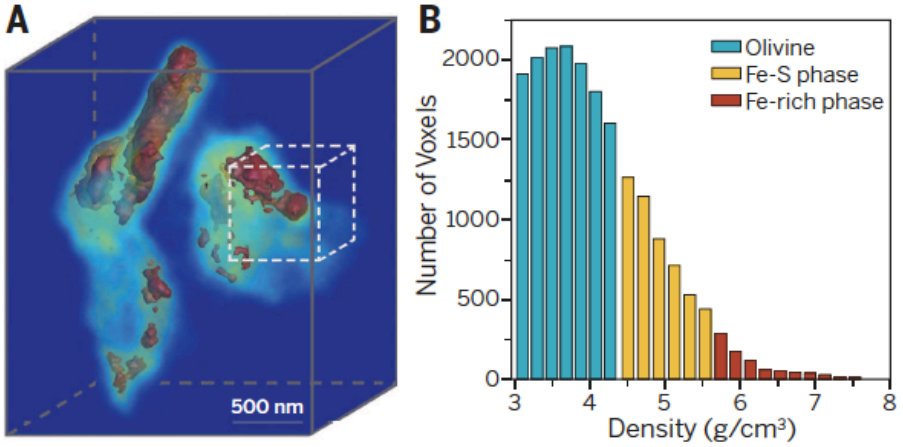
Coherent diffraction imaging at synchrotron sources

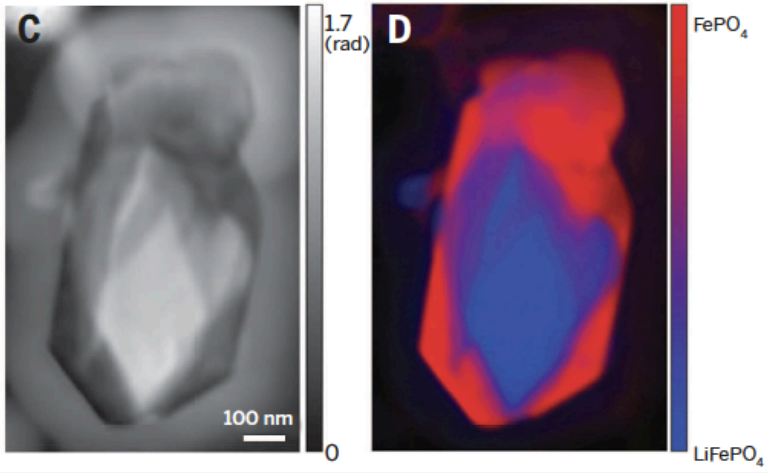
V. Chamard
Institut Fresnel, Marseille France

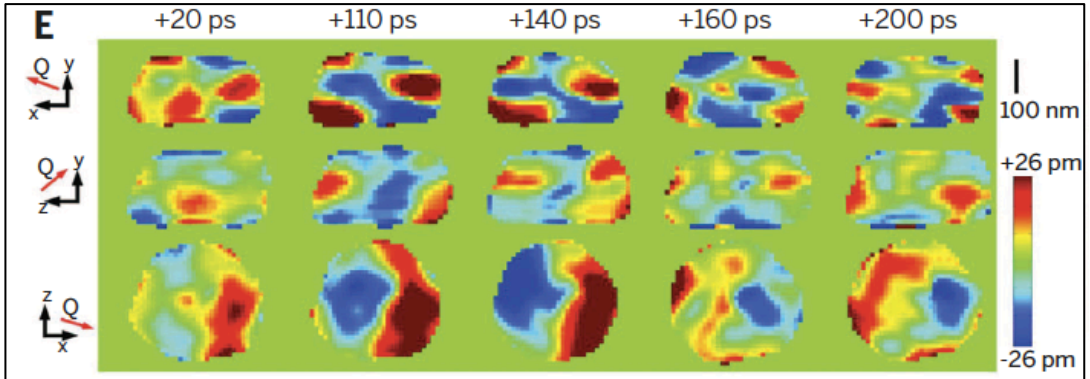
Before we start, what are we talking about?

3D Highly-resolved chemical identification



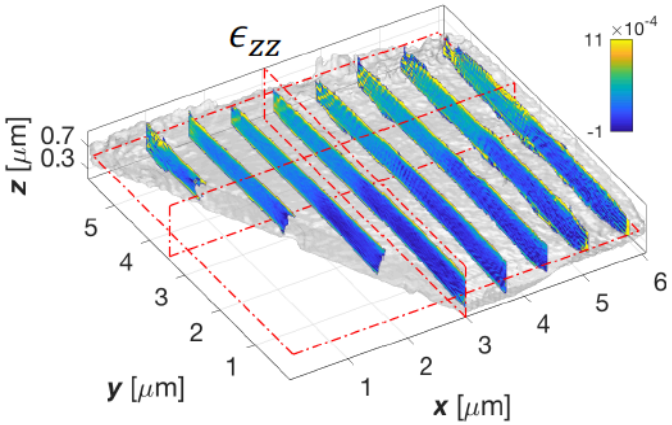
Highly-resolved spectroscopy microscopy





Crystalline lattice dynamics under external stimulus

Miao et al., Science 348 (2015)



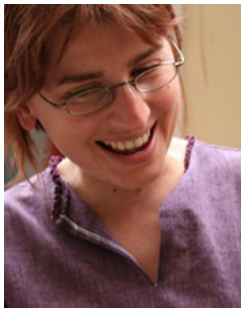
Highly sensitive 3D strain map

Li *et al.*, Nature Commun. (2021)

→ *3D quantitative imaging at 10-100 nm resolution*

The COMiX team at Institut Fresnel

Coherent Optical Microscopy and X-rays



V. Chamard
Coherent X-ray microscopy

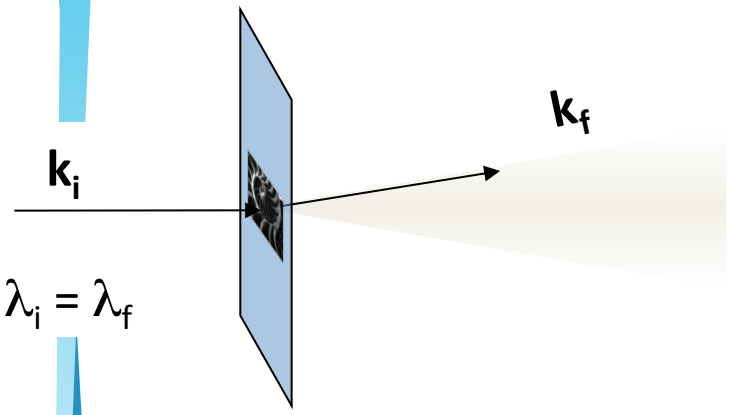
M. Allain
Inversion problems

P. Ferrand
Optical

T. Grünewald
Incoherent x-ray microscopy

→ Development of coherent-diffraction based microscopy methods with x-rays and optics

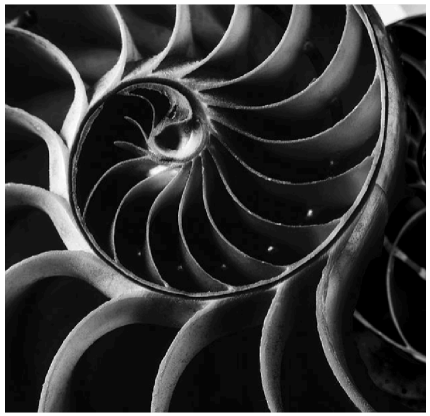
An ideal microscopy set-up



Resolution = $\lambda/2NA$

λ: illumination wavelength
NA: numerical aperture

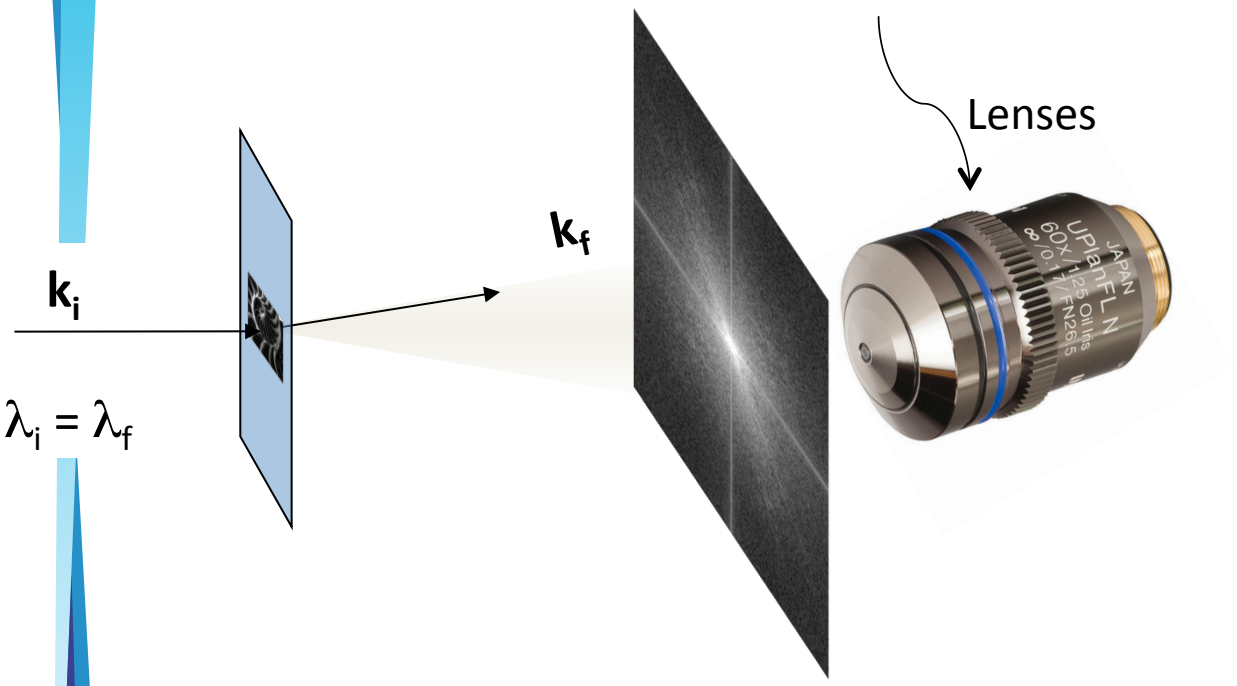
Magnified image



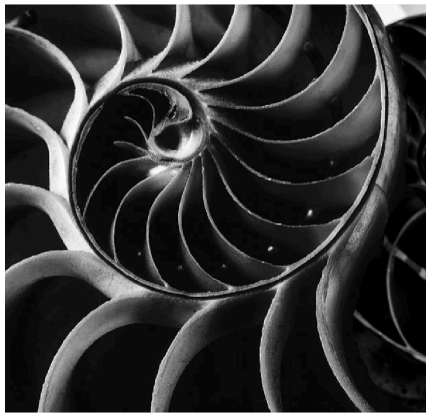
An ideal microscopy set-up

Resolution = $\lambda/2NA$

λ: illumination wavelength
NA: numerical aperture



Magnified image



How to improve the resolution?

- NA ≈ 1
  → Optical microscopy
- Decrease λ
  → X-ray microscopy (λ = 0.1 - 1 nm)

Why x-ray microscopy?

- Decrease λ
  → X-ray microscopy (λ = 0.1 - 1 nm)

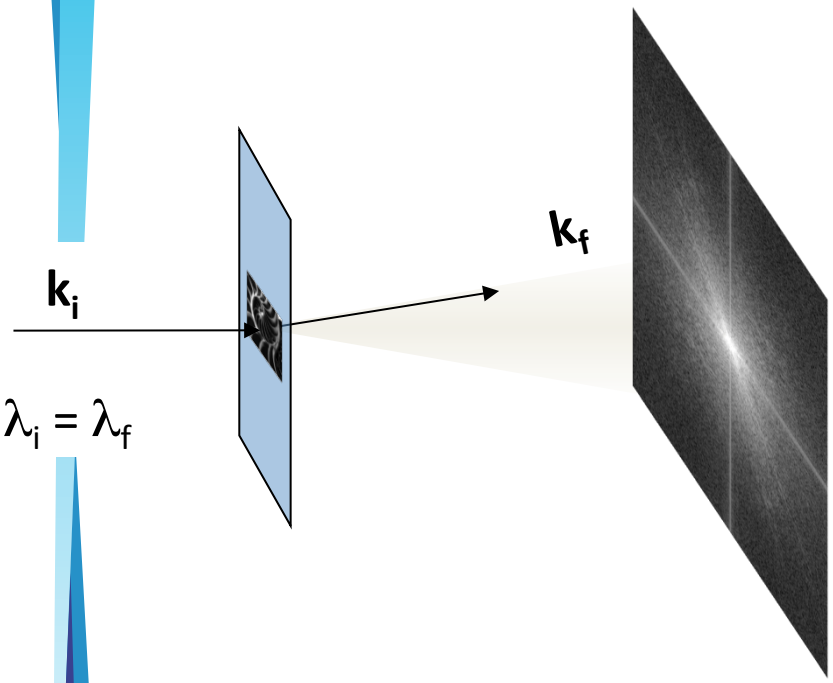
- Weak interaction with matter
  → Bulky sample
  → Complex sample environment

- Label-free chemical sensitivity

X-ray microscopy!?

Resolution = $\lambda/2NA$

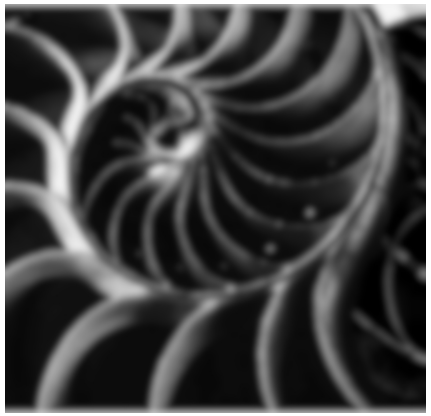
λ: illumination wavelength
NA: numerical aperture



X-ray lens

$NA \approx 10^{-2} - 10^{-3}$

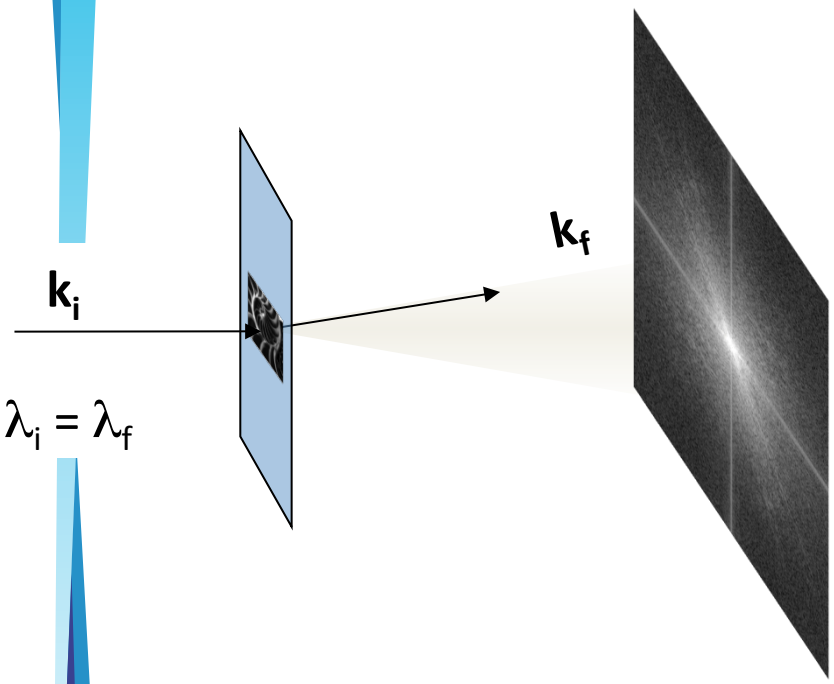
Blurred image



X-ray microscopy!?

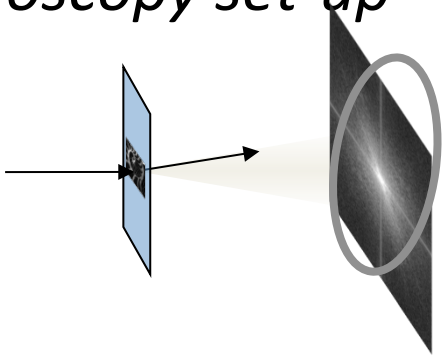
Resolution = $\lambda/2NA$

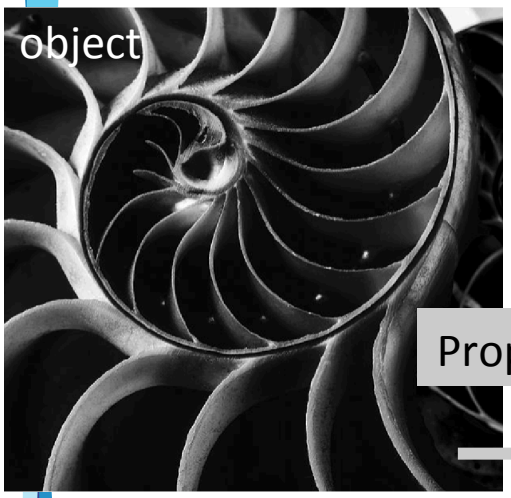
λ: illumination wavelength
NA: numerical aperture



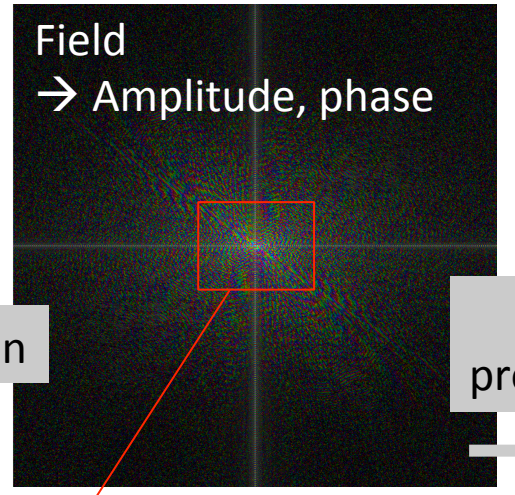
→ Can we deal with the information collected in the diffraction plane?

