJ, UK
[4] Department of Cell and Molecular Biology, Uppsala University, 75124 Uppsala, Sweden
[5] Department of Physics, National University of Singapore, Singapore 117551

E-mail: simone.sala.14@ucl.ac.uk

Abstract. We present some preliminary results from a study aimed at the characterization of the wavefront of X-ray free electron laser (XFEL) beams in the same operation conditions as for single particle imaging (or flash X-ray imaging) experiments. The varying illumination produced by wavefront fluctuations between several pulses leads to a partially coherent average beam which can be decomposed into several coherent modes using ptychographic reconstruction algorithms. Such a decomposition can give insight into pulse-to-pulse variations of the wavefront. We discuss data collected at the Linac Coherent Light Source (LCLS) and FERMI.

1. Introduction

Many X-ray experiments require precise knowledge of the beam. One example is the characterization of the focusing optics in operation conditions aimed at selecting a plane where optics-induced aberrations are minimized. Such aberrations may have a strongly detrimental effect on any experiment performed at high power density and with a small focal spot, which is often the case at X-ray free-electron lasers (XFELs). Time-resolved characterization of the beam is also beneficial in the case of pulsed sources in general, as these might show shot-to-shot fluctuations potentially affecting any experiment extended in time. Furthermore, wavefront sensing is also instrumental in producing an accurate initial estimate of the complex-valued illumination function, useful to some phase retrieval algorithms for imaging experiments as it is the case of flash X-ray imaging [1] which has been the target application for this study.

XFELs often combine all these requirements. These extremely bright sources most frequently exploit self-amplified spontaneous emission (SASE). The stochastic nature of the spontaneous microbunching of the electron beam translates into a small but measurable stochastic variation of both temporal and spectral distribution between X-ray pulses.

Many approaches are available for beam diagnostics at XFELs such as Shack-Hartmann sensors, ablative imprints [2], Young's double-slit experiments [3], grating interferometry [4], aerosol spheres diffraction [5], coherent scattering speckles analysis [6] and ptychography [7]. This latter technique has been chosen to carry out this study as it has been already successfully applied to recover the full wavefront at high-brilliance X-ray sources [8, 9].

IOP Conf. Series: Journal of Physics: Conf. Series **849** (2017) 012032 doi:10.1088/1742-6596/849/1/012032

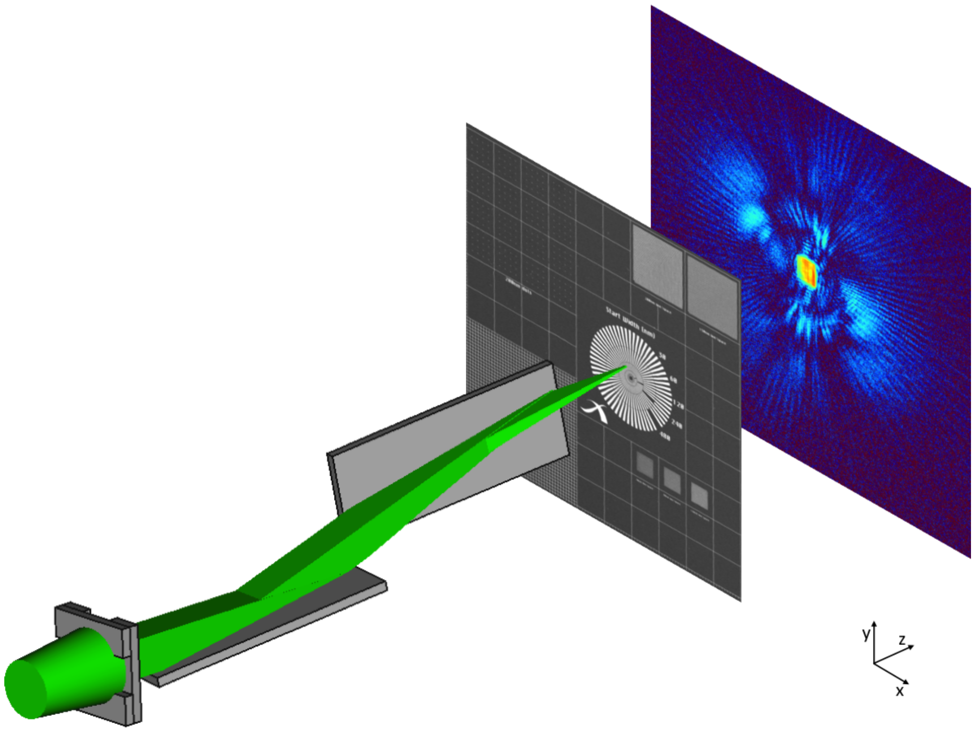

Figure 1. Sketch of the ptychographic setup used for the experiments performed at LCLS and FERMI. The beam is shaped by an aperture and focussed by KB-mirrors. The sample is scanned perpendicularly to the beam and diffraction patterns are collected by a detector downstream.

