

## Quantitative X-ray ptychographic imaging: present and future innovations

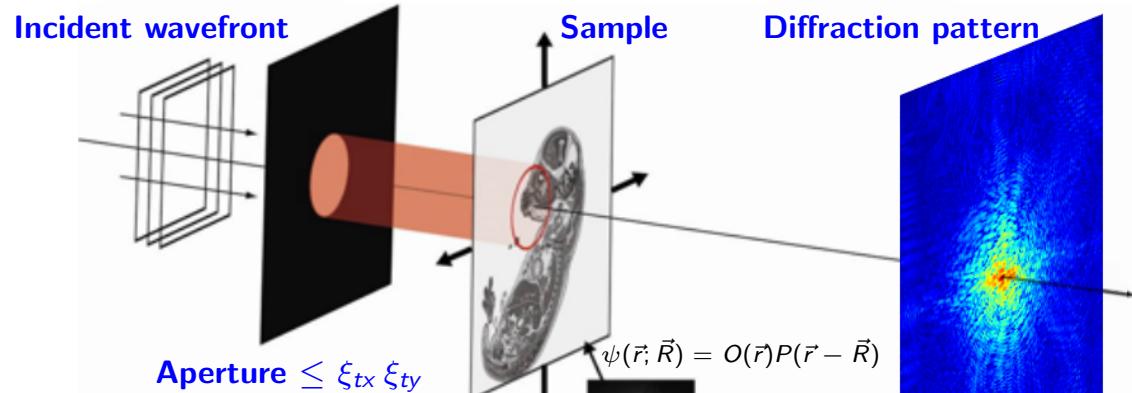
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Julio Cesar da Silva<sup>1,\*</sup>

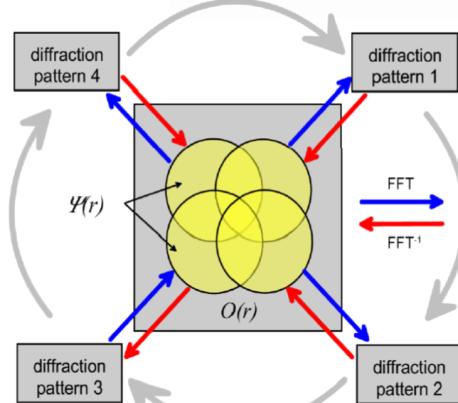
<sup>1</sup>ID16A Nano-imaging beamline  
ESRF - The European Synchrotron, France  
\*e-mail: [jdasilva@esrf.fr](mailto:jdasilva@esrf.fr)



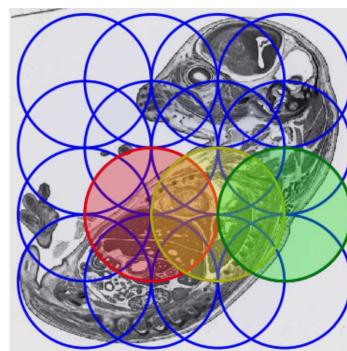
# Transverse diversity - Far-field X-ray Ptychography exploiting the transverse diversity



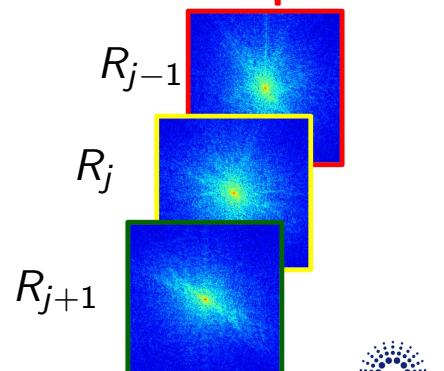
## Reconstruction algorithm



## Scanned area

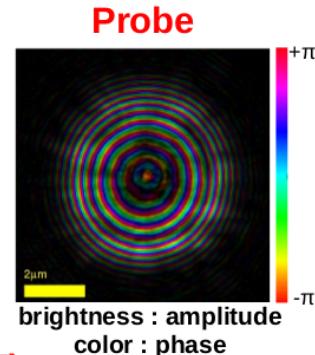
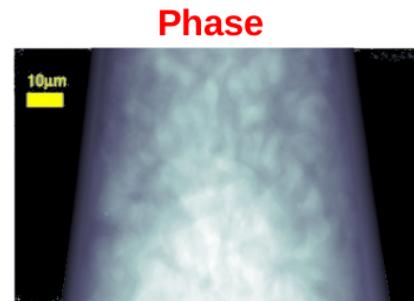


## Diffraction patterns



J. C. da Silva, A. Menzel, Opt. Express 23 (2015) 33812. / J.M. Rodenburg et al., Phys. Rev. Lett. 98 (2007) 034801

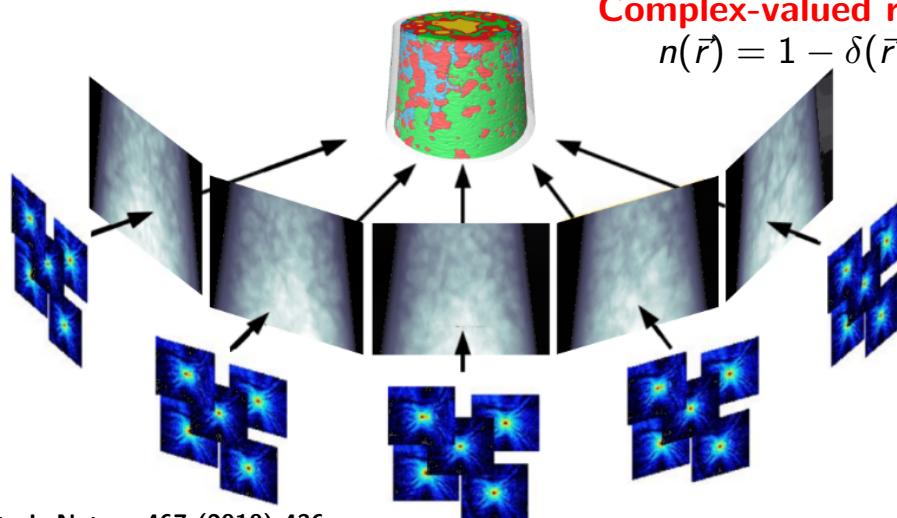
# Welcome to the third dimension



J. C. da Silva et al. Langmuir 31 (2015) 3779

## Ptychographic X-ray Computed Tomography (PXCT)

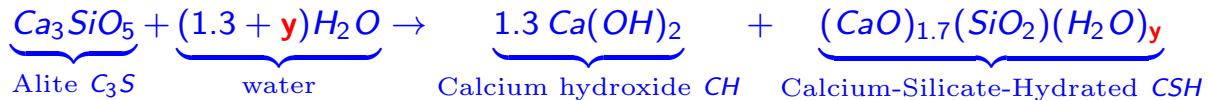
Complex-valued refractive index  
 $n(\vec{r}) = 1 - \delta(\vec{r}) + i\beta(\vec{r})$