A lens-less microscopy set-up

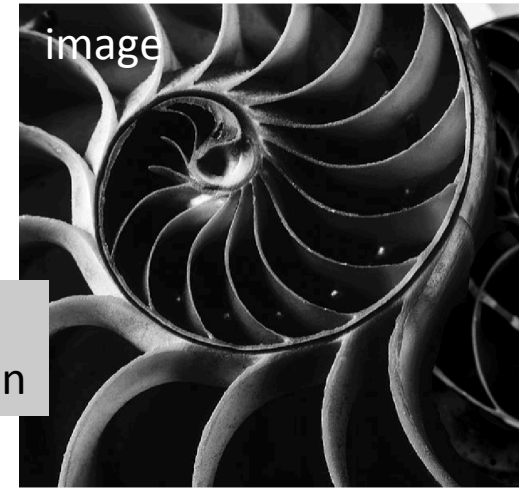


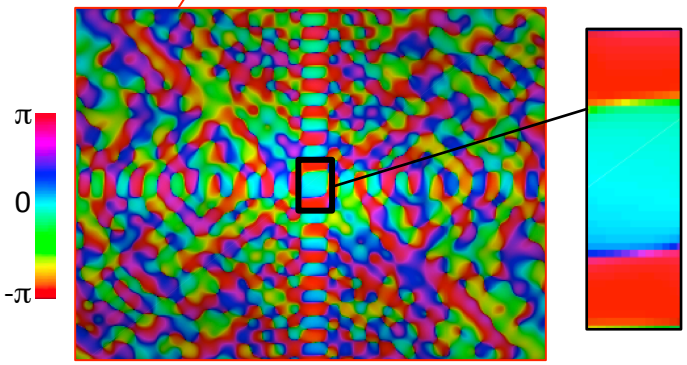


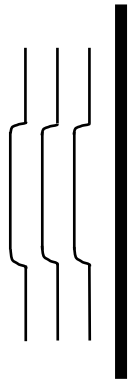
Propagation



Back propagation



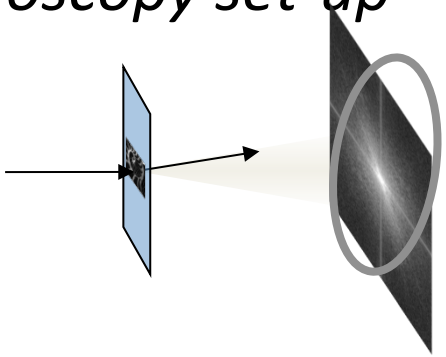


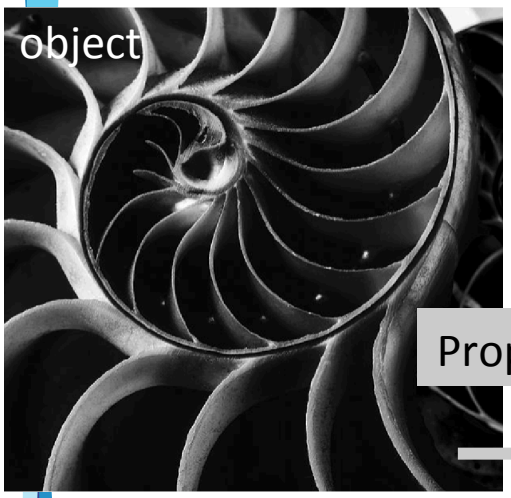


Detector plane

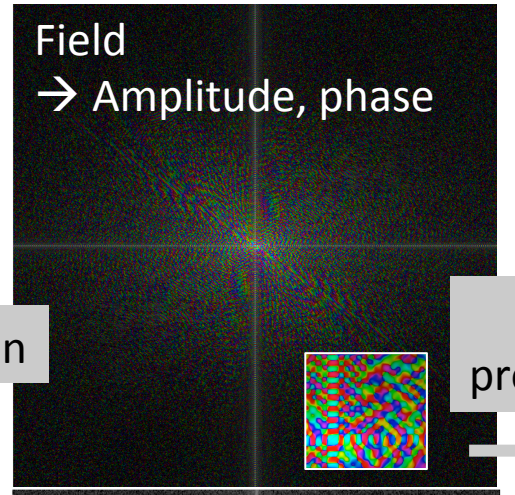
Phase: some parts of the wave field are ‘delayed’
→ *not in phase*

A lens-less microscopy set-up

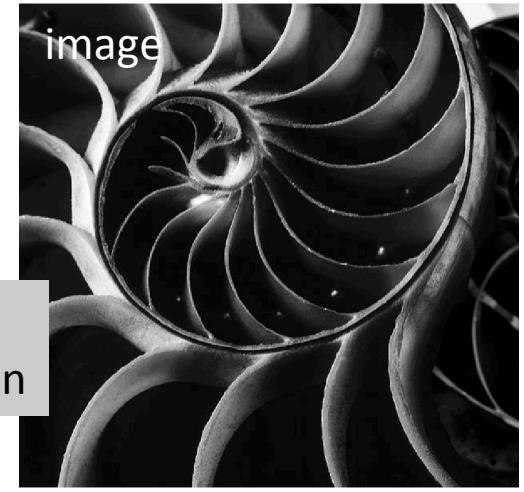




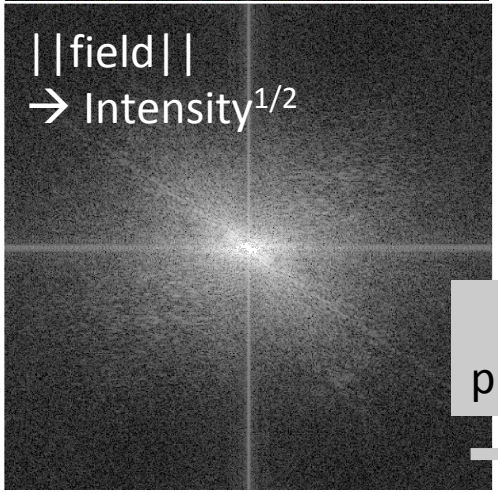
Propagation



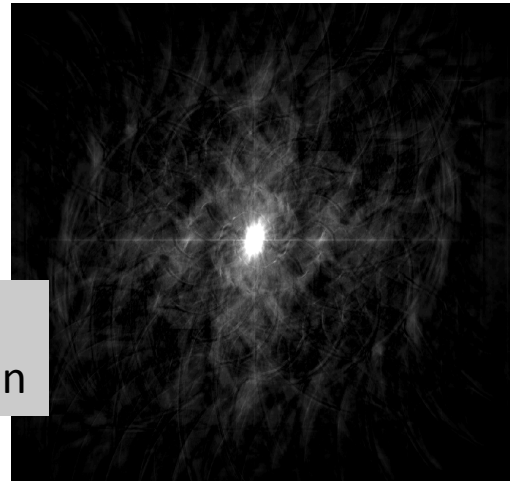
Back propagation



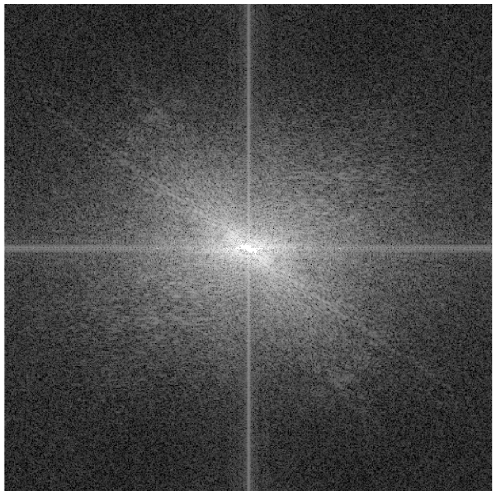
- Lost phase



Back propagation

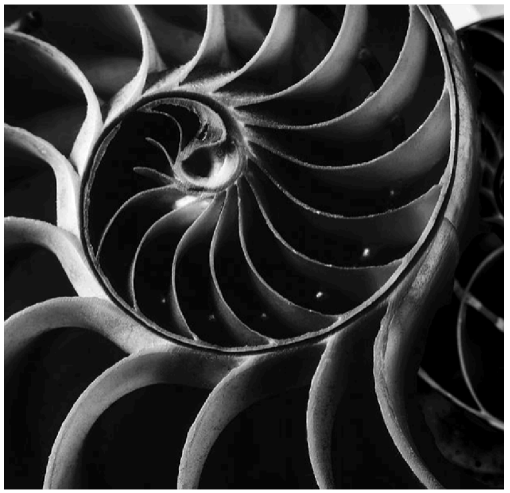


Solving the phase problem: strategies



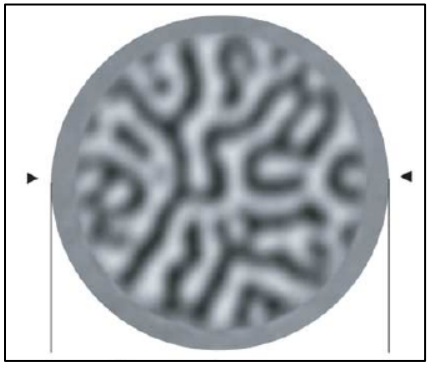
Inverse problem

with intensity data



Experimental set-up

- Encode phases into a ***known*** reference
  → Holography



Eisebitt *et al.*, Nature (2004)

Sample information

- Add ***known*** constraint

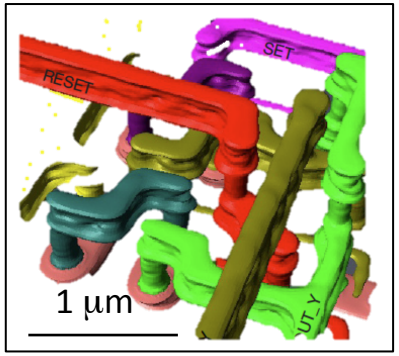
→ **Finite support CDI**

Chapman *et al.* (2006). J. Opt. Soc. Am. A, **23**, 1179–1200.

Exploit the probe

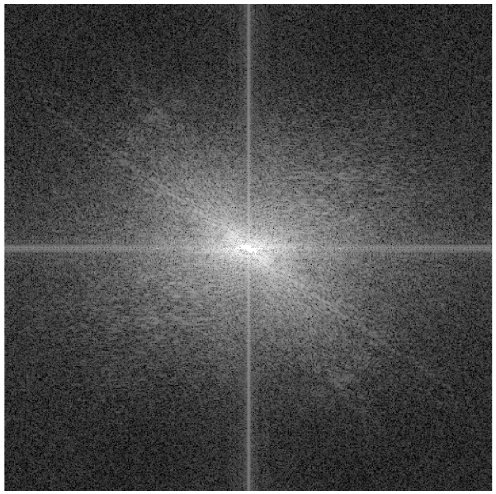
- **Divide the problem into simpler sub-problems with partial *redundancy***

→ **Ptychography**



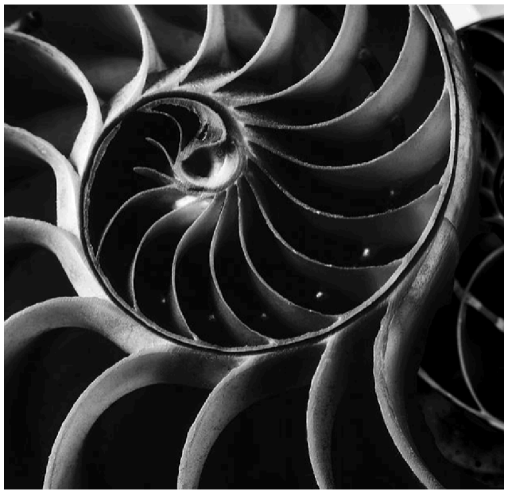
Holler *et al.*, Nature (2017)

Solving the phase problem: strategies



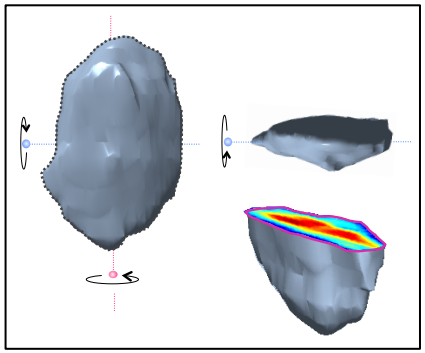
Inverse problem

with intensity data



Experimental set-up

- Encode phases into a ***known*** reference
  → Holography

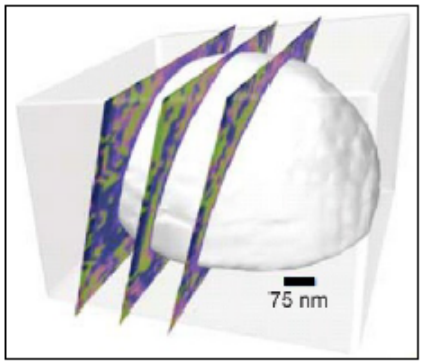


Chamard *et al.*,
Phys. Rev. Lett. (2010)

Sample information

- Add ***known*** constraint

→ **Finite support CDI**

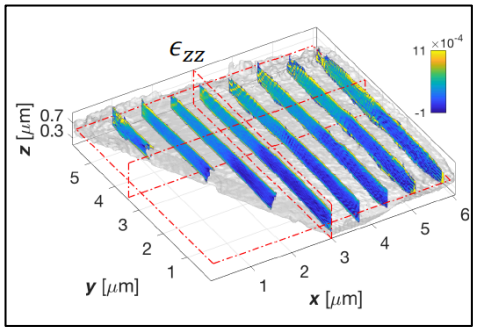


Pfeifer *et al.* (2006).
Nature, **442**, 63–66.

Exploit the probe

- **Divide the problem into simpler sub-problems with partial *redundancy***

→ **Ptychography**



Li *et al.*, Nature Commun. (2021)

I − Solving the phase problem from diffraction intensity information

II − Coherent diffraction imaging modalities

III − Biomineralization & coherent diffraction imaging

I – Solving the phase problem from diffraction intensity information

Finite support coherent diffraction imaging

It all started with this article

Acta Cryst. (1952). **5**, 843

Some implications of a theorem due to Shannon.

By D. Sayre, *Johnson Foundation for Medical Physics, University of Pennsylvania, Philadelphia* 4, *Pennsylvania, U. S. A.*

(*Received* 3 *July* 1952)

Shannon (1949), in the field of communication theory, has given the following theorem: If a function $d(x)$ is known to vanish outside the points $x = \pm a/2$, then its Fourier transform $F(X)$ is completely specified by the values which it assumes at the points $X = 0, \pm 1/a, \pm 2/a, \ldots$. In fact, the continuous $F(X)$ may be filled in merely by laying down the function $\sin \pi aX/\pi aX$ at each of the above points, with weight equal to the value of $F(X)$ at that point, and adding.

Now the electron-density function $d(x)$ describing a single unit cell of a crystal vanishes outside the points $x = \pm a/2$, where a is the length of the cell. The reciprocal-lattice points are at $X = 0, \pm 1/a, \pm 2/a, \ldots$, and hence the experimentally observable values of $F(X)$ would suffice, by the theorem, to determine $F(X)$ everywhere, if the phases were known. (In principle, the necessary points extend indefinitely in reciprocal space, but by using, say, Gaussian atoms both $d(x)$ and $F(X)$ can be effectively confined to the unit cell and the observable region, respectively.)

For centrosymmetrical structures, to be able to fill in the $|F|^2$ function would suffice to yield the structure, for sign changes could occur only at the points where $|F|^2$ vanishes. The structure corresponding to the $|F|^2$ function is the Patterson of a single unit cell. This has twice the width of the unit cell, and hence to fill in the $|F|^2$ function would require knowledge of $|F|^2$ at the half-integral, as well as the integral h's. This is equivalent to a statement made by Gay (1951).

I think the conclusions which may be stated at this point are:

1. Direct structure determination, for centrosymmetric structures, could be accomplished as well by finding the sizes of the $|F|^2$ at half-integral h as by the usual procedure of finding the signs of the F's at integral h.

2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where $|F|^2$ was observed at non-integral h, it would suffice to have only the values at half-integral h.

The extension to three dimensions is obvious.

References

Boyes-Watson, J., Davidson, E. & Perutz, M. F. (1947). *Proc. Roy. Soc.* A, **191**, 83.

Gay, R. (1951). Paper presented at the Second International Congress of Crystallography, Stockholm.

Shannon, C. E. (1949). *Proc. Inst. Radio Engrs., N.Y.* **37**, 10.

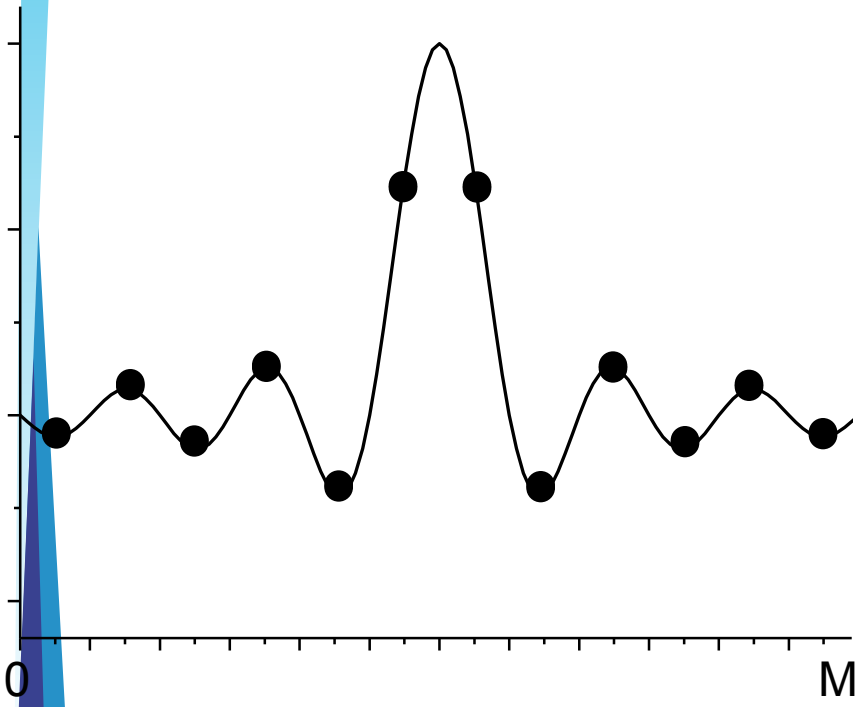
→ The solution to the phase problem!