2. Methods

Ptychography is a lensless scanning diffraction technique [10]. It requires the beam to be scanned through a specimen non-destructively and its image reconstruction algorithm relies on the overlap among adjacent illuminated areas of the specimen. Such an overlap ensures data redundancy to a degree that makes phase retrieval algorithms robust enough to relax several constraints. Ptychography allows to achieve the simultaneous reconstruction of both the transmission function of the specimen (object) and the illumination function (probe) [11].

Several sources of decoherence can be accounted for by exploiting multimodal decomposition of the probe [12] which improves the quality of the reconstructed images in most experimental conditions [13]. This approach is applied here to XFEL data in order to retrieve the wavefront of the average beam and the individual pulses.

A first set of data has been collected at the AMO end station at the Linac Coherent Light Source (LCLS), SLAC's SASE XFEL, at 1.25 keV.

A second set of data has been collected at the DiProI beamline [14, 15] at FERMI, Elettra's seeded EUV / soft X-rays FEL, at 83 eV.

In both cases a setup based on the one shown in Fig. 1 has been used. Homogeneous attenuation of the beam's intensity by several orders of magnitude was needed to avoid damaging the sample. Except for this attenuation, all other conditions have been the same as those used in flash X-ray imaging experiments.

The sample used is a 100×100 μm^2 gold resolution and calibration test pattern including a 30×30 μm^2 Siemens star 150 nm thick and with a 30 nm smallest feature mounted on top of a 100 nm thick silicon nitride chip. A SEM image of the sample is shown within the sketch in Fig. 1.

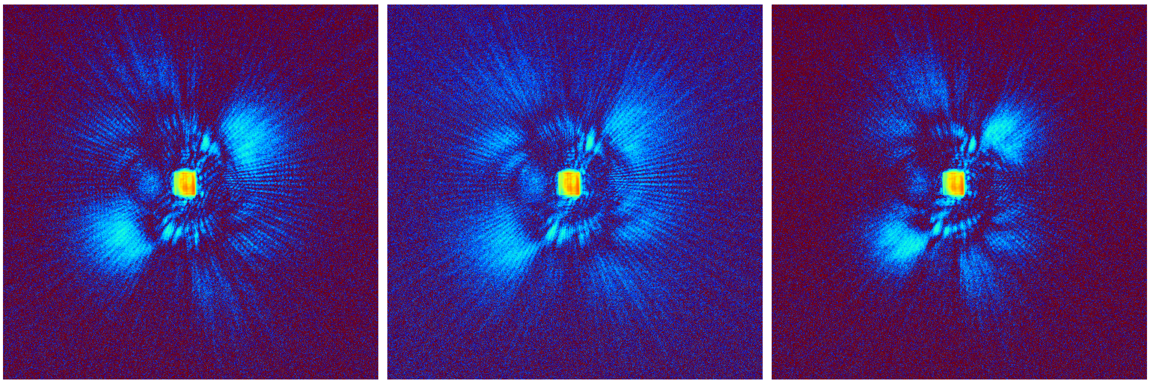

Figure 2. Three diffraction patterns collected at FERMI at the same sample position show that at least intensity and pointing vary between pulses. Each frame is plotted in a logarithmic scale and reaches a resolution of 83 nm on the edges of the frame.

3. Results

Several diffraction patterns have been collected at every scanning position in order to gather enough statistical significance and to make possible the analysis of the average beam before moving on to the single shot analysis.

FERMI data have been complicated by a significant jitter of the beam. Fig. 2 for example shows how different diffraction patterns have been generated by different pulses collected at the same sample position. The observed differences are the result of beam pointing variations as well as flux and intensity distribution fluctuations. The pulses produced by a seeded XFEL are expected to be more stable and reproducible than those produced by SASE XFELs, but due to the observed jitter a more elaborate position refinement analysis has been necessary. This position refinement can be included in the reconstruction algorithm as an orthogonal probe relaxation [16] which allows to correct for the difference between the recorded motor positions and the actual positions of the scanned beam onto the sample as well as for other pulse-to-pulse fluctuations.

At LCLS, the average beam has been investigated exploiting diffraction patterns obtained by averaging over 300 pulses collected at each sample position. Three of them are shown in Fig. 3. Using multimodal ptychographic reconstruction algorithms a first estimate of the average beam has been produced. The first three coherent modes of the average probe shown in Fig. 4 reveal an average beam profile a few micrometers wide which is consistent with the expected focal spot size. The relative intensity of each mode suggests that pulse-to-pulse fluctuations resulting in decoherence effects on the average probe are present though limited.

4. Conclusions

The data analysis is still in progress. The implementation of flexible position refinement methods within existing ptychographic algorithms will widen the experimental conditions in which these can be applied. Furthermore the outcome of these experiments is expected to shed new light on pulse-to-pulse fluctuations of the wavefront at XFELs and advance the development of fast and reliable beam diagnostic techniques for high-brilliance sources.

Acknowledgments

The research leading to these results has received funding from the European Research Council, the Swedish Research Council, the Knut and Alice Wallenberg Foundation and the Swedish Foundation for Strategic Research.