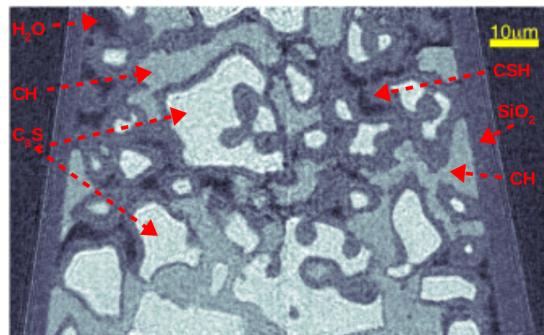
M. Dierolf et al. Nature 467 (2010) 436



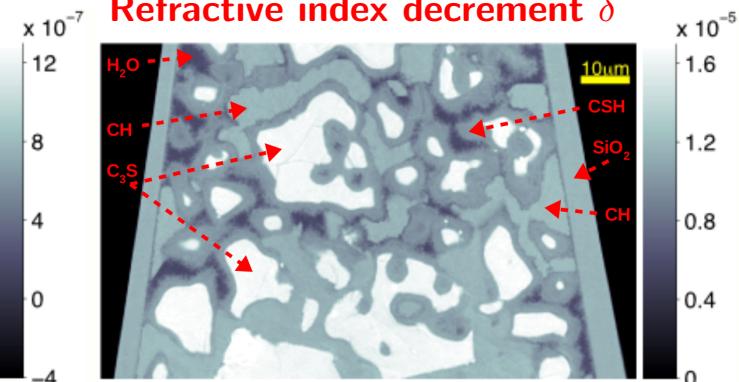
# Chemical imaging of hydrated ordinary cement



Absorption index  $\beta$



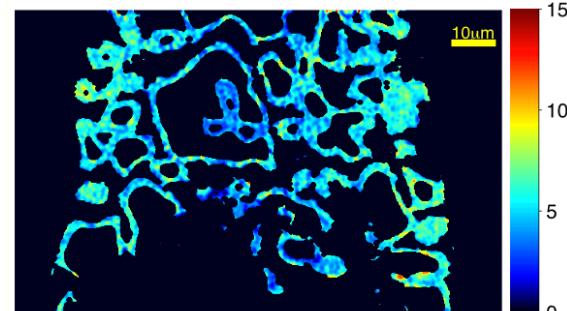
Refractive index decrement  $\delta$



$$\left(\frac{\mu}{\rho}\right)_{CSH} = \omega_{CaO} \left(\frac{\mu}{\rho}\right)_{CaO} + \omega_{SiO_2} \left(\frac{\mu}{\rho}\right)_{SiO_2} + \omega_{H_2O} \left(\frac{\mu}{\rho}\right)_{H_2O}$$

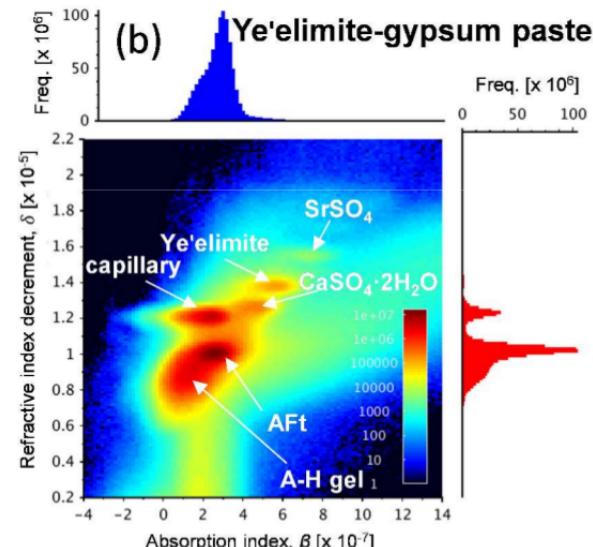
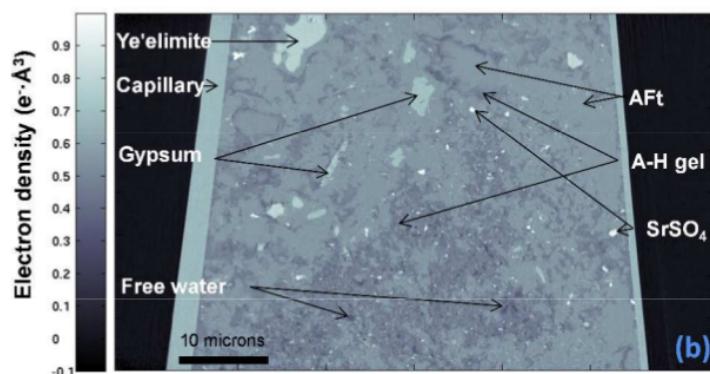
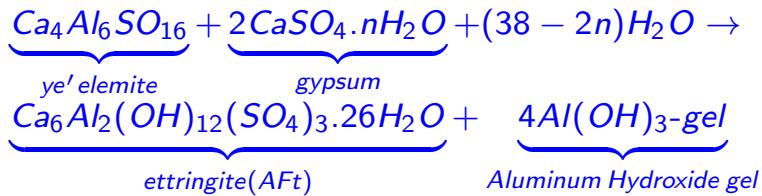
Materials	$\rho \text{ (g.cm}^{-3})$	$\rho_{att.} \text{ (g.cm}^{-3})$
Water	$0.99 \pm 0.01$	1.00
$CH$	$2.18 \pm 0.01$	2.211
$C_3S$	$3.10 \pm 0.01$	3.064
Capillary	$2.19 \pm 0.01$	2.203
$CSH_{(y=5.2 \pm 0.4)}$	$1.83 \pm 0.01$	$1.83(y = 5)$

Water content of  $CSH$ :



J. C. da Silva et al., Langmuir 31 (2015) 3779.

# Hydration of eco-friendly cement based on ye' elemite

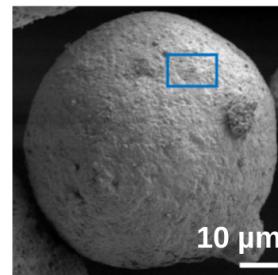


Materials	vol%	mass density ( $g \cdot \text{cm}^{-3}$ )	Expected ( $g \cdot \text{cm}^{-3}$ )
Ye'elemite	3.6	2.58	2.60
Ettringite (AFt)	69.7	1.77	1.78
Al hydroxide gel <sup>α</sup>	25.4	1.48	1.53

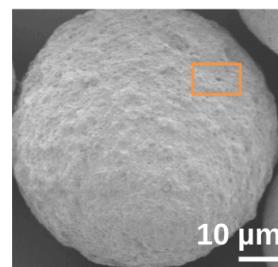
$$\alpha: (CaO)_{0.04}Al(OH)_3 \cdot 2.3H_2O$$

A. Cuesta et al. J. Phys. Chem. C 121, 3044-3054 (2017).

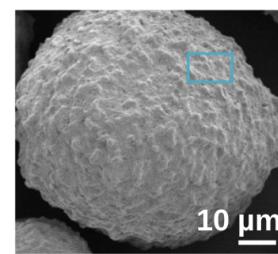
# Fluid Catalytic Cracking (FCC) catalysis