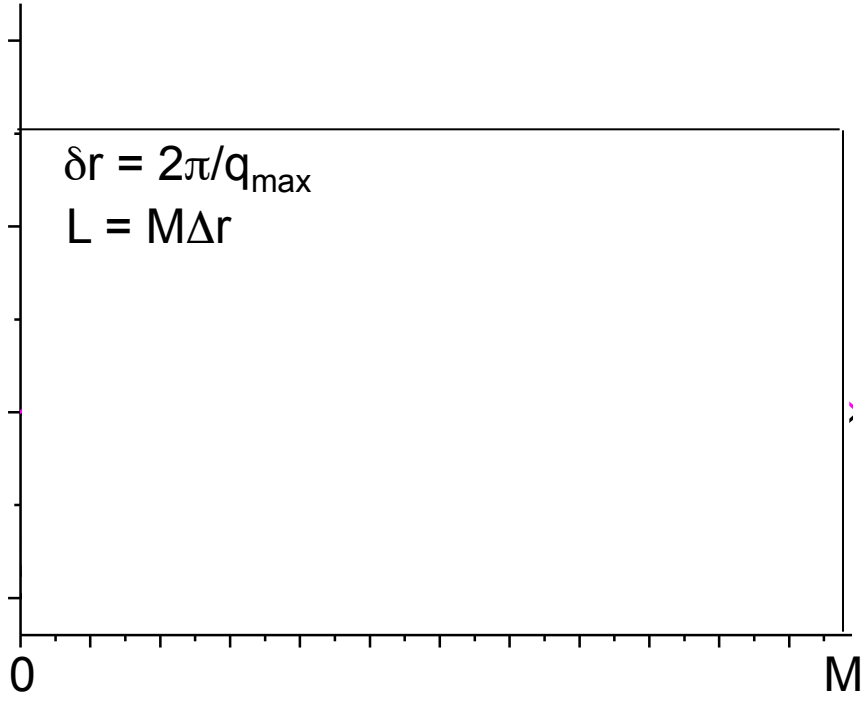
Possibility of phase retrieval

- Shannon theorem + oversampling (2 × Nyquist frequency)

$$\rho(r) = FT^{-1}[\, |A(q)| \exp^{i\varphi(q)} \,]$$

experimentally → $I(q) = |A(q)|^2$





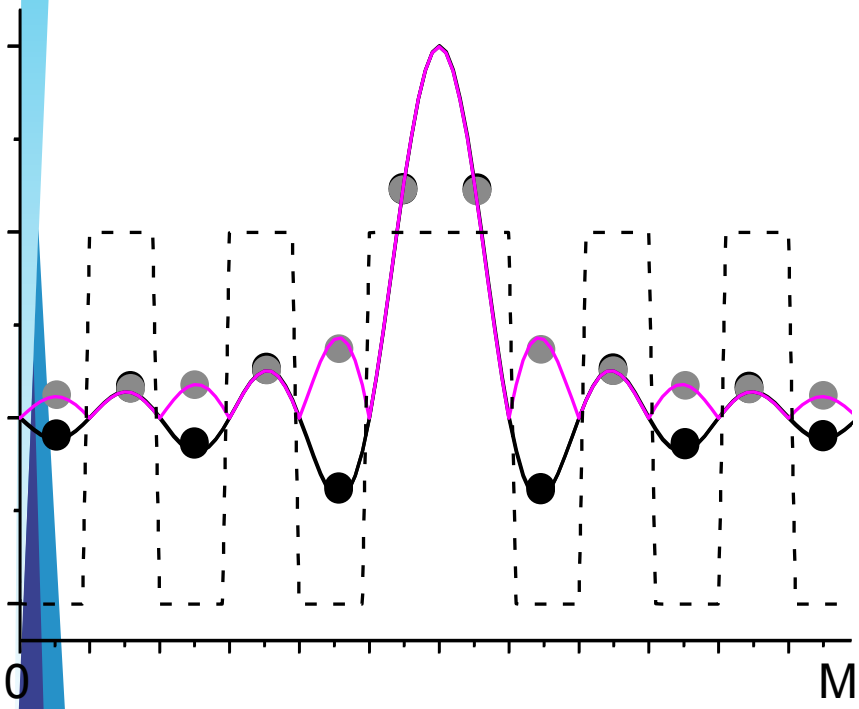
Possibility of phase retrieval

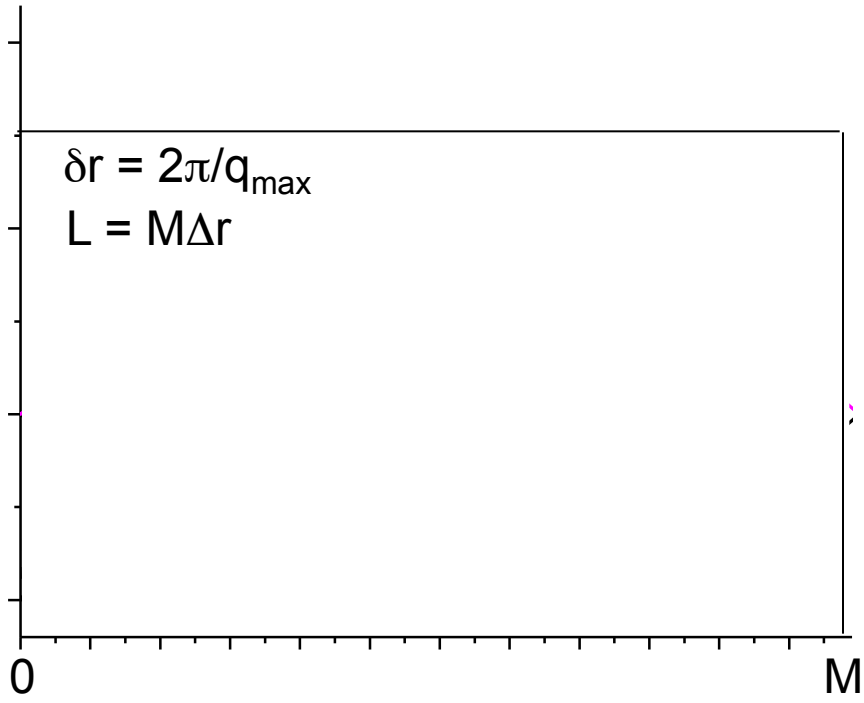
- Shannon theorem + oversampling (2 × Nyquist frequency)

$$\rho(r) = FT^{-1}[\, |A(q)| \exp^{i\varphi(q)} \,]$$

experimentally → $I(q) = |A(q)|^2$

- the phase information is lost





Possibility of phase retrieval

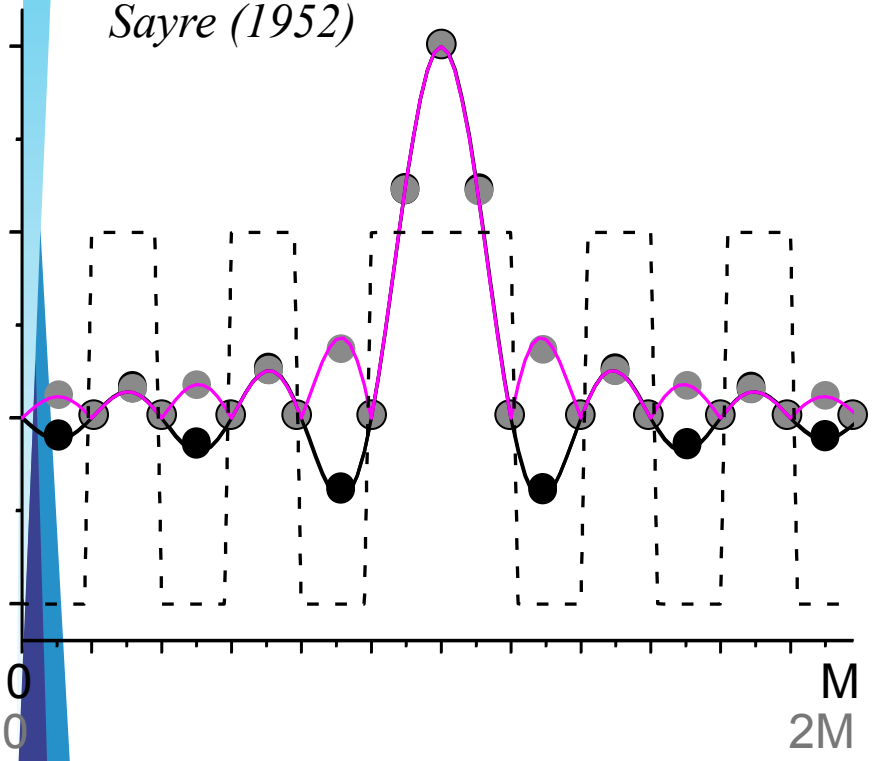
- Shannon theorem + oversampling (2 × Nyquist frequency)

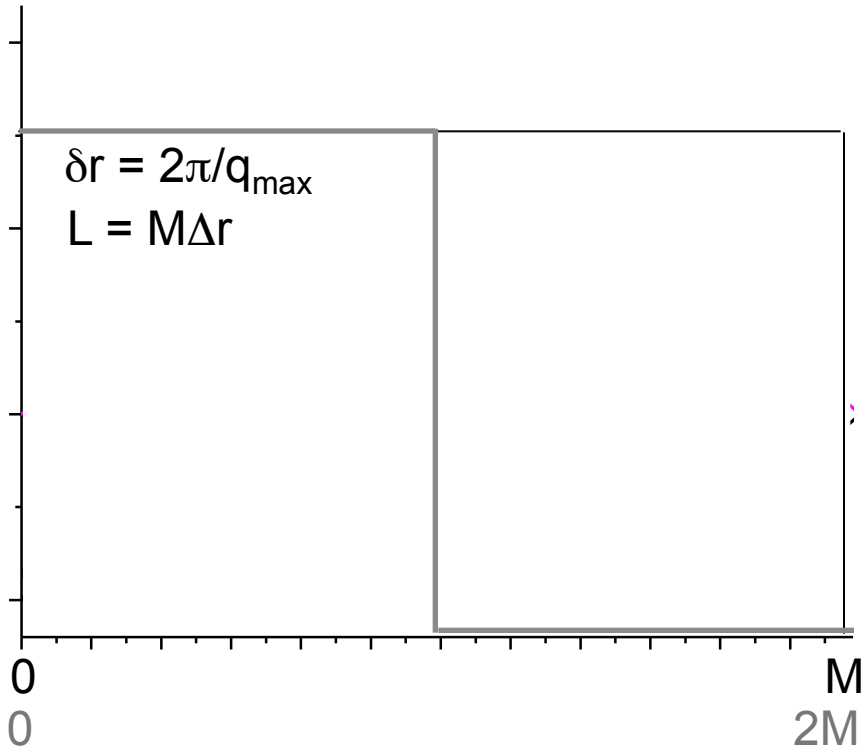
$$\rho(r) = FT^{-1}[\ |A(q)|\ \exp^{i\varphi(q)}\ ]$$

experimentally → $I(q) = |A(q)|^2$

- the phase information is lost
- \+ Oversampling: a solution can be found (in principle !) → zero padding the sample

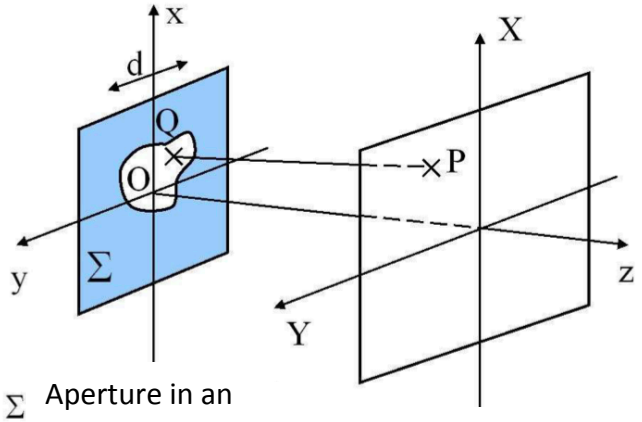
Sayre (1952)





→ Fourier transform?

The diffraction plane (Fraunhoffer formalism)



Σ Aperture in an opaque screen

Observation plane

Sum of spherical waves emitted by the aperture

$$\psi(P) = \int_{\Sigma} K\psi_i(Q)\frac{e^{ikQP}}{QP}dxdy$$

with the incident plane wave:

$$\psi_i(Q) \propto \exp(i\vec{k_i}.\vec{OQ})$$

→ Plane wave? (coherent beam)

Paraxial approximation

$$1/QP \sim 1/z$$

$$QP = z[1 + \frac{(X-x)^2 + (Y-y)^2}{z^2}]^{1/2} \sim z + \frac{(X-x)^2 + (Y-y)^2}{2z}$$

Fraunhoffer conditions

$$d^2 << \lambda.z$$

$$\psi(\vec{k}) \propto \int_{\Sigma} T(x,y).\exp(-i(\vec{k} - \vec{k_i}).\vec{OQ})dxdy$$

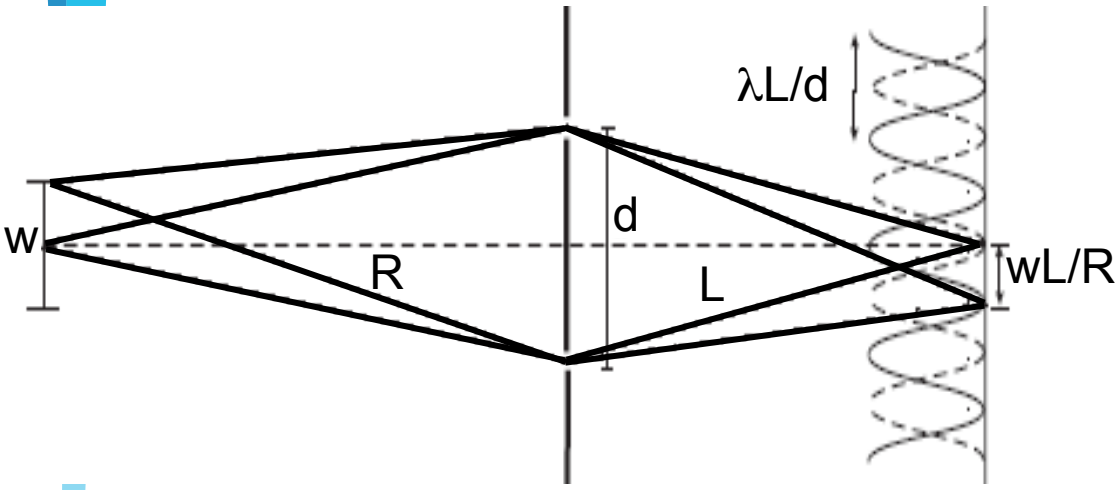
→ **Fourier transform** of the aperture transmission function

L3 lecture from O. Jacquin, Grenoble-Alpes Univ.

Coherence volume: $\xi_{//}\xi_{\perp}^{2}$

See V. Jacques's talk on friday

- Transverse coherence length: the Young's slits experiment

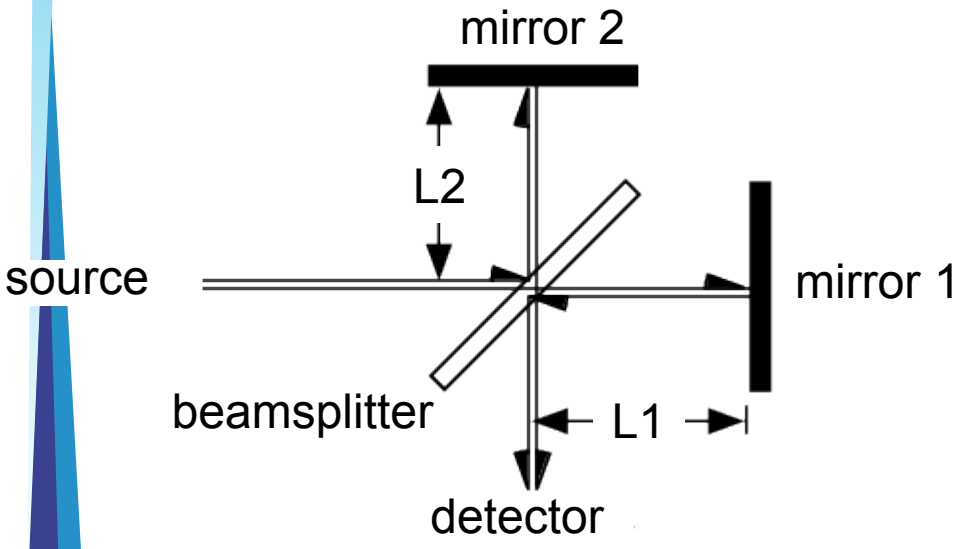


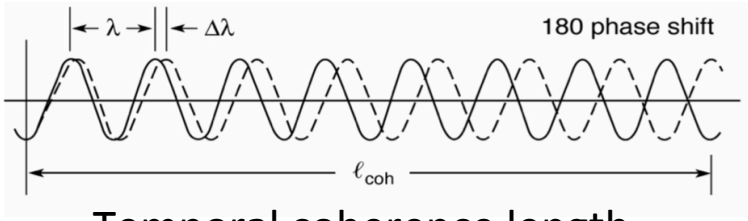
Spatial coherence length

$$\xi_{\perp} = \tfrac{1}{2}\,\lambda R/w$$

λ= 1.5 Å, R ≈ 50 m, w = 100 μm
→ $\xi_{\perp} \approx 40$ μm

- Longitudinal coherence length: the Michelson interferometer





Temporal coherence length

$$\xi_{//} = \tfrac{1}{2}\,\lambda^{2}/\Delta\lambda$$

λ= 1.5 Å, $\Delta\lambda/\lambda \approx 10^{-4}$ (Si (111))
→ $\xi_{//} \approx 1$ μm

F. van der Veen and F. Pfeiffer, J. Phys: Condens. Matter 16 (2004) 5003

Producing a coherent beam from an incoherent source

Most of x-ray sources are incoherent sources

Transverse coherence length

$\xi_{\perp} = ½\ \lambda R/w$

→ Decrease source size w

→ Increase distance to the source R

Longitudinal coherence length

$\xi_{//} = ½\ \lambda^2/\Delta\lambda$

→ Increase energy filtering $\Delta\lambda/\lambda$

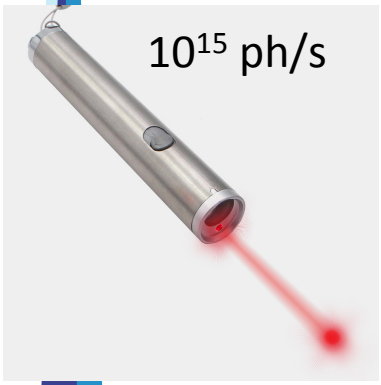
→ Throwing away a lot of photons!