IOP Conf. Series: Journal of Physics: Conf. Series **849** (2017) 012032 doi:10.1088/1742-6596/849/1/012032

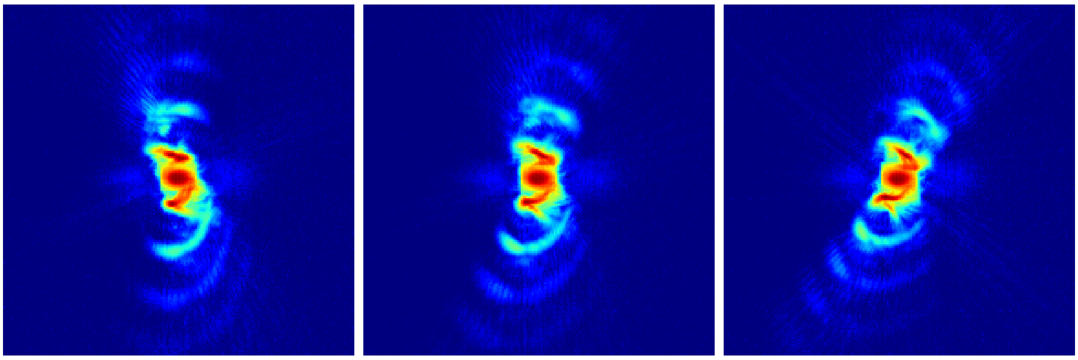

Figure 3. Preliminary analysis of LCLS average data: three diffraction patterns obtained by averaging over 300 pulses each. Each frame is plotted in a logarithmic scale and reaches a resolution of 100 nm on the edges of the frame.

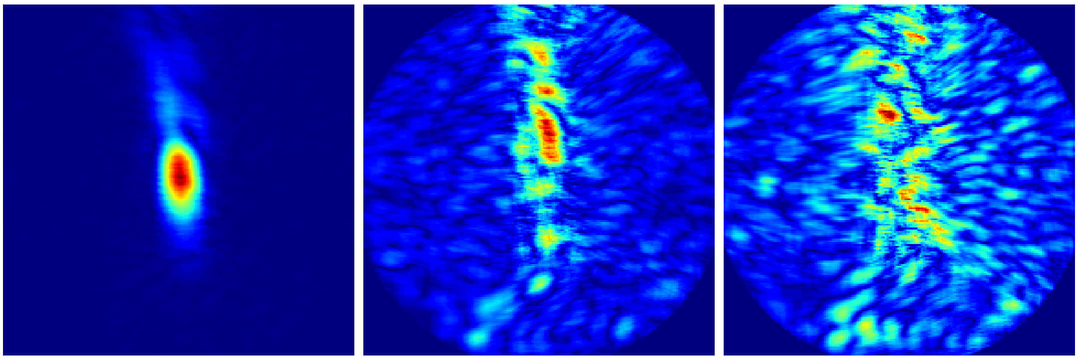

Figure 4. Preliminary analysis of LCLS average data: first three coherent modes of the probe obtained from a 10-mode ptychographic reconstruction. They contribute to the overall intensity of the probe by respectively 89.00%, 2.01% and 1.42%. Each frame is 9.7×9.7 μm^2 and is plotted in a linear scale.

References

[1] Ekeberg T *et al.* 2015 *Physical Review Letters* **114** 1–6
[2] Chalupsky J *et al.* 2011 *Nucl. Instrum. Meth. A* **631** 130–133
[3] Vartanyants I A *et al.* 2011 *Physical Review Letters* **107** 1–5
[4] Rutishauser S, Samoylova L, Krzywinski J, Bunk O, Grünert J, Sinn H, Cammarata M, Fritz D M and David C 2012 *Nature communications* **3** 947
[5] Loh N D *et al.* 2013 *Optics express* **21** 12385–94
[6] Sikorski M *et al.* 2015 *Journal of Synchrotron Radiation* **22** 599–605
[7] Schropp A *et al.* 2013 *Scientific reports* **3** 1633
[8] Kewish C M, Thibault P, Dierolf M, Bunk O, Menzel A, Vila-Comamala J, Jefimovs K and Pfeiffer F 2010 *Ultramicroscopy* **110** 325–329
[9] Vila-Comamala J, Diaz A, Guizar-Sicairos M, Mantion A, Kewish C M, Menzel A, Bunk O and David C 2011 *Optics Express* **19** 21333
[10] Rodenburg J M and Faulkner H M L 2004 *Applied Physics Letters* **85** 4795–4797
[11] Thibault P, Dierolf M, Bunk O, Menzel A and Pfeiffer F 2009 *Ultramicroscopy* **109** 338–343
[12] Thibault P and Menzel A 2013 *Nature* **494** 68–71
[13] Enders B, Dierolf M, Cloetens P, Stockmar M, Pfeiffer F and Thibault P 2014 *Appl. Phys. Lett.* **104** 171104
[14] Pedersoli E *et al.* 2011 *Review of Scientific Instruments* **82**
[15] Capotondi F *et al.* 2015 *Journal of Synchrotron Radiation* **22** 544–552
[16] Odstrcil M, Baksh P, Boden S A, Card R, Chad J E, Frey J G and Brocklesby W S 2016 *Optics Express* **24** 8360