Pristine



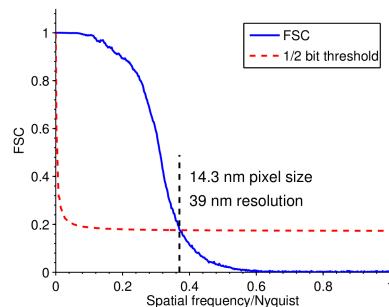
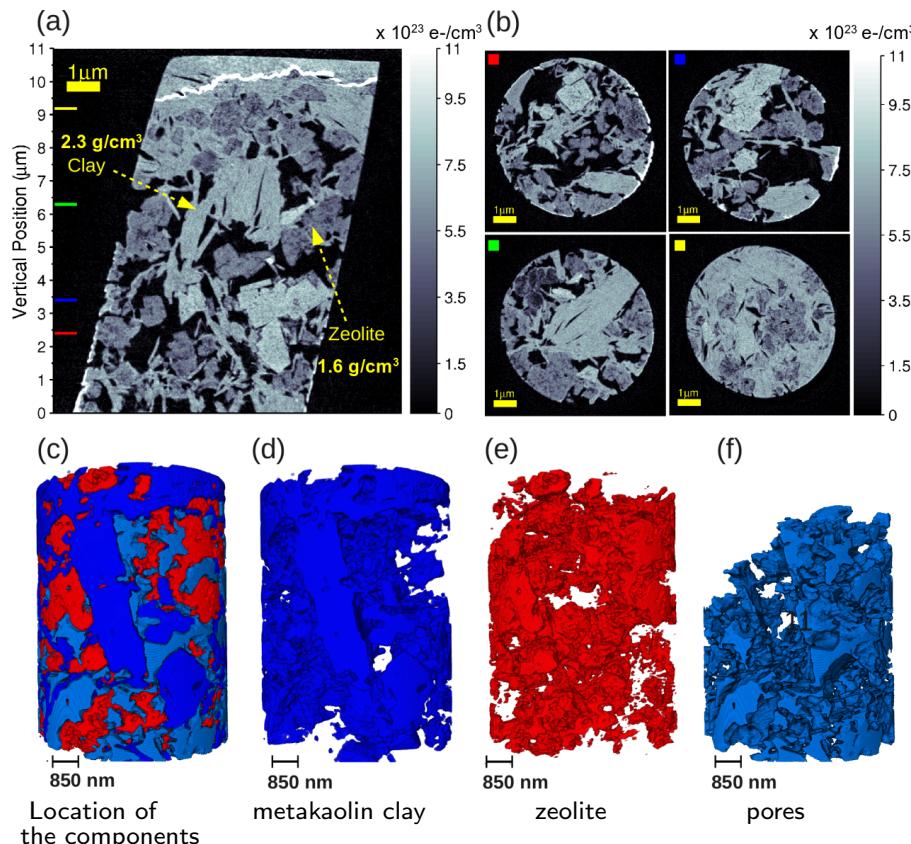
Middle  
life



End of life  
(deactivated)



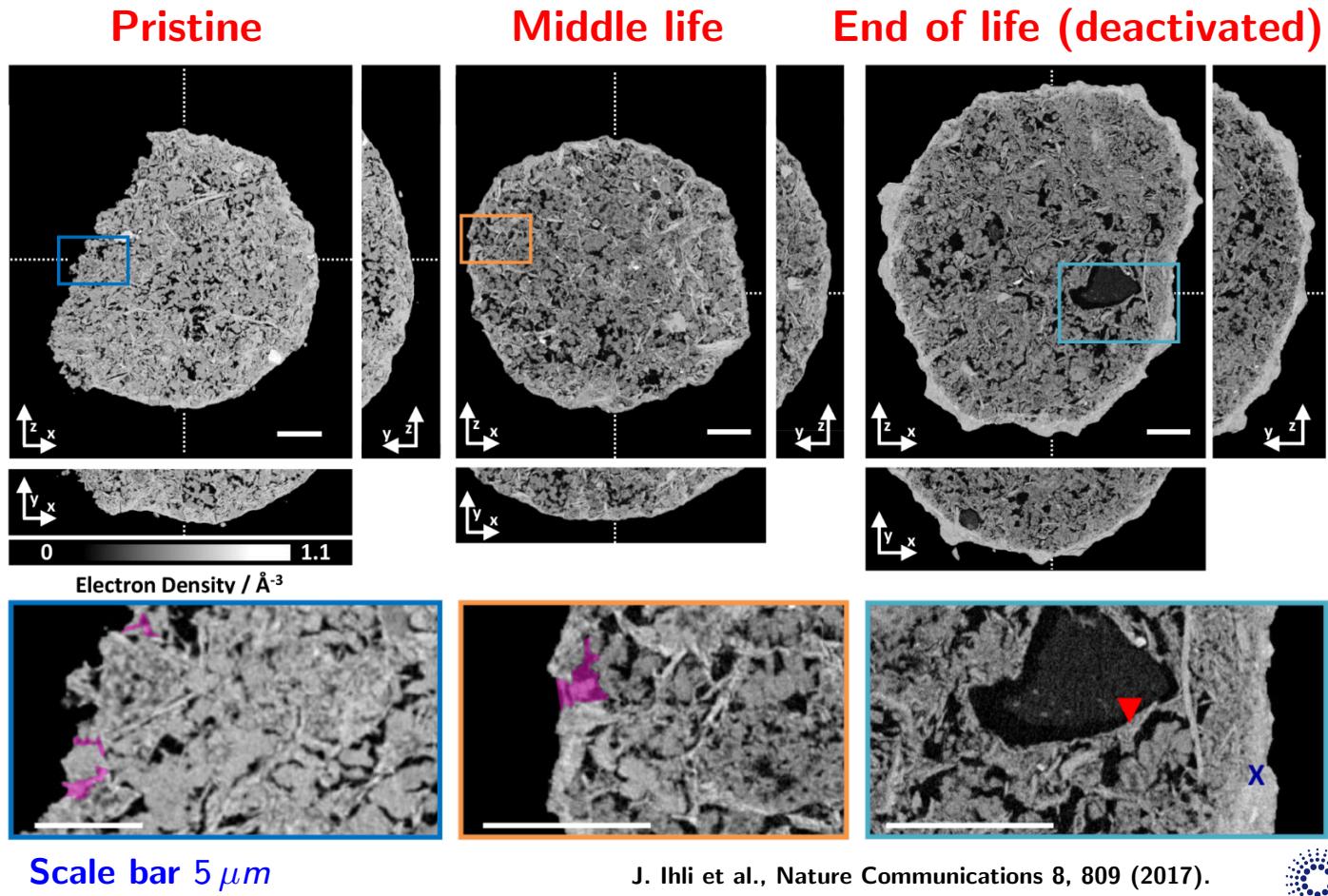
# PXCT - pre-shaped FCC catalyst - pristine



M. van Heel, M. Schatz,  
J. Struc. Biol. 151 (2005) 250.  
[gitlab.com/jcesardasilva/FSCimaging](https://gitlab.com/jcesardasilva/FSCimaging)