Flux → Brilliance (photons/s/mm^2/mrad^2/0.1%bw)

$F_c = B\ w_h\ w_v\ \Delta\Omega\ \Delta\lambda/\lambda$

with $\Delta\Omega = \xi_h\xi_v/R^2$

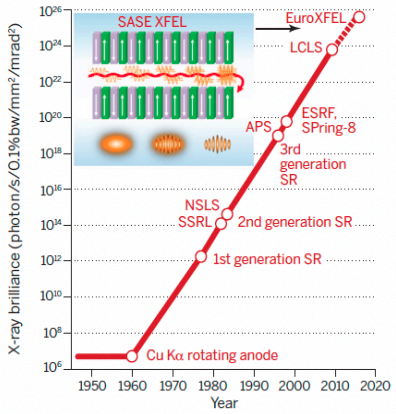
$F_c = B\ \lambda^2\ \Delta\lambda/\lambda$



3rd generation synchrotron

$\Delta\lambda/\lambda = 10^{-4}$, $\lambda = 10^{-10}$ m, $B = 10^{20}$

→ **Fc = 10^{11} ph/s**



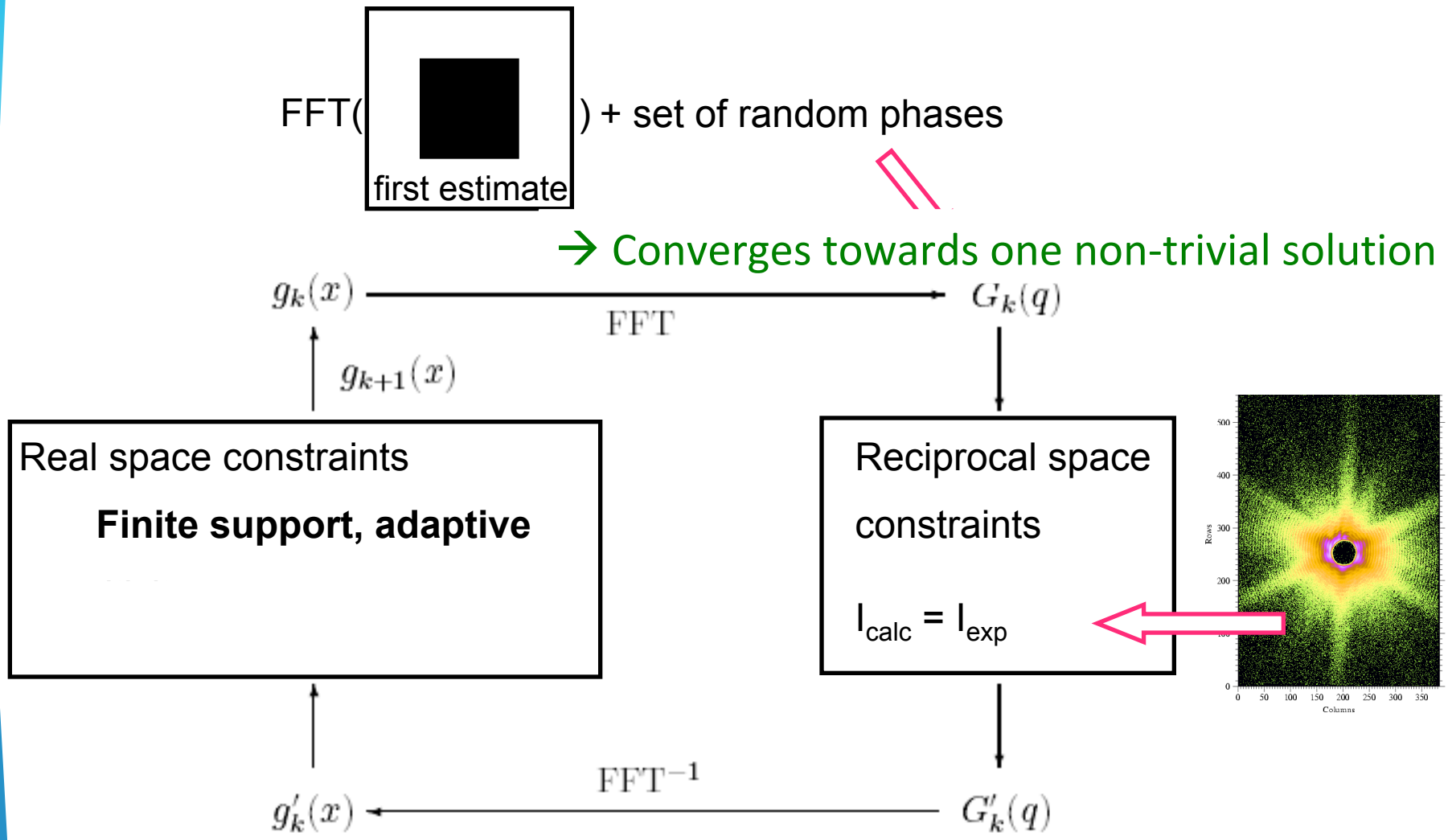
In summary

- Shannon theorem → Phase retrieval is possible from the knowledge of oversampled Fourier components (ie finite size sample)
- Fourier components → Possible in the Fraunhoffer regime, but needs coherent illumination
- Highly brilliant x-ray source → Possibility to extract a coherent beam from an incoherent x-ray source
- *Solutions to the phase problem → Numerical approaches based on high power computing*

II – Coherent diffraction imaging modalities

1 - **CDI** - *Inversion iterative algorithm for isolated particle*

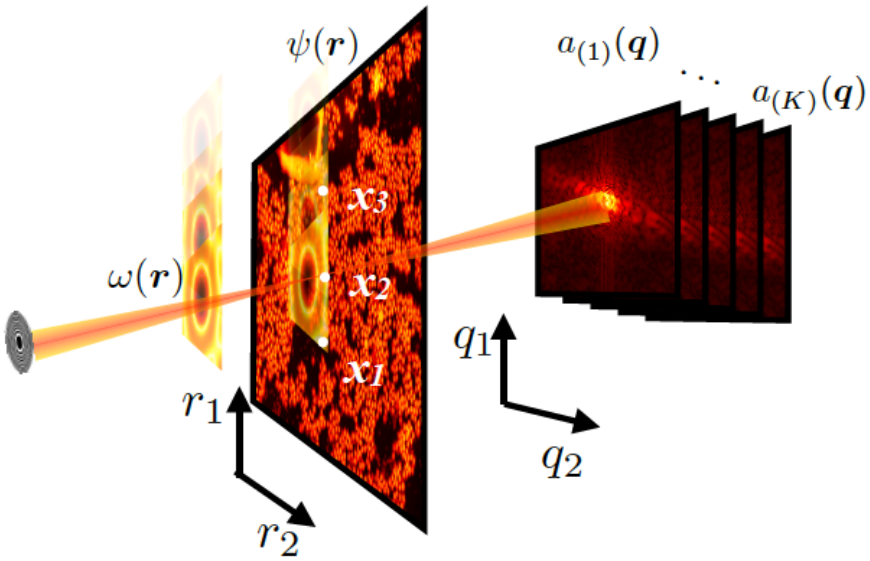
Inversion algorithm : weak scattering regime and far-field detection



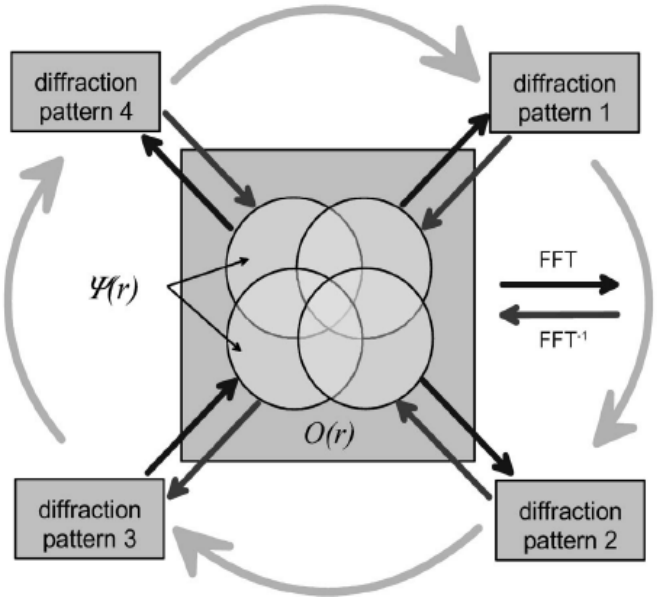
J. R. Fienup, Appl. Opt. ***21****, 2758 (1982),*
R. W. Gerchberg et al., Optik (Stuttgart) ***35****, 237 (1972).*

2 - **Ptychography** - *Inversion algorithm for extended sample*

An alternative to the finite support approach
→ using a scanned 'structured' illumination



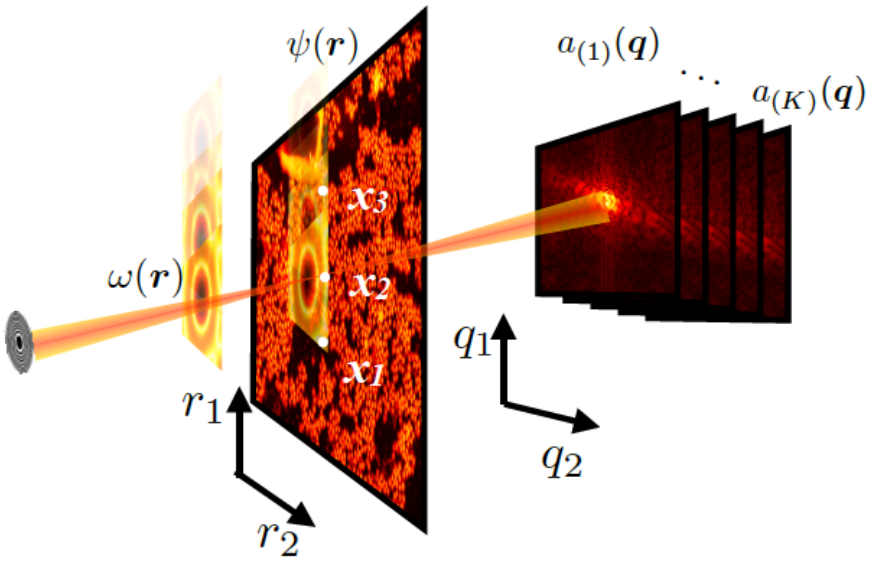
Marchinesi et al.



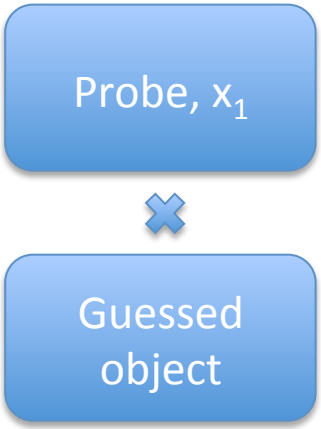
Rodenburg et al., PRL 2007

*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*

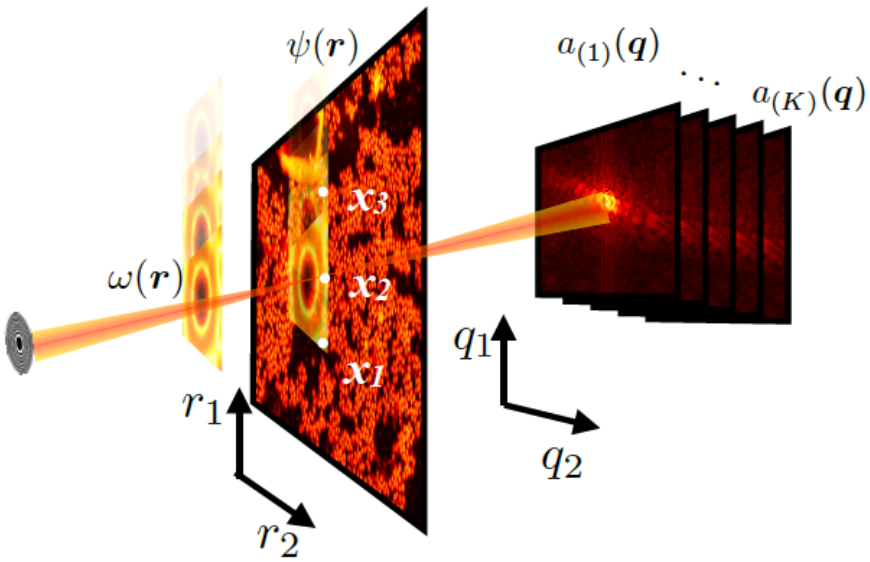


Marchinesi et al.

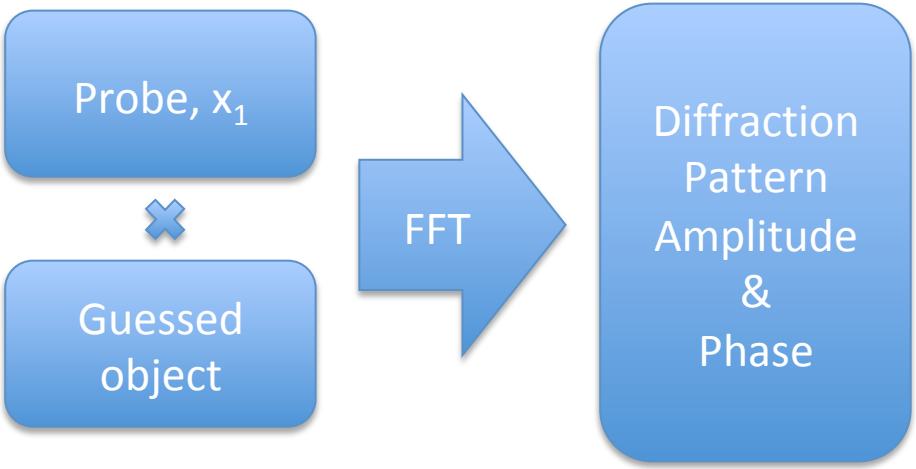


*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*

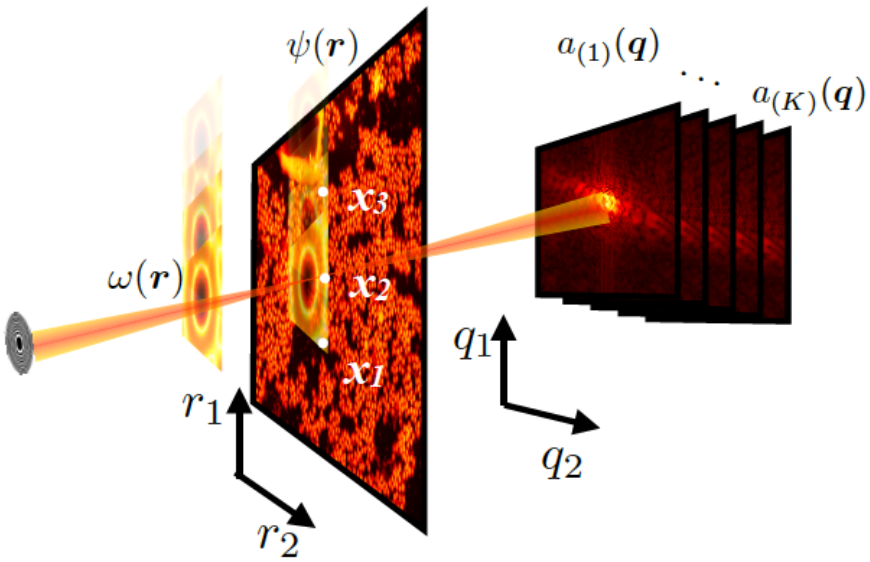


Marchinesi et al.



*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*



Marchinesi et al.

Probe, x_1

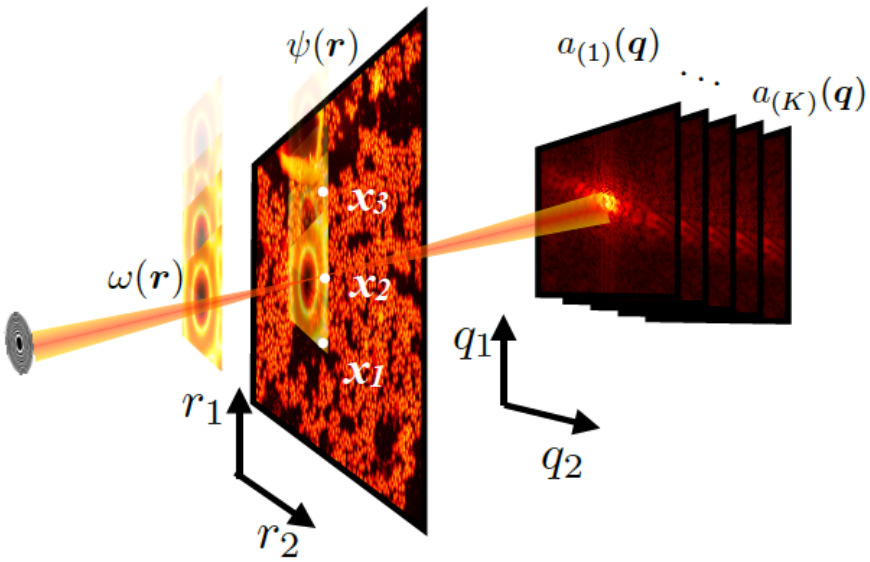
✖

Guessed object

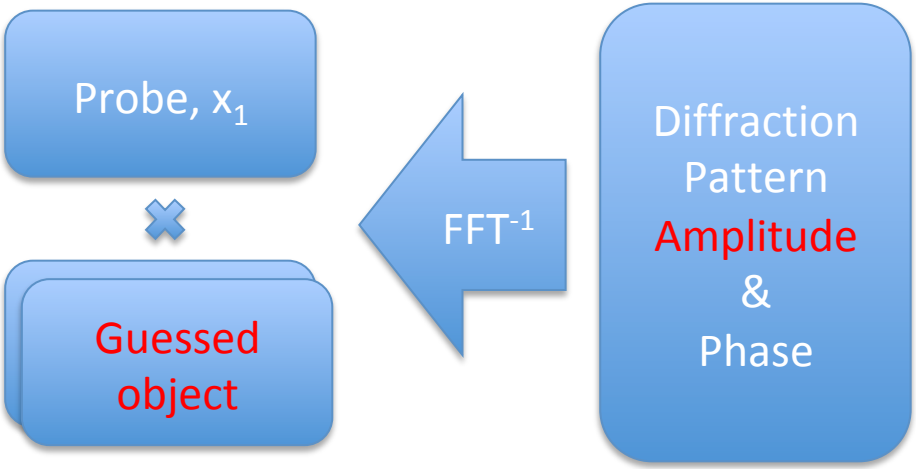
Diffraction Pattern
Amplitude
&
Phase

*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*



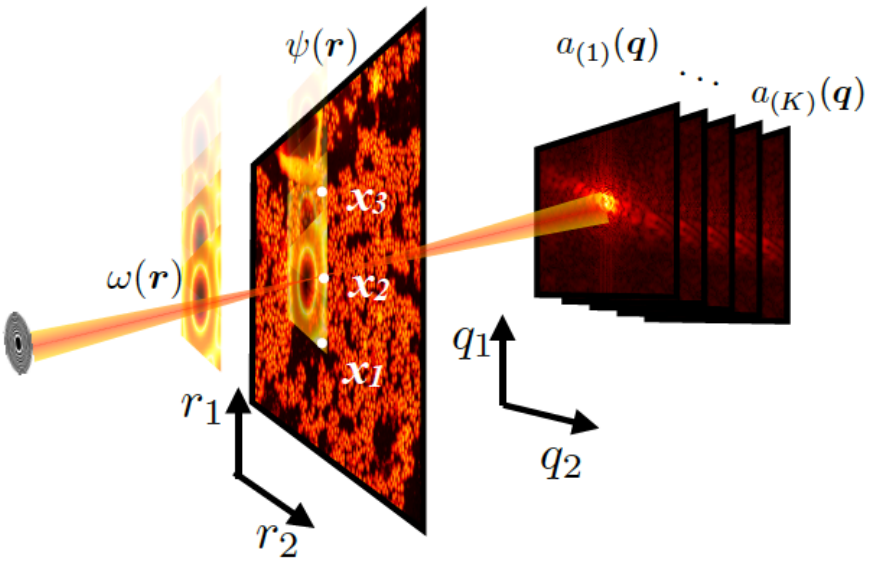
Marchinesi et al.



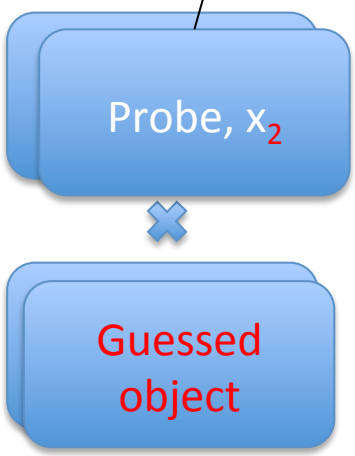
*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

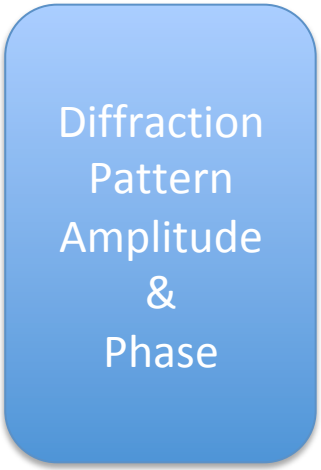
2 - **Ptychography** - *Inversion algorithm for extended sample*

Partial redundancy:
A small amount of unknowns is introduced at x_2



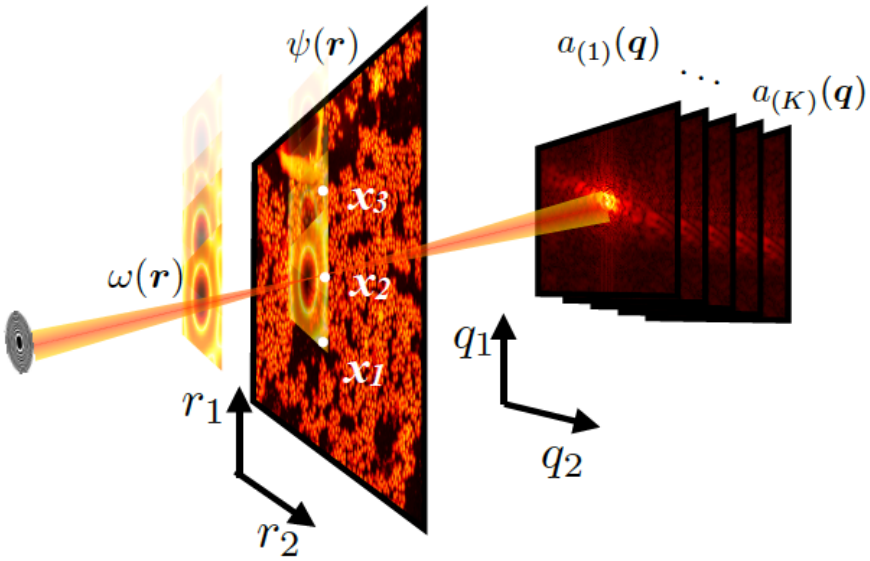
Marchinesi et al.





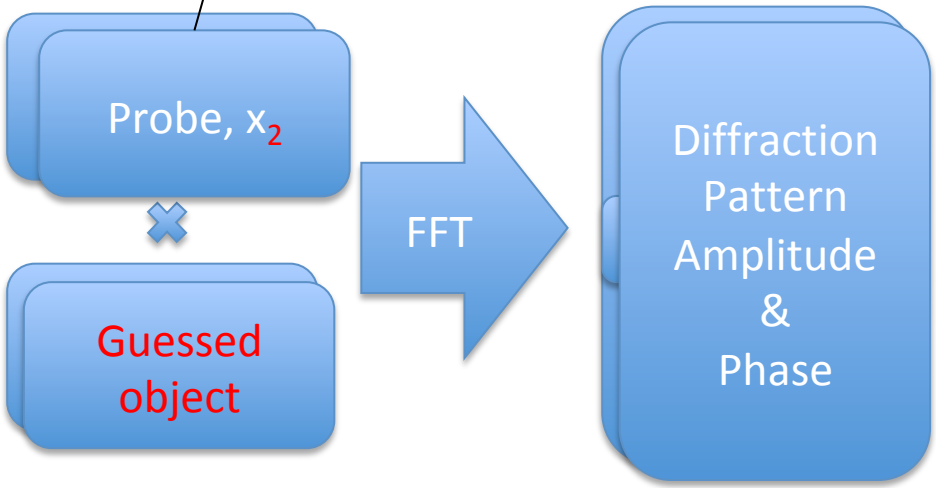
*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*



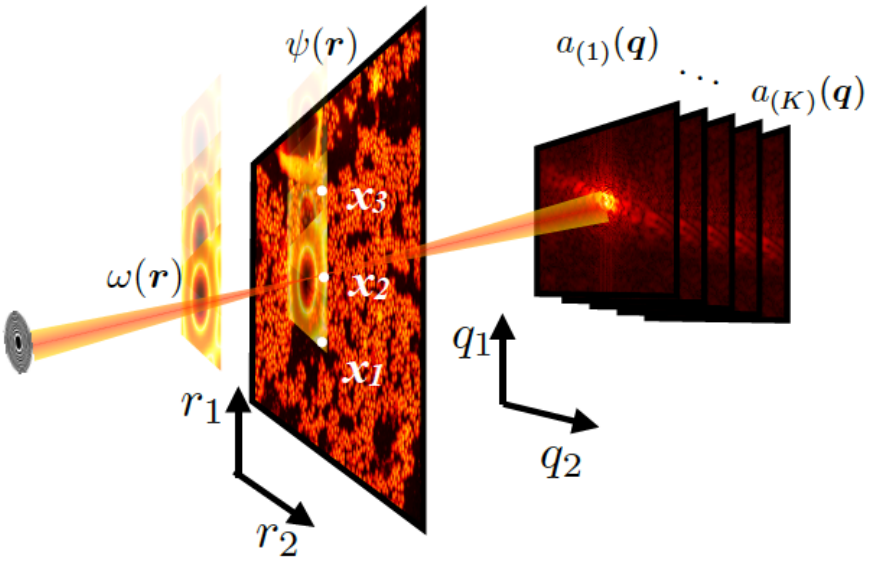
Marchinesi et al.

Partial redundancy:
A small amount of unknowns is introduced at x_2



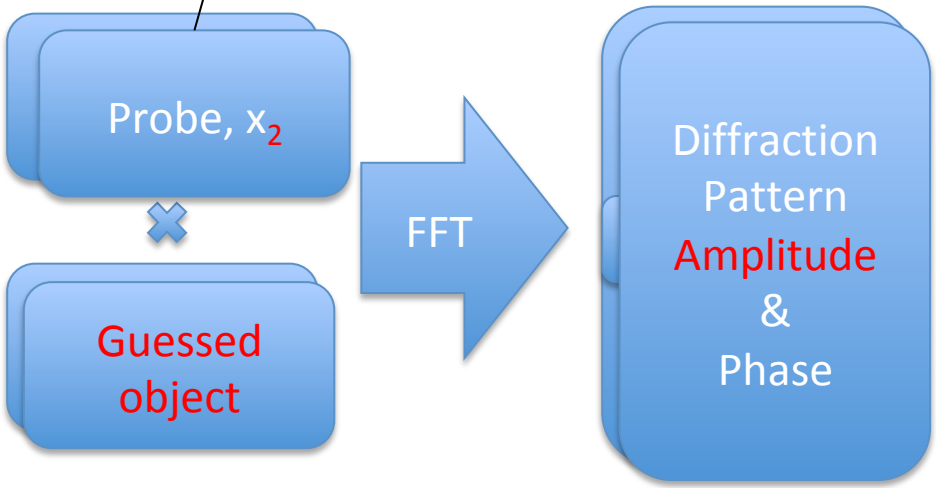
*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*



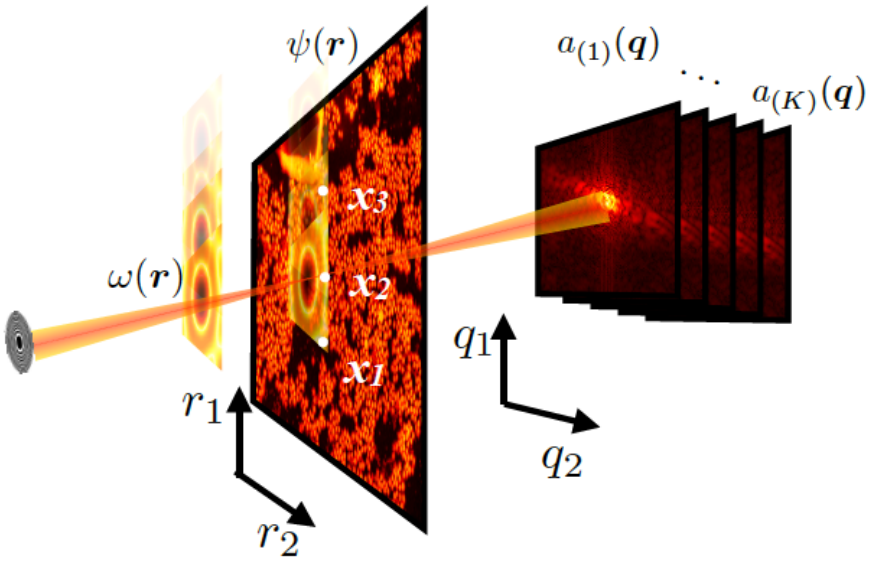
Marchinesi et al.

Partial redundancy:
A small amount of unknowns is introduced at x_2



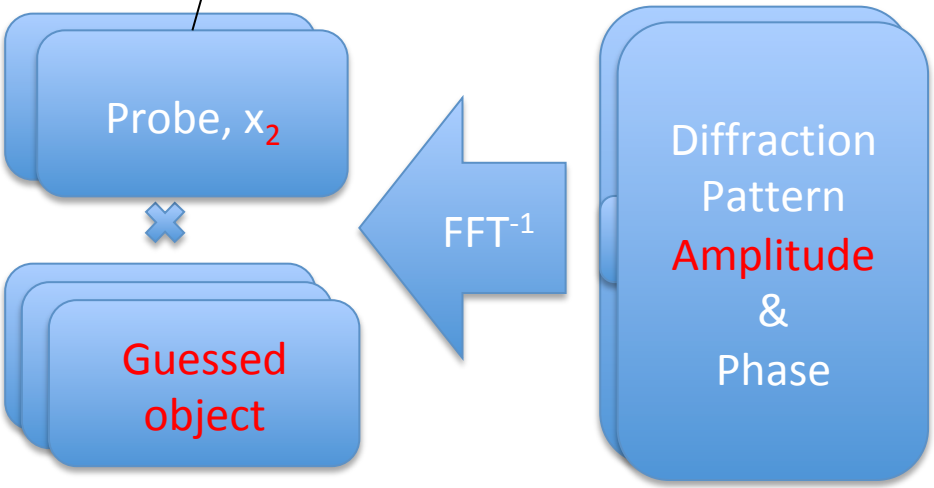
*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

2 - **Ptychography** - *Inversion algorithm for extended sample*



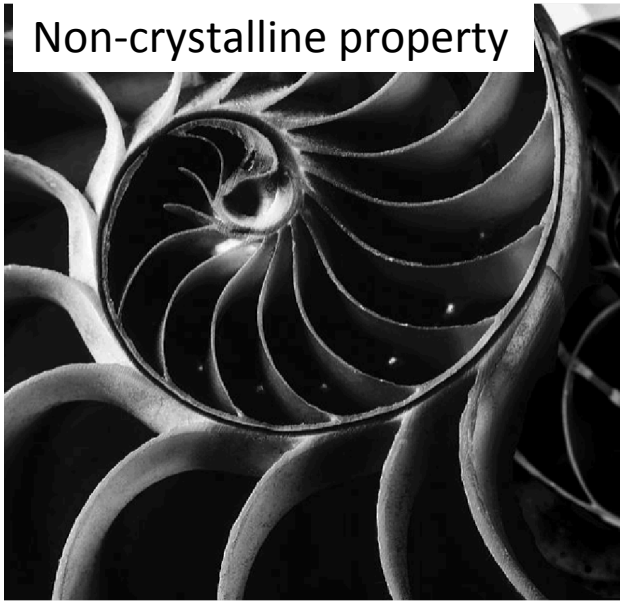
Marchinesi et al.

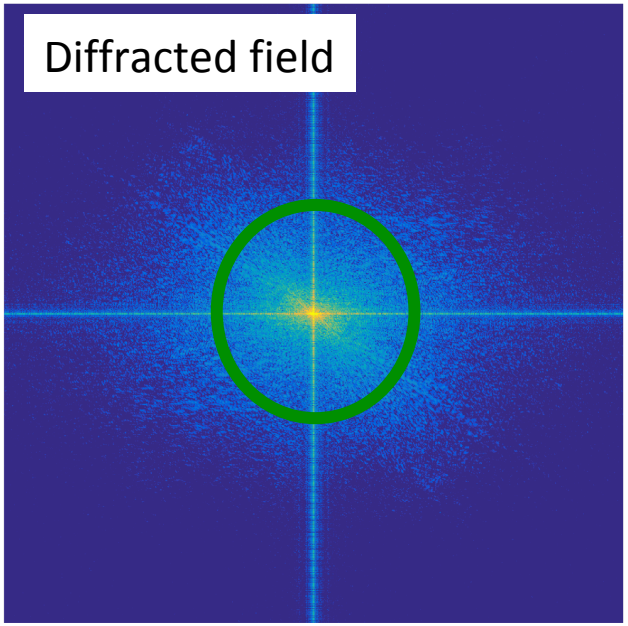
Partial redundancy:
A small amount of unknowns is introduced at x_2

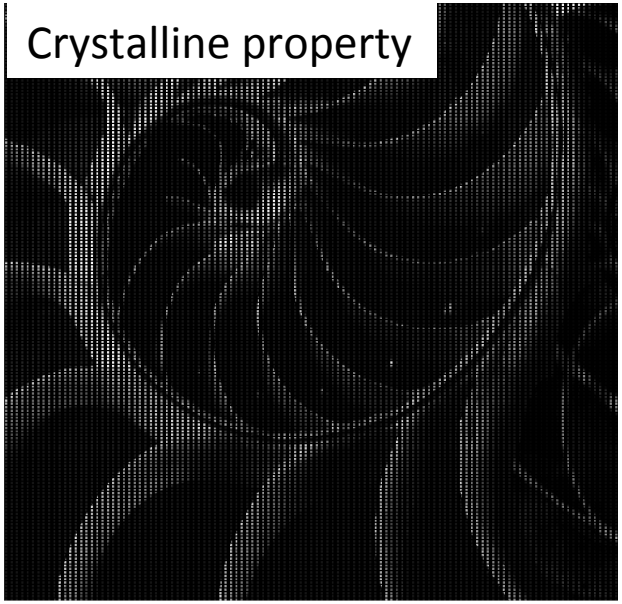


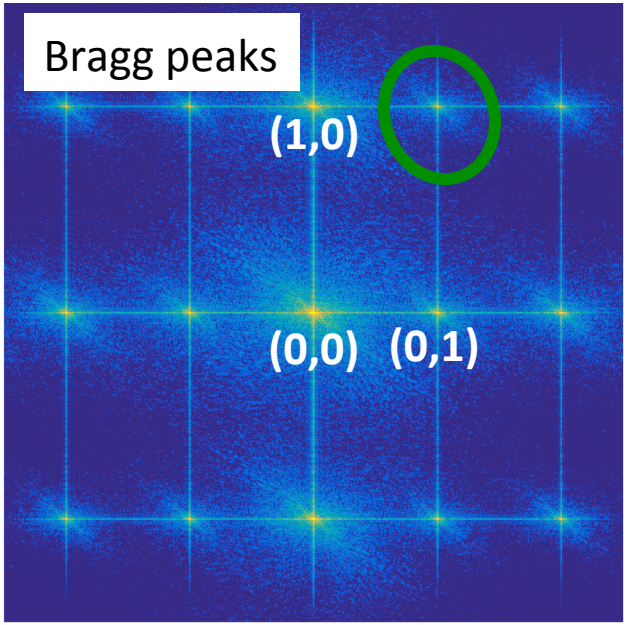
*Faulkner et al. PRL **93** (2004); Rodenburg et al. APL **85** (2004)*