$E = 6.2 \text{ keV} (\lambda = 2 \text{\AA})$   
419 diff. patterns per proj.  
450 projections  
 $12 \times 12 \times 11 \mu\text{m}^3$   
14.3 nm of voxel size  
39 nm of spatial resolution

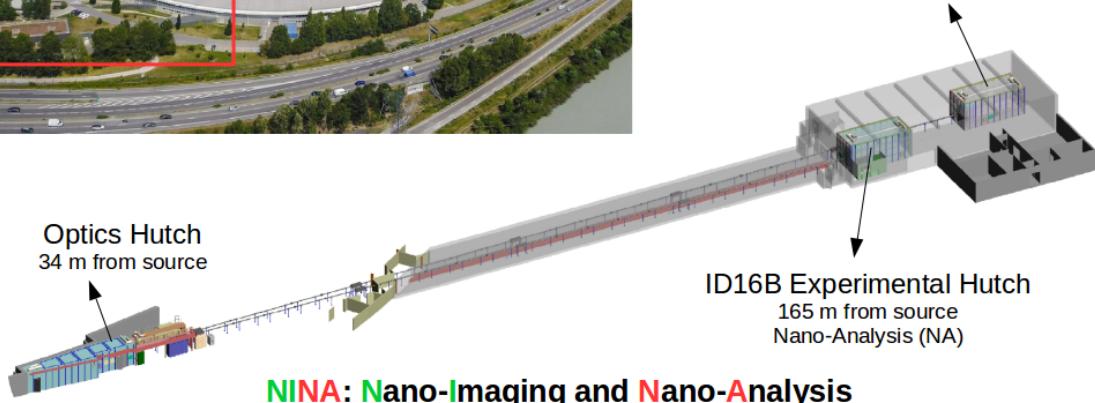
# FCC – Coked and uncoked catalysts



# ID16A nano-imaging beamline



ID16A Experimental Hutch  
185 m from source  
Nano-imaging (NI)



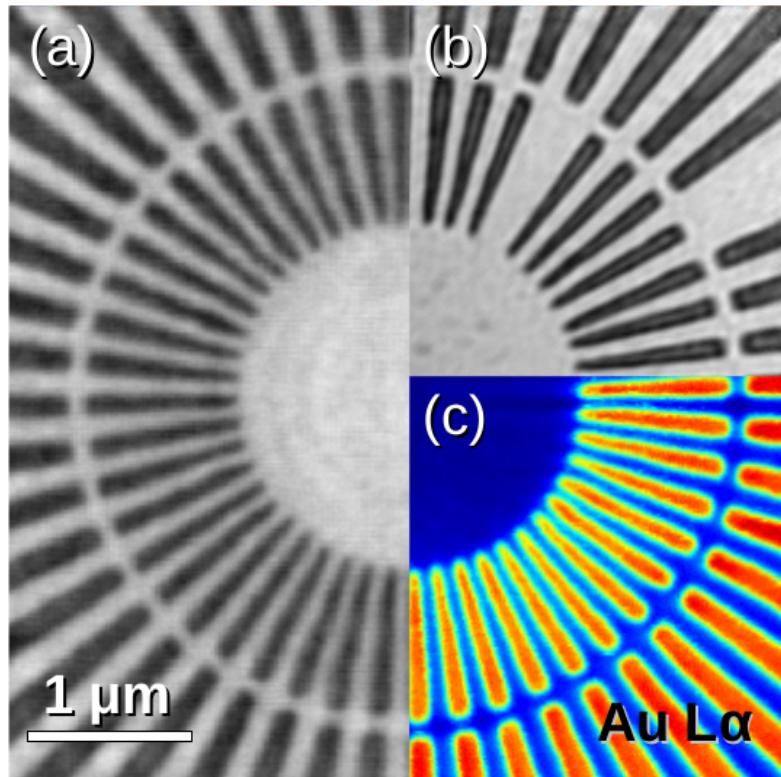
**NINA: Nano-Imaging and Nano-Analysis**

J. C. da Silva et al., Proc. SPIE 10389, 103890F (2017).

# The main techniques available at ID16A beamline

## Holography

- full field microscopy
- large FOV
- quantitative



J. C. da Silva et al., Proc. SPIE 10389, 103890F (2017).

## Ptychography

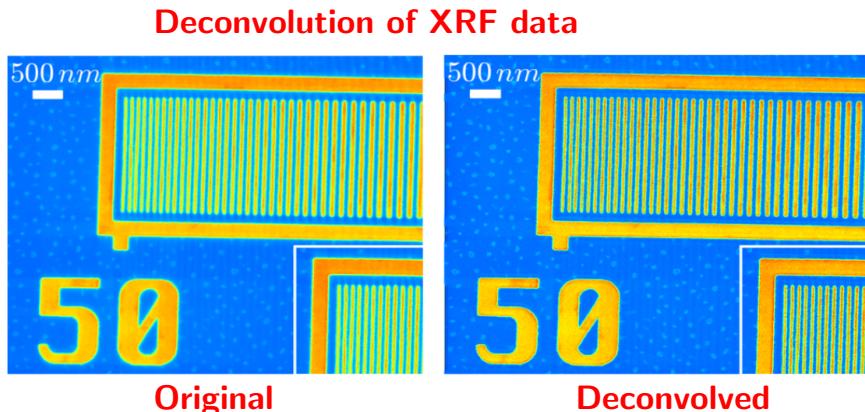
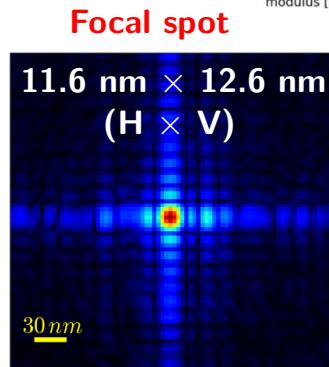
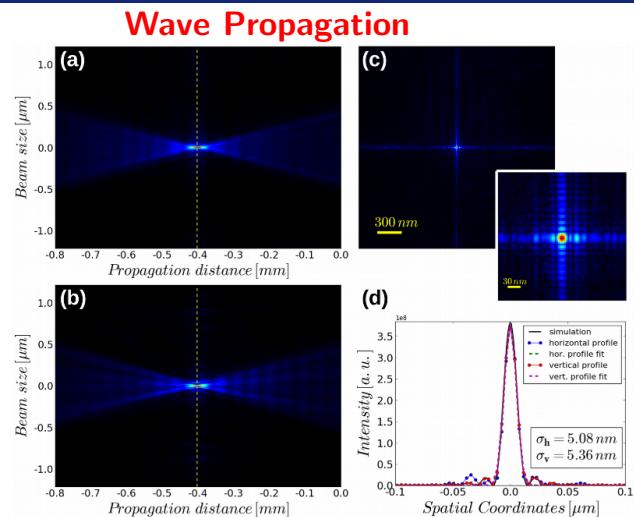
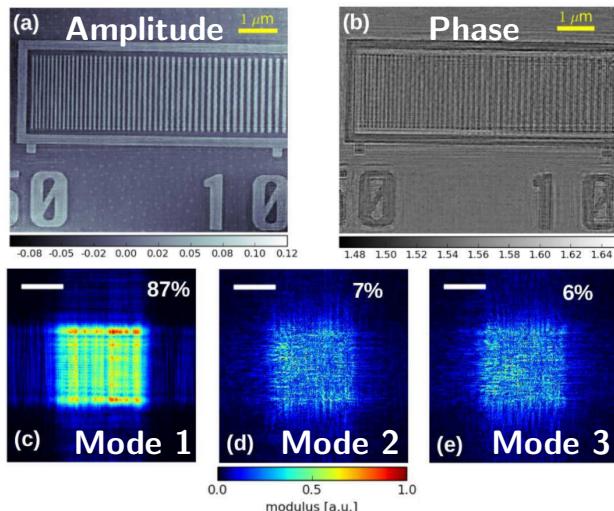
- scanning microscopy
- high resolution
- high sensitivity
- fully quantitative