From non-crystalline to crystalline microscopy

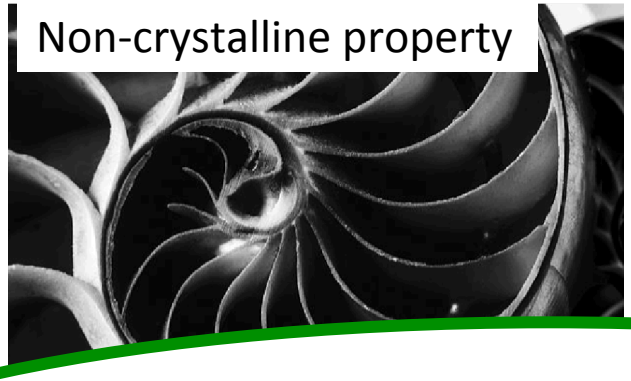


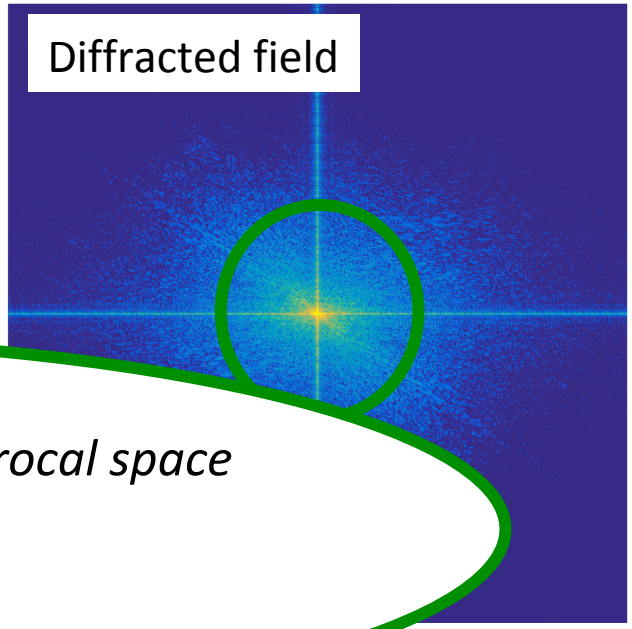






From non-crystalline to crystalline microscopy



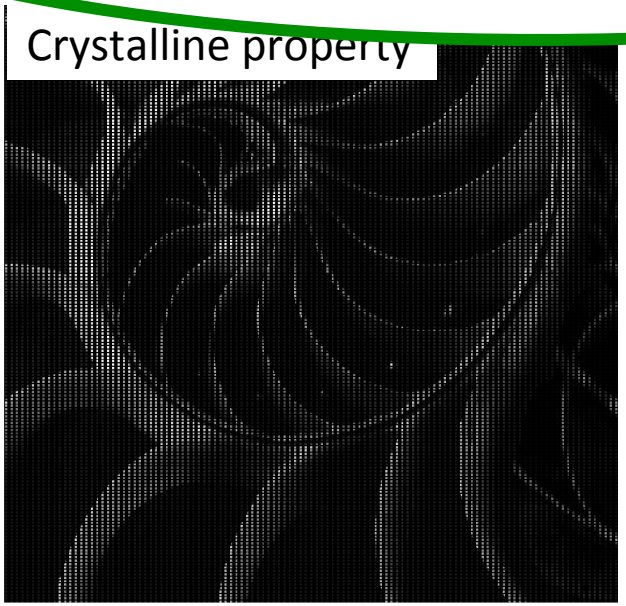


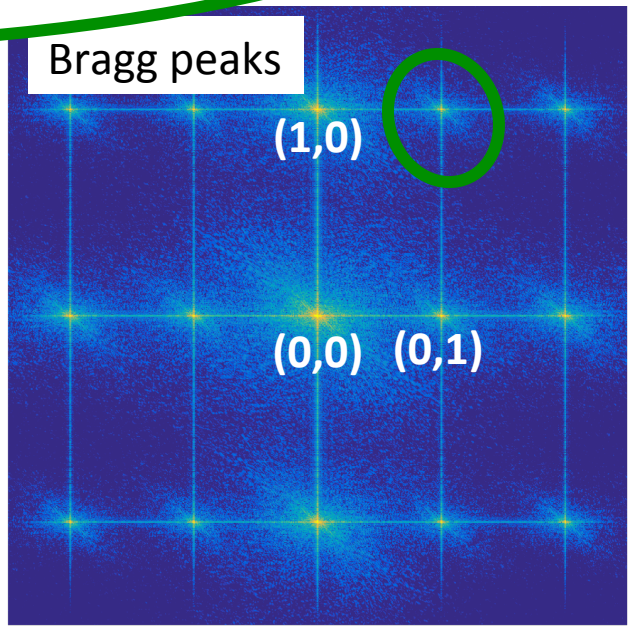
In the vicinity of the origin of the reciprocal space

→ *Non crystalline information*

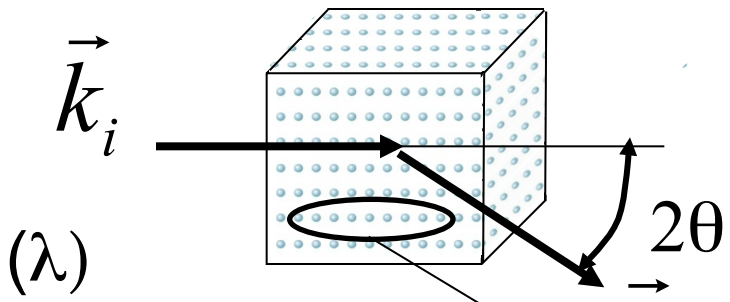
In the vicinity of a Bragg peak

→ *Crystalline information*

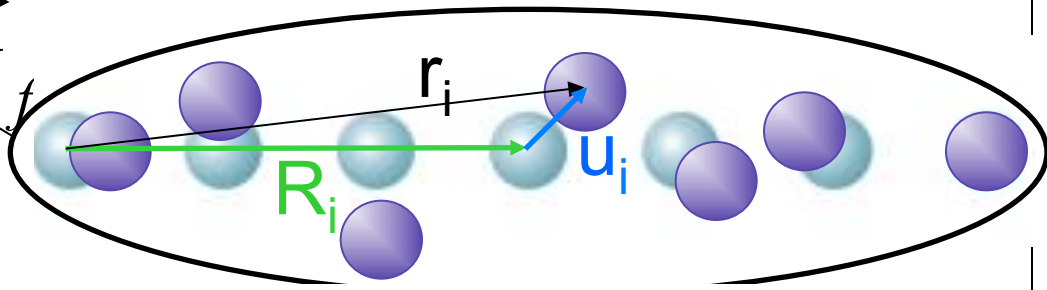




Mathematical model introducing the displacement field



$\vec{q} = \vec{k}_f - \vec{k}_i$ In the vicinity of the Bragg vector $\vec{G}$



$$I(\vec{q}) \propto \left|F(\vec{q})\right|^2$$

$$F(\vec{q}) = \int \rho(\vec{r}) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r}$$

$$\vec{r} = \vec{R} + \vec{u}(\vec{R})$$

$$I(\vec{q}) \propto \left| FT\left\{ \rho(\vec{R}) e^{i\vec{G}\cdot\vec{u}(\vec{R})} \right\} \right|^2$$

complex-valued electron density

$\vec{r}$: strained solid

$\vec{R}$: unstrained solid

$\vec{u}(\vec{R})$: displacement field

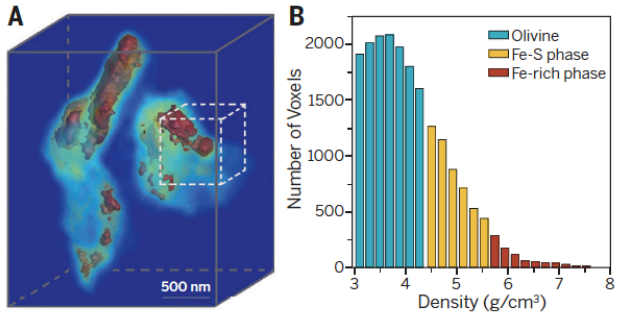
From the spatial derivatives of $\vec{G}\cdot\vec{u}(\vec{R})$, strain and orientation fields are extracted

Main coherent x-ray microscopy modalities

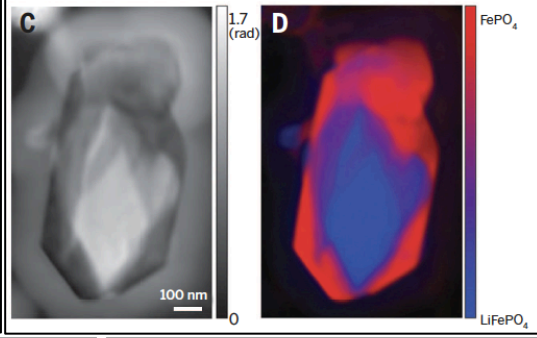
	Density information	**Crystalline properties**
Finite-size sample	Coherent Diffraction Imaging (CDI)	Bragg-Coherent Diffraction Imaging (BCDI)
Extended sample	Ptychography	Bragg ptychography

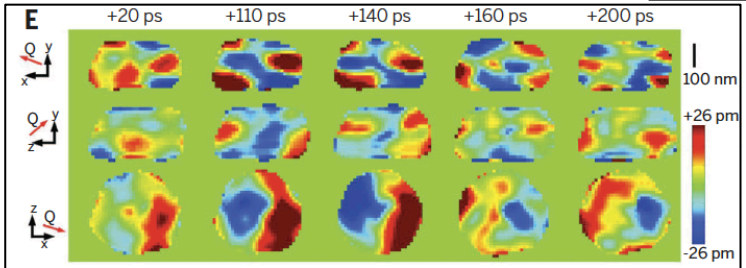
Review: see *Miao et al., Science 348 (2015)*

CDI of mantle olivine

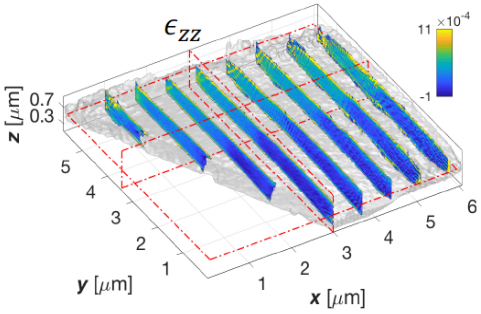


Spectro-ptychography of an electrochemical energy storage material





BCDI of lattice displacement after IR-laser pulse



Invisible defects seen from Bragg ptychography in implanted materials

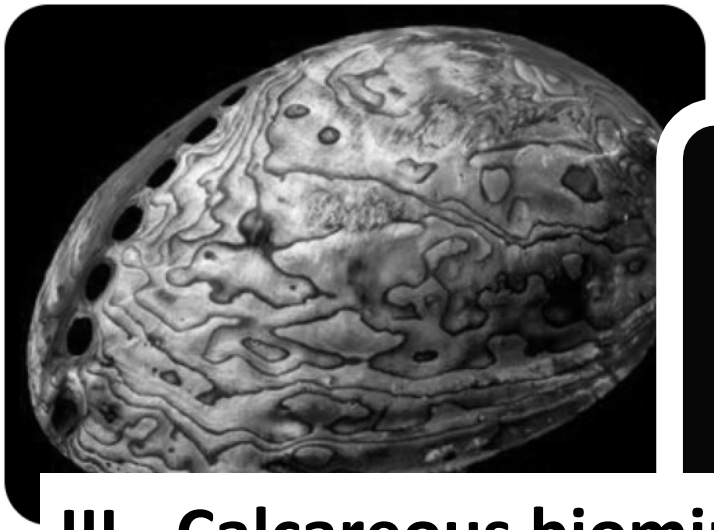
Li *et al.*, Nature Commun. (2021)

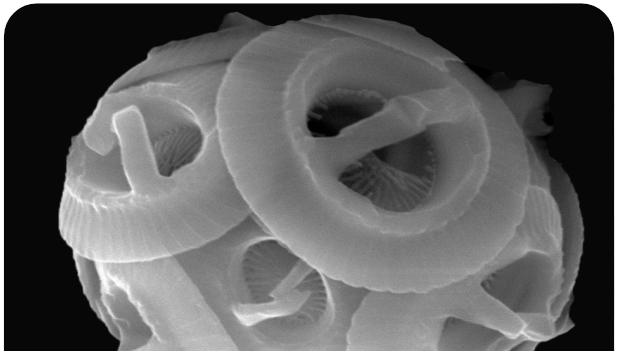
Main coherent x-ray microscopy modalities

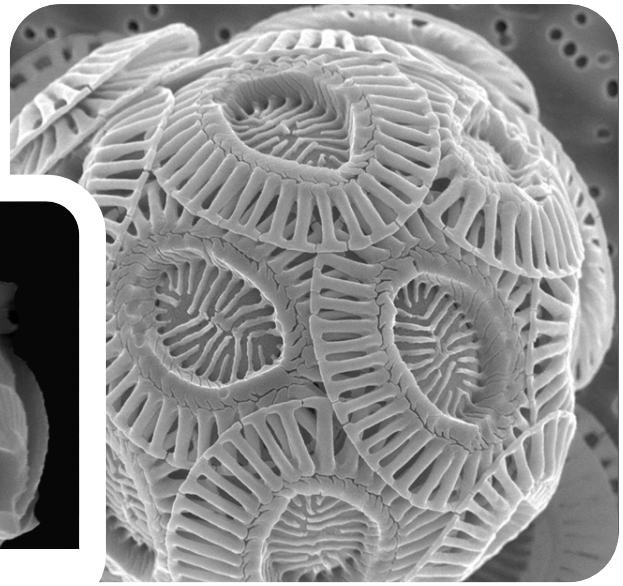
	Density information	**Crystalline properties**
Finite-size sample	Coherent Diffraction Imaging (CDI)	Bragg-Coherent Diffraction Imaging (BCDI)
Extended sample	Ptychography	Bragg ptychography

- **3D field of view**
  - → CDI: 0.1 − 4 μm
  - → BCDI: 0.1 − 2 μm
  - → Ptychography: 2 - 30 μm
  - → Bragg ptychography: extended x 2 μm
- **Sensitivity**
  - → CDI, ptychography: 1-2%
  - → BCDI − Strain, lattice rotation: 10^{-4} - a few 10^{-3}, 0.005 – 0.01°
  - → Bragg ptychography − Strain, lattice rotation: up to 10^{-2}, up to 1°
- **Spatial resolution**
  - → 3D, down to 7 nm, but contrast-dependent, anisotropic
- **Total acquisition time**
  - → From a few hours to 10 min
- **Inversion time**
  - → From a few hours to a few min

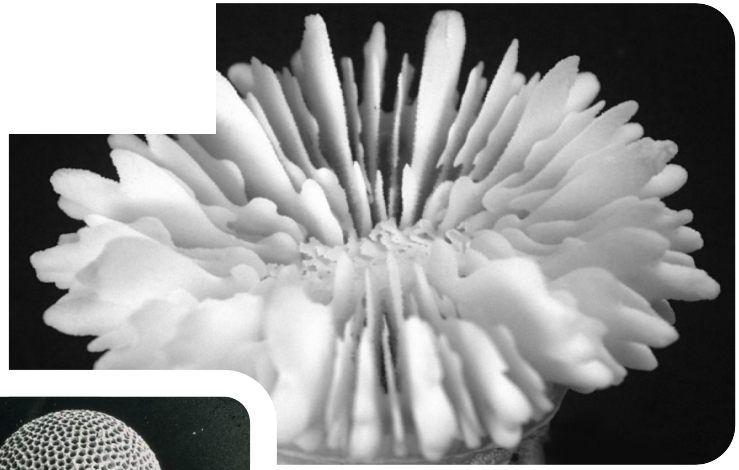
III – Applications of coherent diffraction imaging