## Fluorescence

- scanning microscopy
- elemental sensitivity

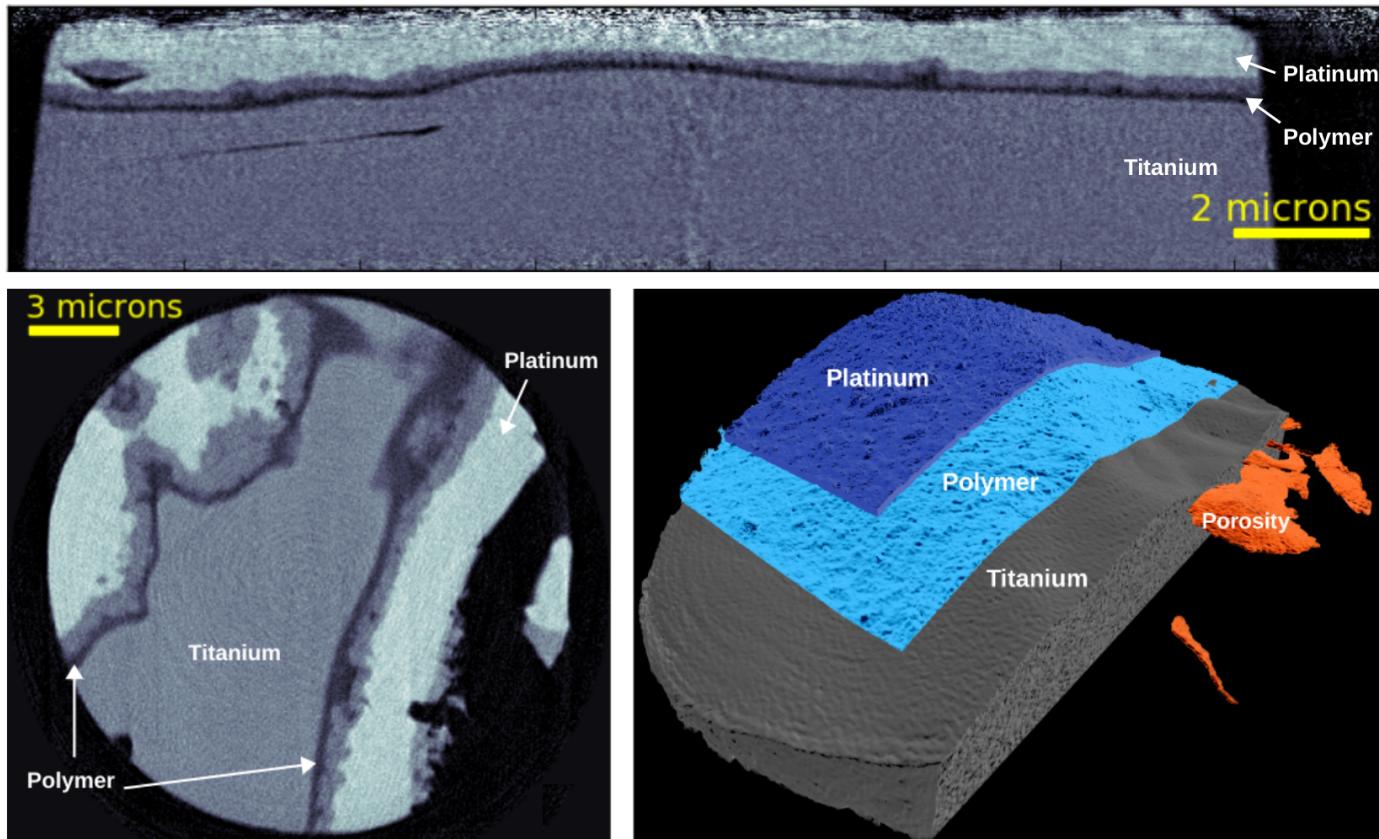


# Smallest ever high energy (33.6 keV) focal spot



J. C. da Silva et al., Optica 4(5), 492-495 (2017).

# PXCT application case: polymer infiltration in metals

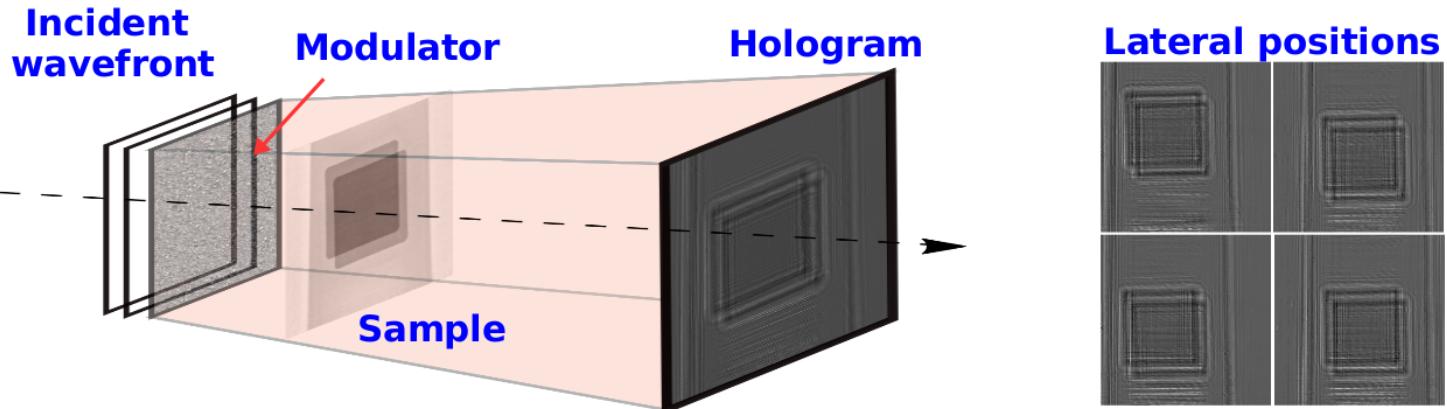


J. Haubrich et al., Applied Surface Science 433, 546-555 (2018).

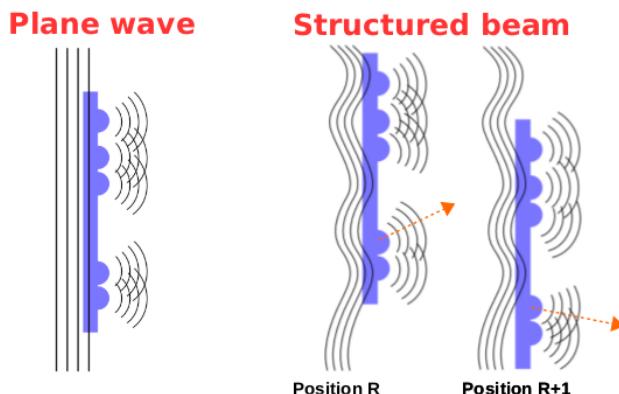
J. C. da Silva et al., Proc. SPIE 10391, 1039106 (2017).