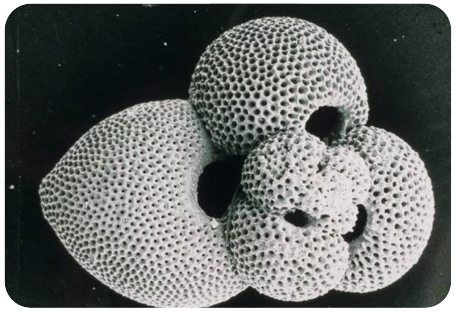






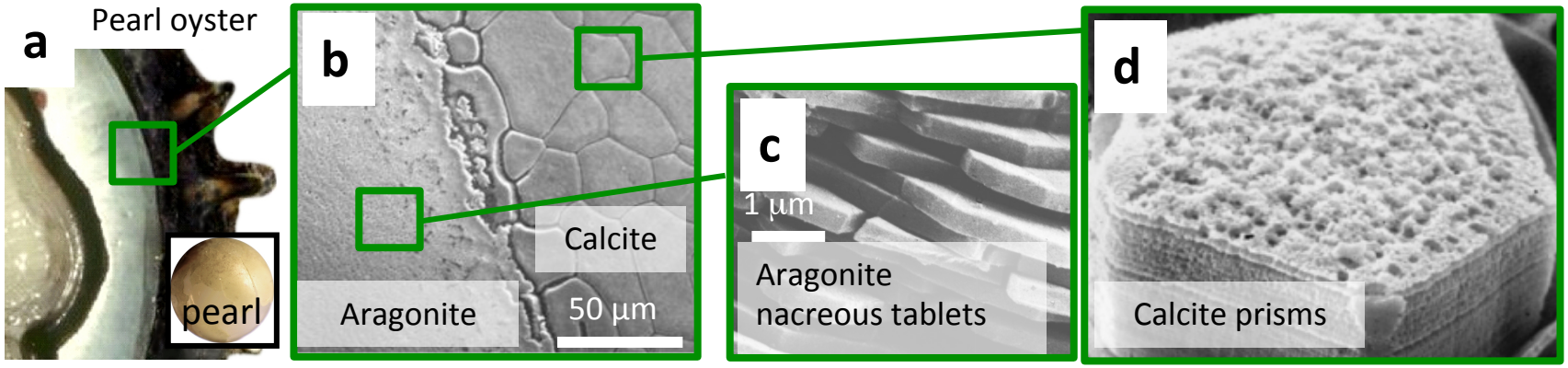
III - Calcareous biomineralisation & coherent diffraction imaging





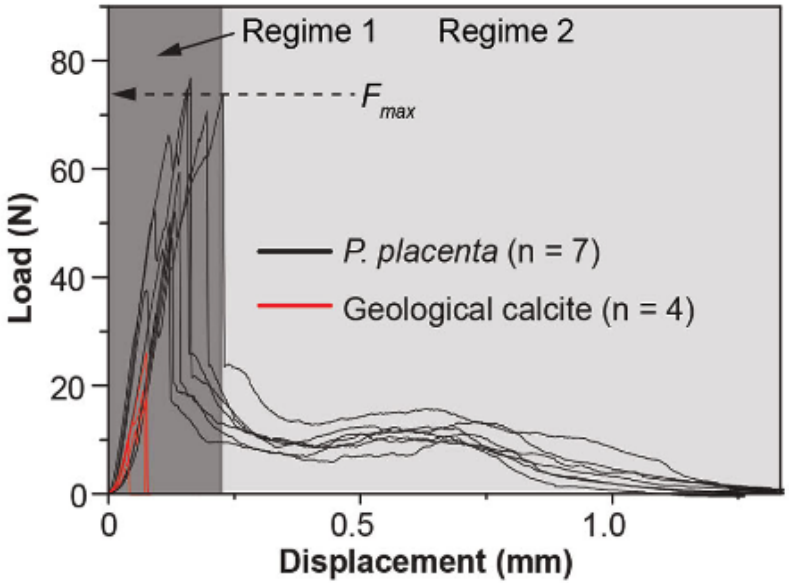
Biominerals in material science

Highly regulated and complex hierarchical organo-mineral structures



J.-P. Cuif, Y. Dauphin and E. Sorauf, Cambridge Univ. Press (2011)

- Damage resistance

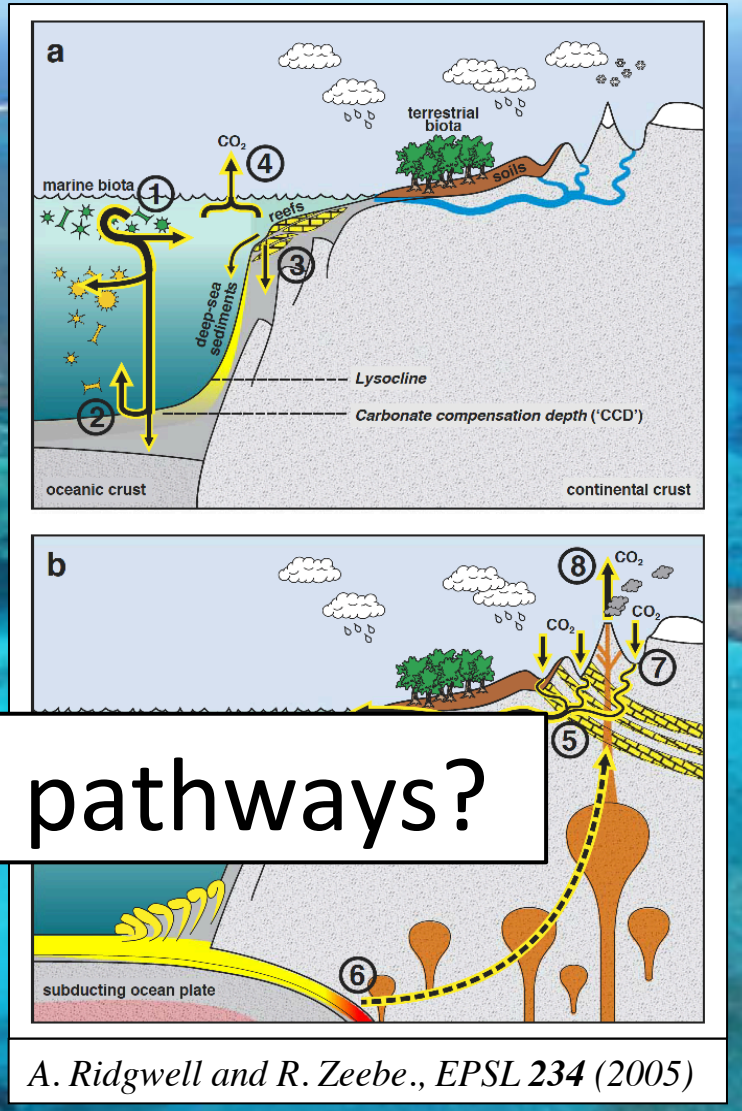


L. Li and C. Ortiz, Adv. Funct. Mater. ***25*** *(2015)*

→ Biomimetism?

Biominerals and environmental science

$CaCO_3$, one of most prominent minerals in Earth's crust



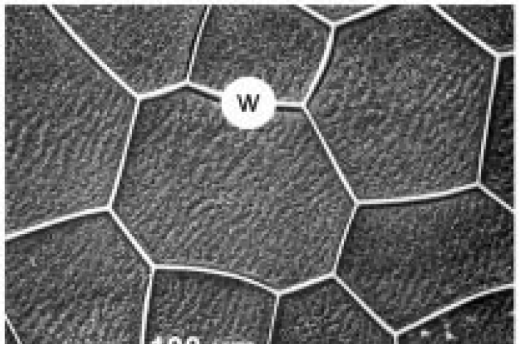
A. Ridgwell and R. Zeebe., EPSL **234** (2005)

→ Physico-chemical pathways?

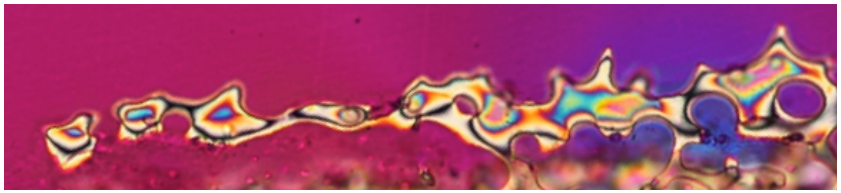
Calcareous biomineralisation

Generic features

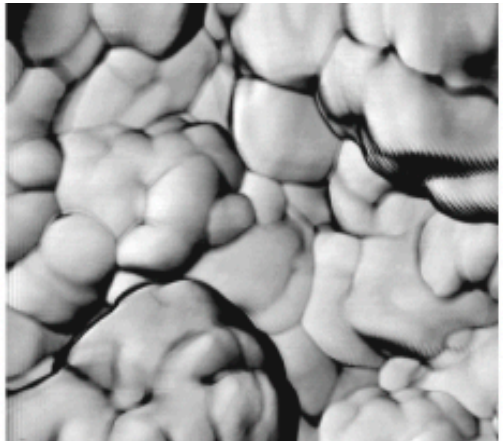
- Mineral/organics materials



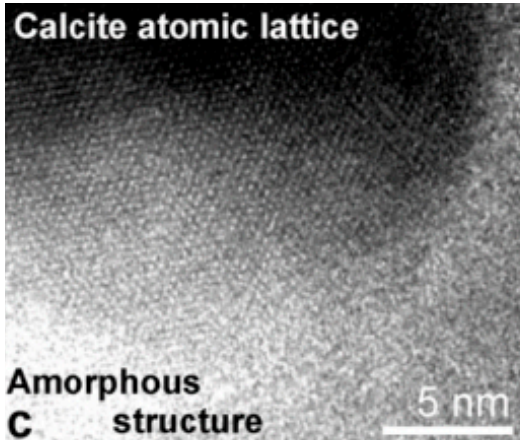
- Single crystalline at the macro-scale (no facet)

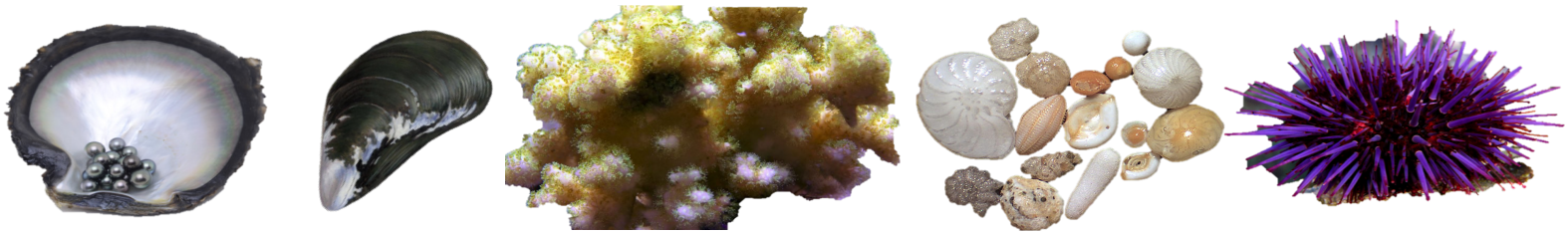


- Granular structure at the nano-scale



- Amorphous precursor(s)



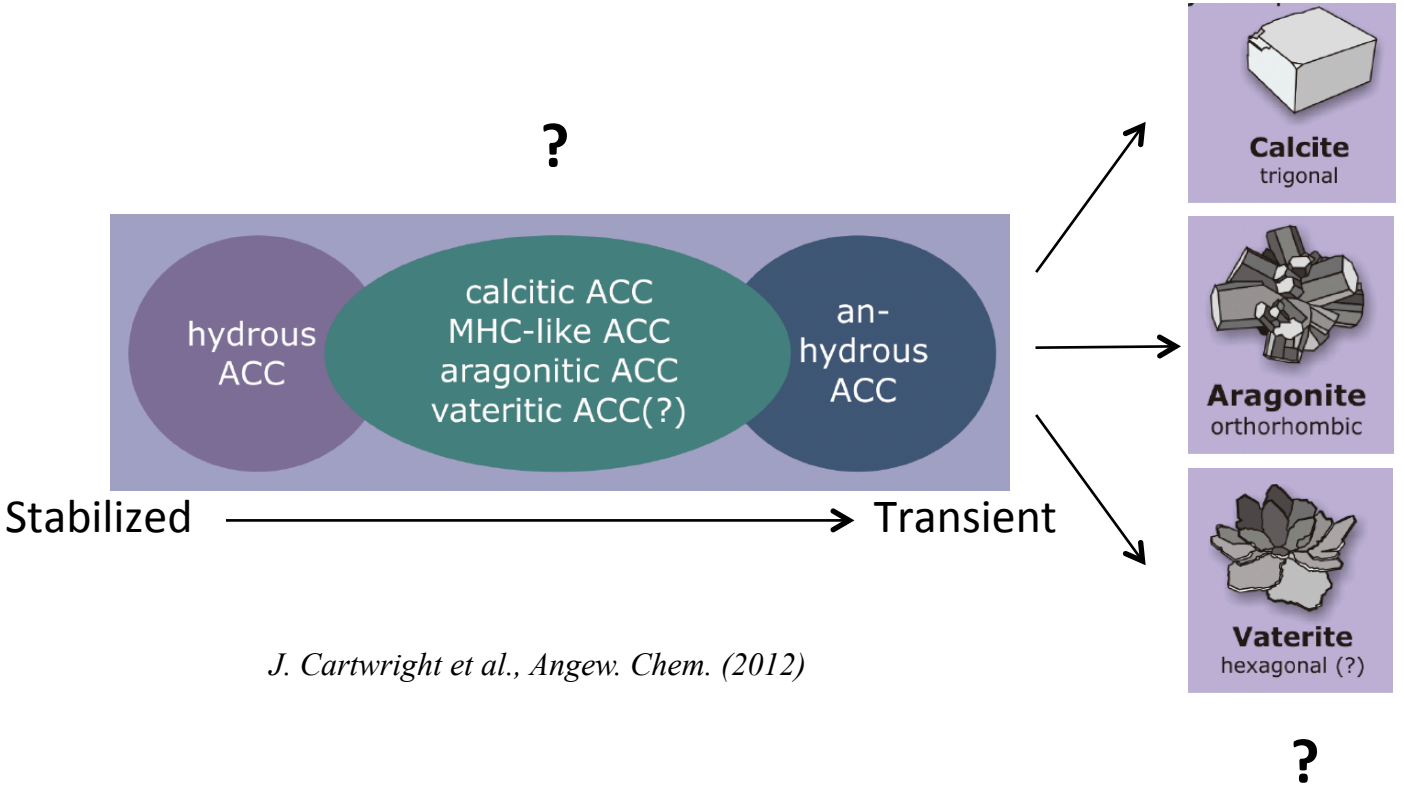


Biocrystallisation related questions

From the amorphous to the crystalline final phase

What are the different transient metastable phases?

What are the nucleation and phase transition mechanisms?

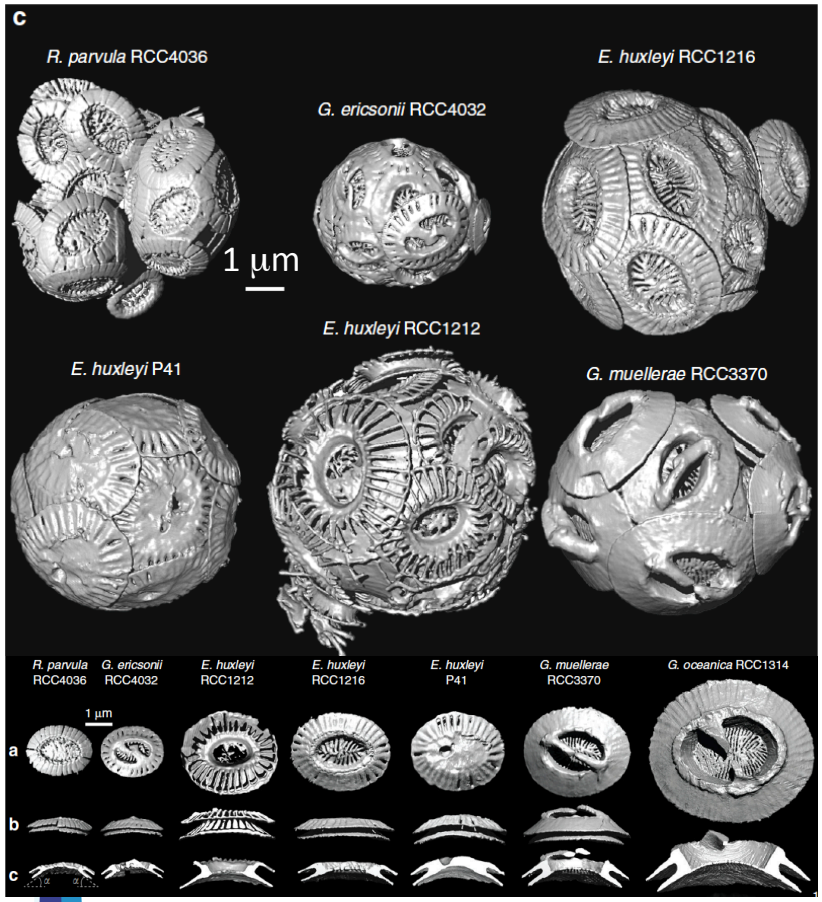


J. Cartwright et al., Angew. Chem. (2012)

CDI – Coccolithophores formation

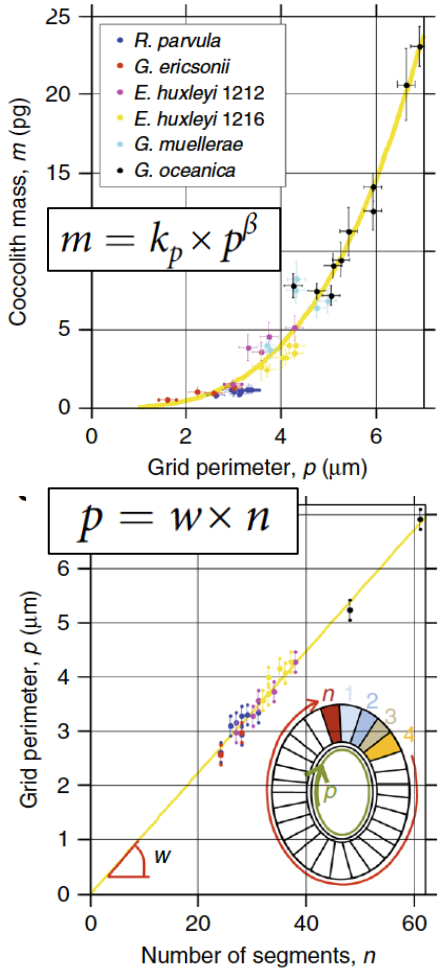
Unicellular marine planktonic algae producing calcareous exoskeleton made of $CaCO_3$ scales