# Near-field ptychography

another way to exploit the transverse diversity



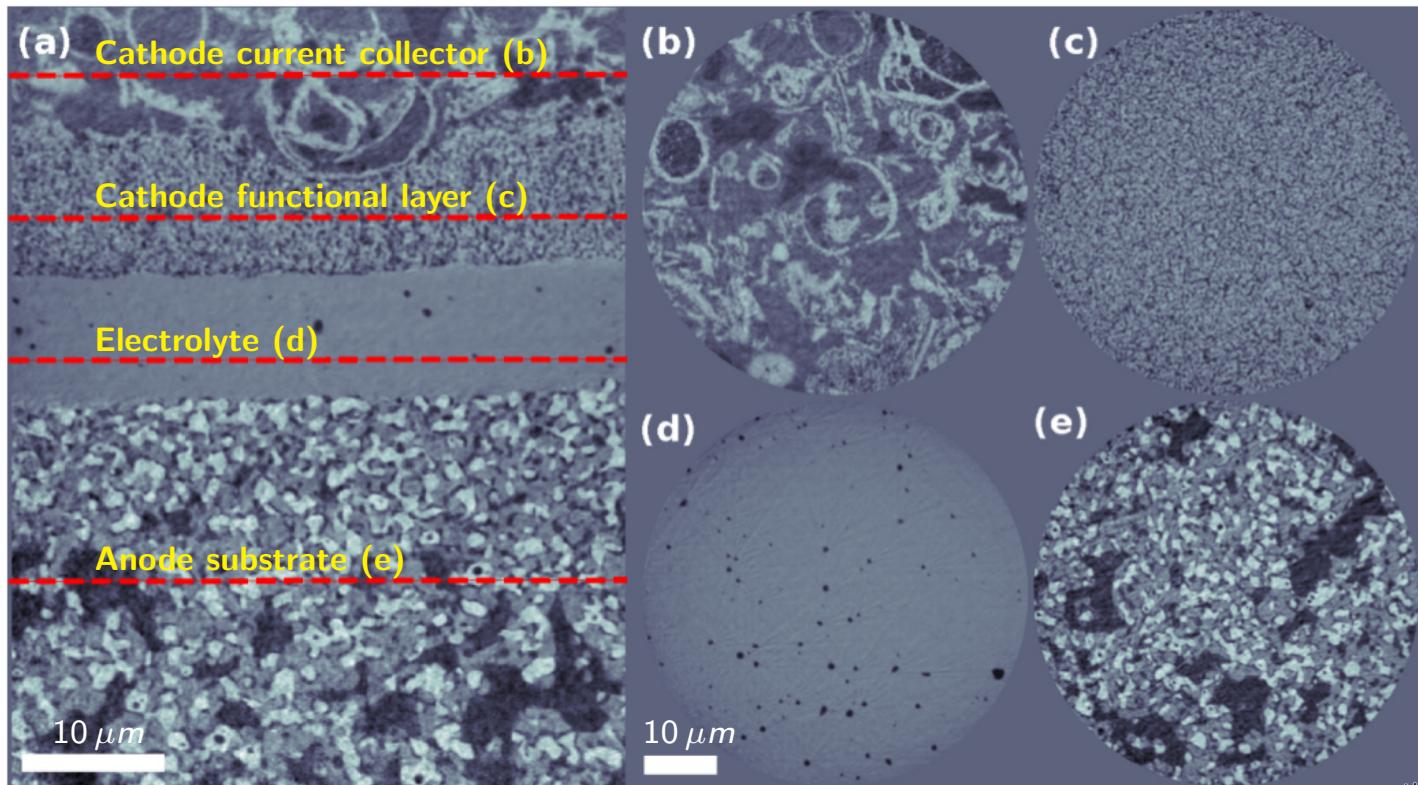
## Transverse diversity



M. Stockmar et al., Sci. Rep. 3, 1927 (2013)

# The different structures of a SOFC

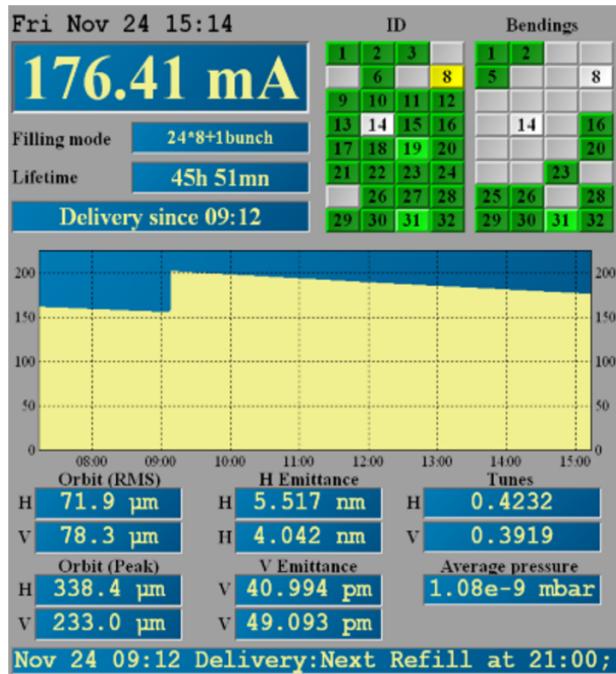
## SOFC: Solid Oxide Fuel Cell



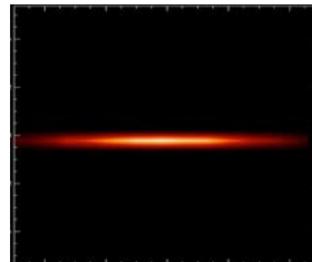
M. Stockmar et al., Opt. Express 23(10), 12720 (2015)



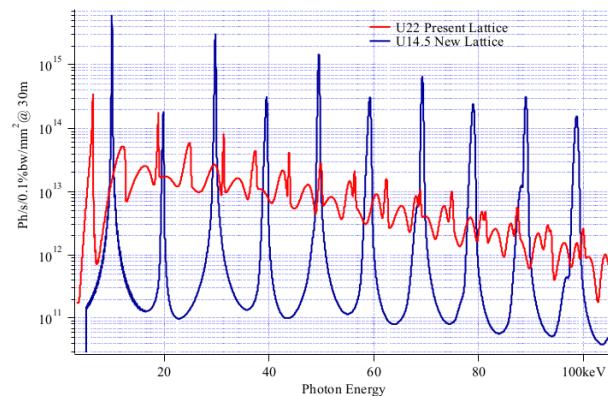
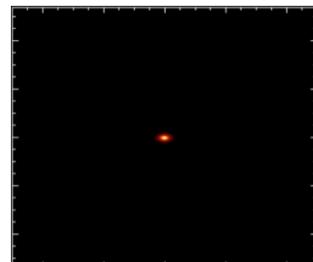
# ESRF - Extremely Brilliant Source (EBS)



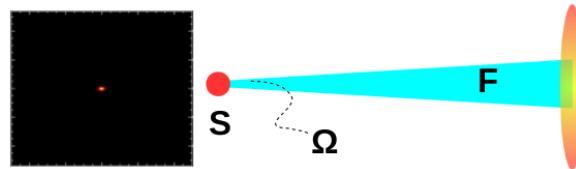
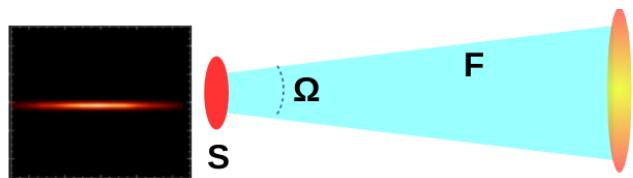
Current source



New source (Expected)

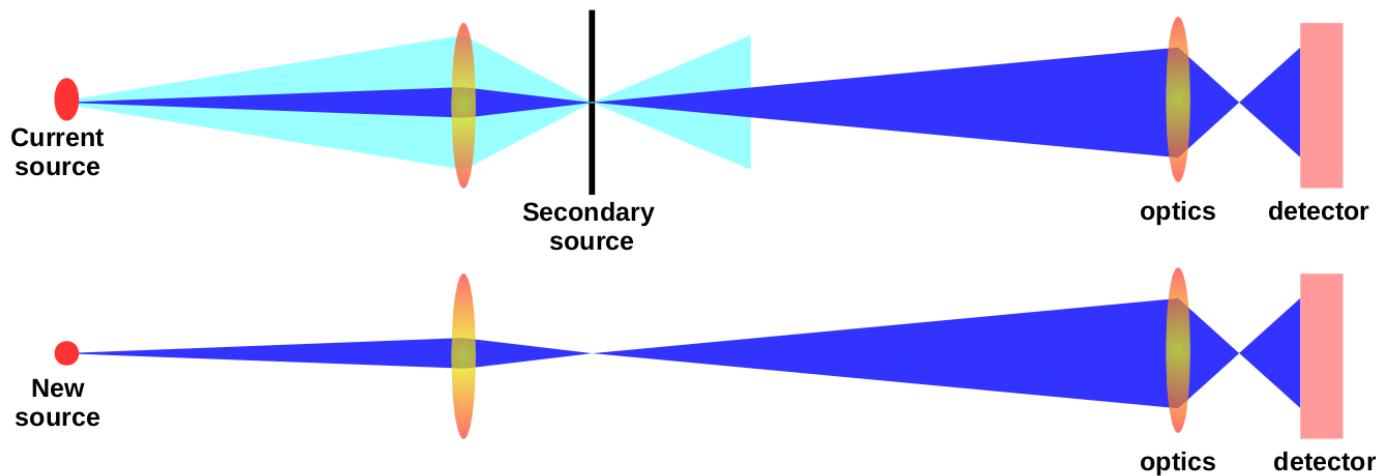


# More brilliance and transverse coherence

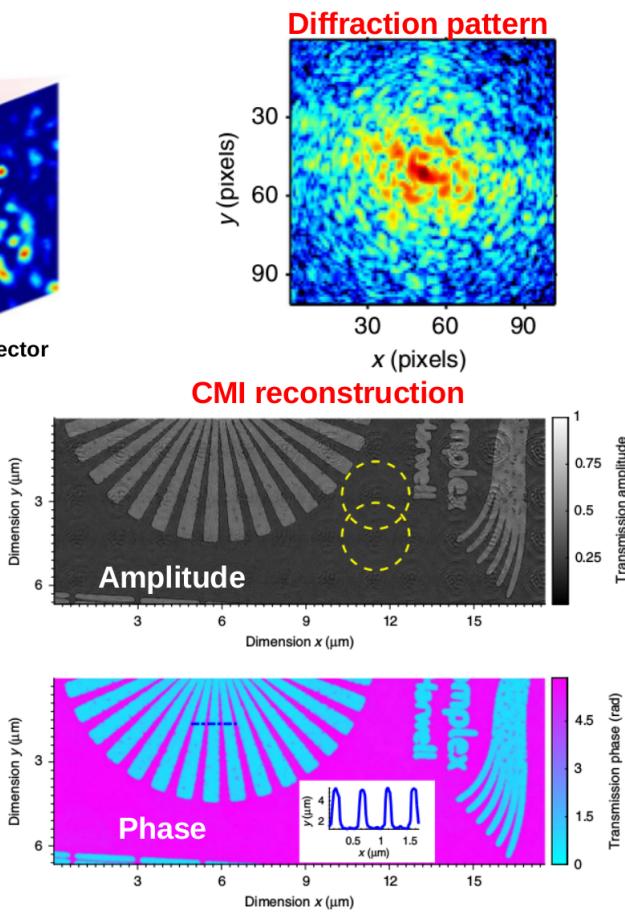
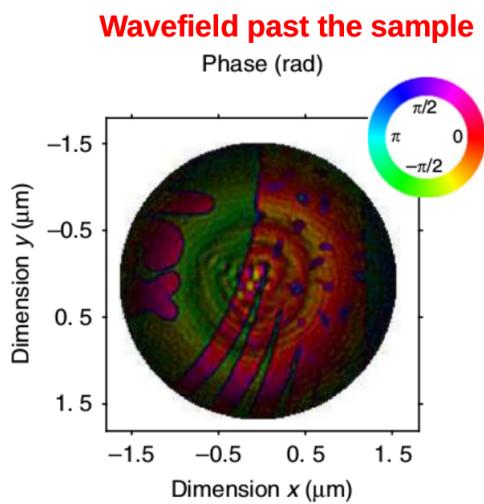
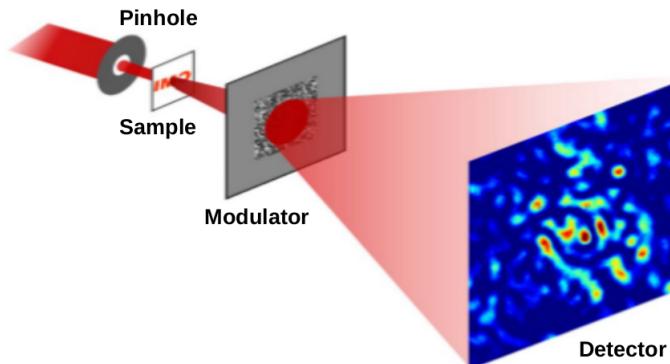


$\Omega$  = angular divergence  
S = source area  
F = Flux

$$\text{Brilliance} = (\text{const.}) \times \frac{F}{S\Omega}$$
$$\text{Emittance} = S\Omega$$



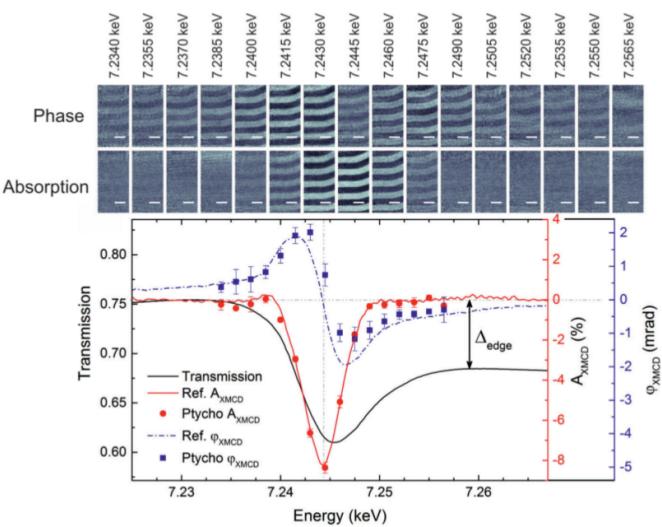
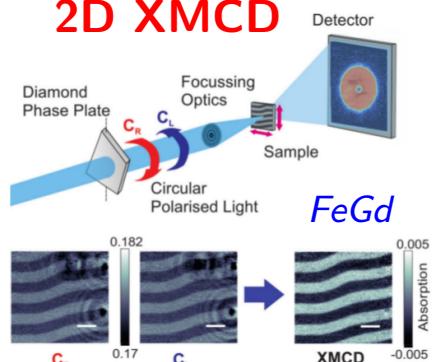
# Innovation I: Coherent X-ray modulation imaging



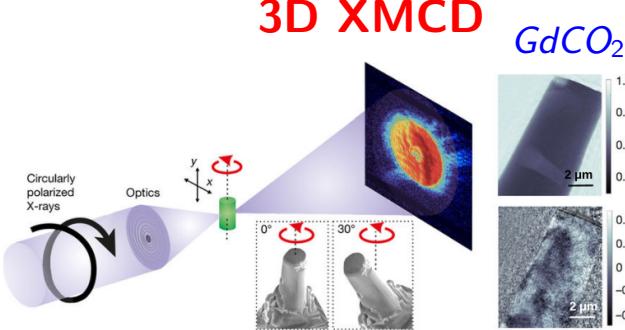
F. Zhang et al., Nature Communications 7, 13367 (2016).

# Innovation II: Magnetic imaging via ptychography

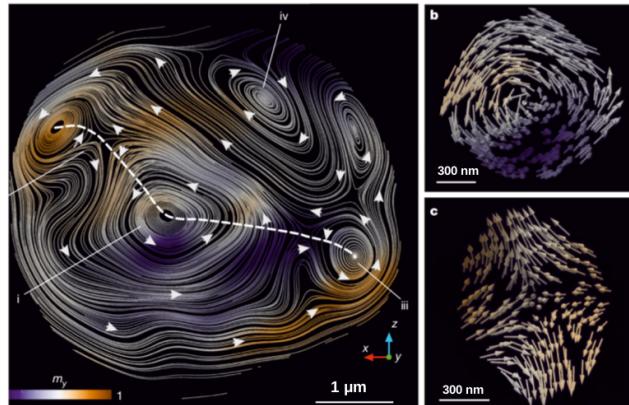
## 2D XMCD



## 3D XMCD



## Reconstructed magnetization vector field



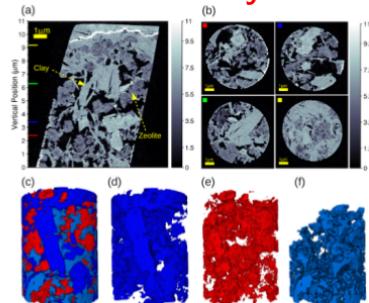
C. Donnelly et al., Nature 547, 328-331 (2017)

C. Donnelly et al., Phys. Rev. B 94, 064421 (2016)

# Ptychography is already an established imaging technique

## Some Application Cases of X-ray ptychography

### FCC catalyst



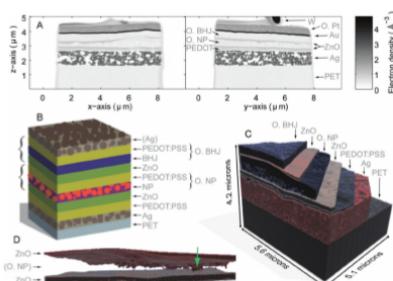
J. C. da Silva et al.,  
*ChemCatChem* 7 (2015) 413.

### Cement hydration



J. C. da Silva et al.,  
*Langmuir* 31 (2015) 3779.

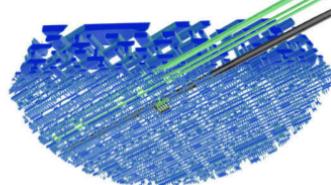
### Tandem solar cells



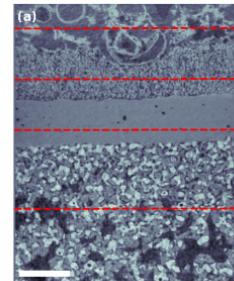
E. B. L. Pedersen et al.,  
*Nanoscale* 7 (2015) 13765.

### Microelectronics

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

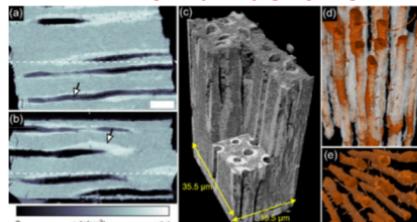


### SOFC



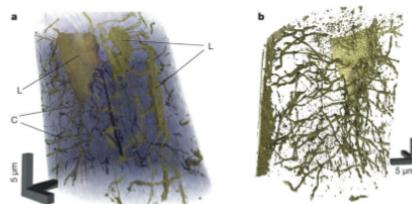
M. Stockmar et al.,  
*Opt. Express* 23 (2015) 12720.

### Human dentine



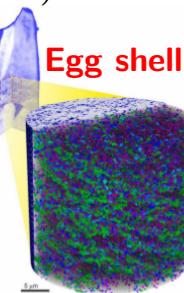
I. Zanette et al.,  
*Sci. Rep.* 5 (2015) 9210.

### Bones



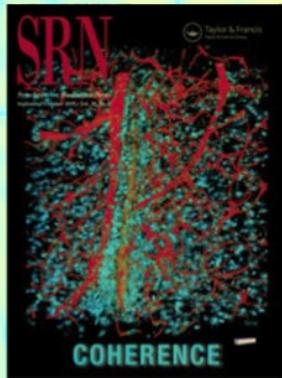
M. Dierolf et al.,  
*Nature* 467 (2010) 436.

### Egg shell



M. Guizar-Sicairos et al.,  
*Optica* 2 (2015) 259.

# Thank you for your attention!



Dynamics and Imaging Using Coherent X-rays at  
the European Synchrotron

V. Favre-Nicolin, Y. Chushkin, P. Cloetens, J. C. da Silva, S. Leake, B. Ruta & F. Zontone

Synchrotron Radiation News 30(5), 13-18 (2017).

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**Thank you for your  
attention!**