3D electron density of several species

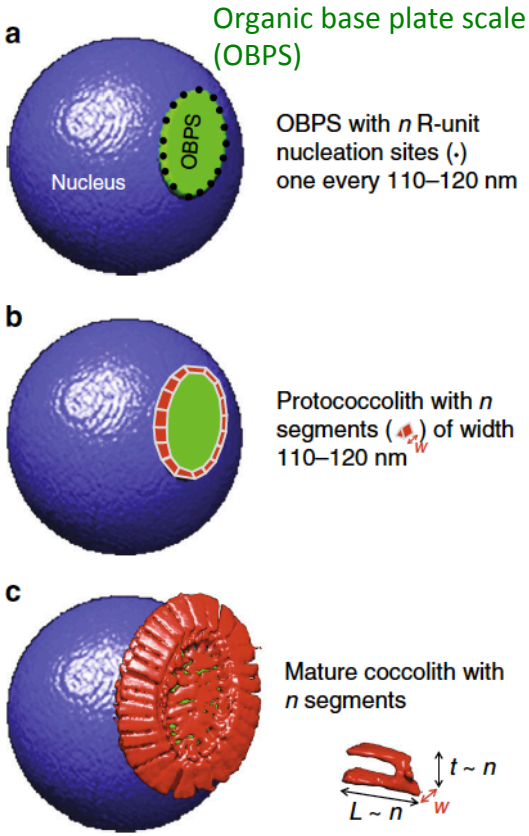


Beuvier et al., Nature Commun. 2019

Universal laws



Nucleation mechanism



→ Unique distance between nucleation sites

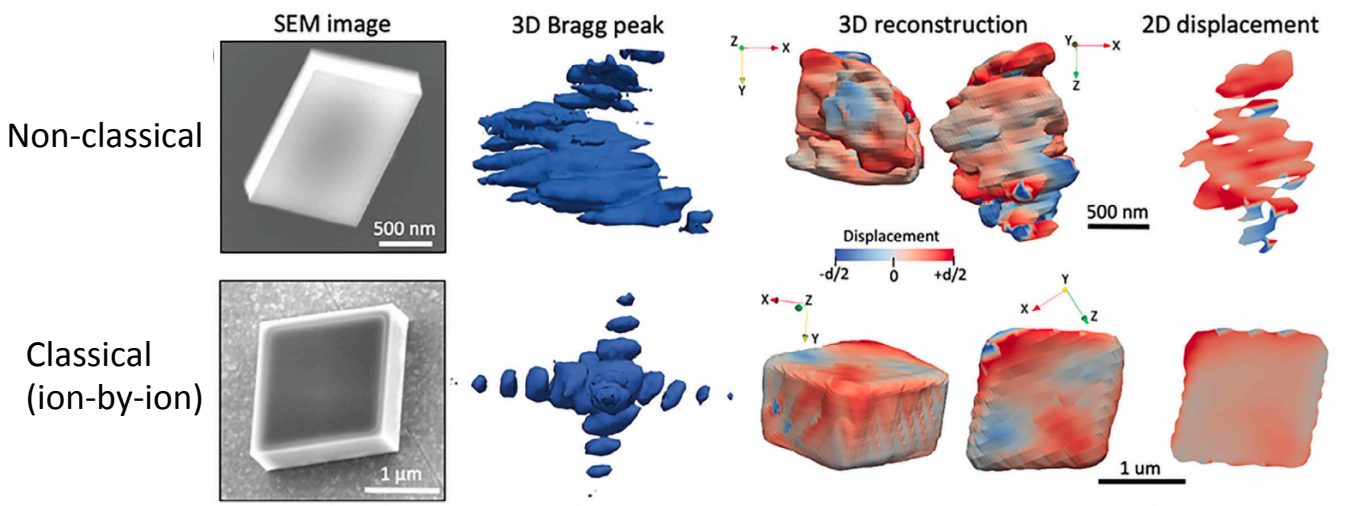
→ Mass directly related to perimeter

BCDI – *Crystallisation pathways from a synthetic model*

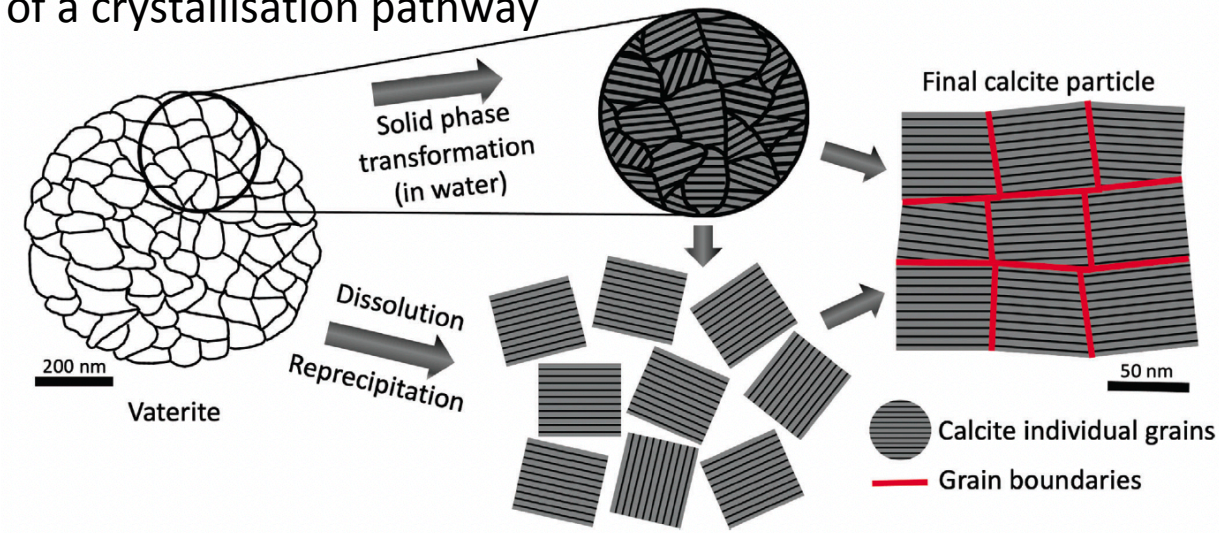
Crystal growth

Classical vs non classical crystallisation of calcite

Suzana et al., Adv. Mat. 2024



→ Proposition of a crystallisation pathway

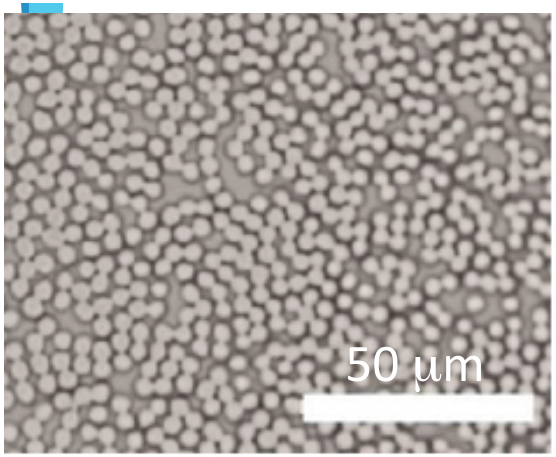


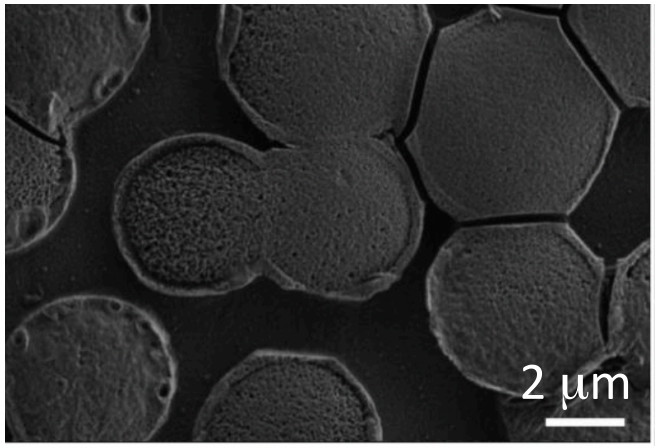
Bragg ptycho. – *Crystallisation pathways from synthetic model*

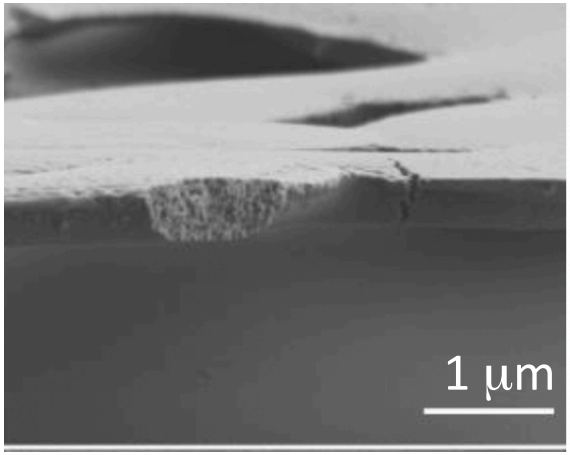
Biomimetic calcareous systems
Amorphous to crystalline transition in synthetic CaCO3

Collab.
C. Chevallard
C. Clément

Production of an **amorphous calcium carbonate** film
(from Ammonia diffusion method into organic-mediated solution)





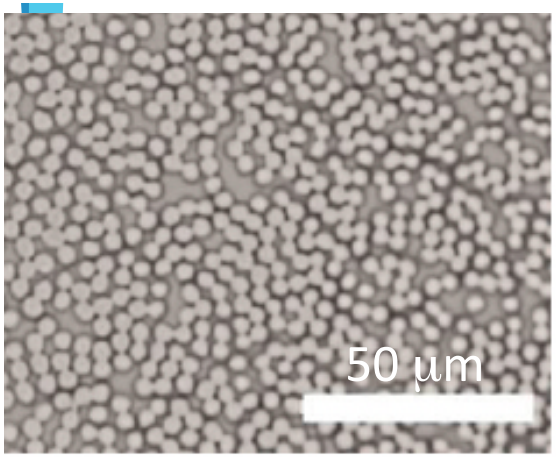


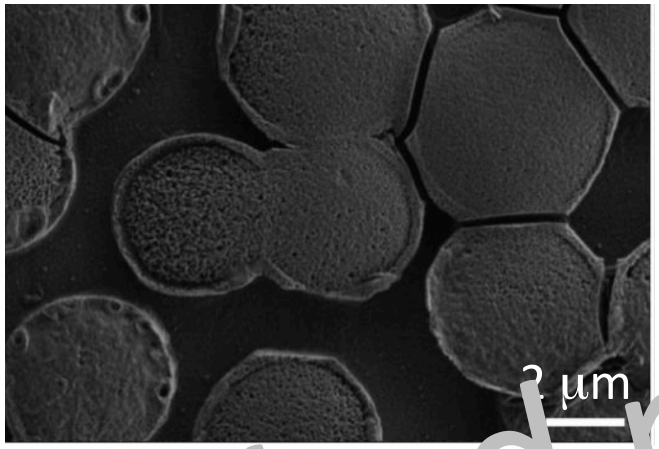
Bragg ptycho. *– Crystallisation pathways from synthetic model*

Biomimetic calcareous systems
Amorphous to crystalline transition in synthetic CaCO3

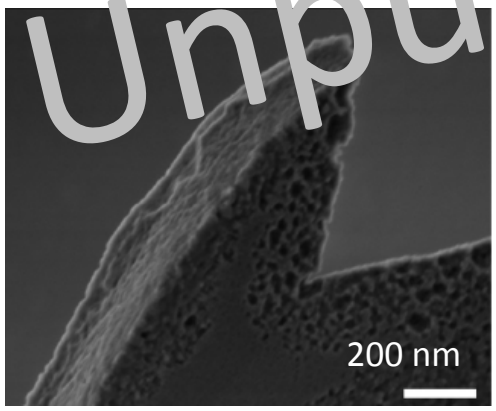
Collab.
C. Chevallard
C. Clément

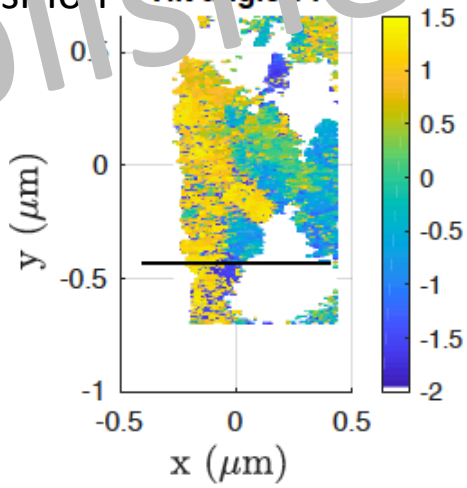
Production of an **amorphous calcium carbonate** film
(from Ammonia diffusion method into organic-mediated solution)

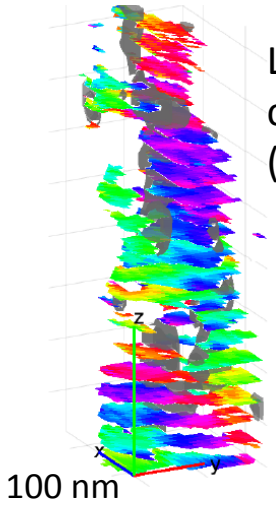




Heat activated crystalline transition
→ Solid/solid transition







Limited
coherence length
(50 x 200 nm²)

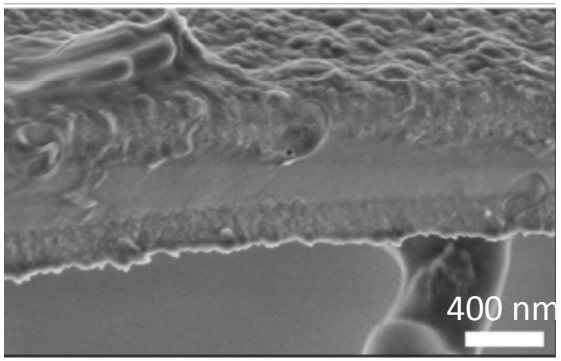
unpublished

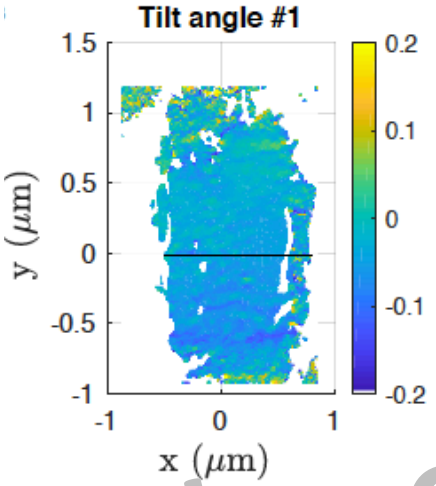
Bragg ptycho. *– Crystallisation pathways from synthetic model*

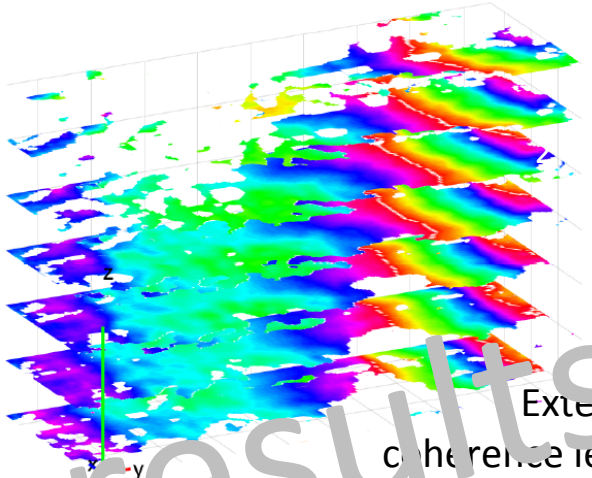
Crystallisation pathways in biomimetic calcareous systems
Amorphous to crystalline transition in synthetic CaCO3

Collab.
C. Chevallard
C. Clément

Humidity activated crystalline transition
→ Localized dissolution/
reprecipitation



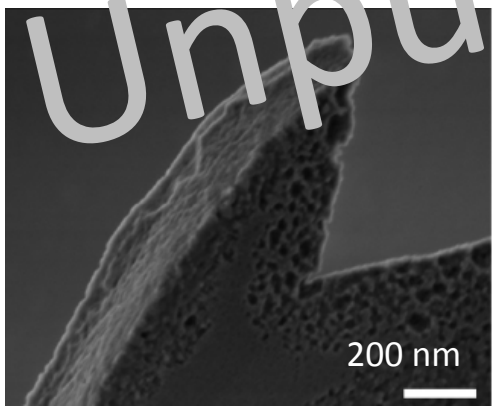


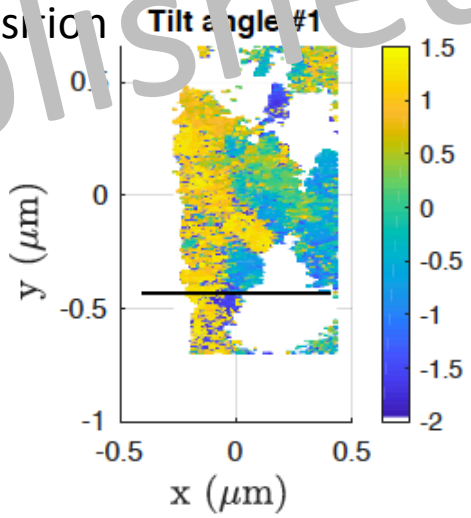


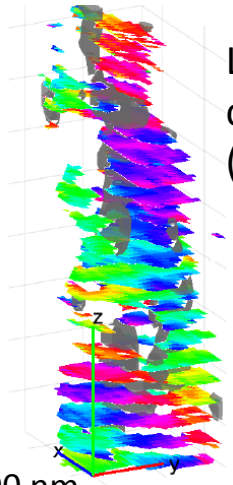
100 nm

Extended
coherence length
(700 x 250 nm²)

Heat activated crystalline transition
→ Solid/solid transition







100 nm

Limited
coherence length
(50 x 200 nm²)

unpublished

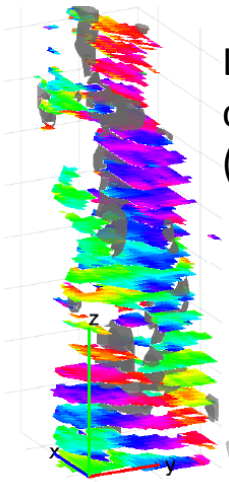
Bragg ptycho. *– Crystallisation pathways from synthetic model*

Biomimetic calcareous systems
Amorphous to crystalline transition in synthetic CaCO3

Collab.
C. Chevallard
C. Clément

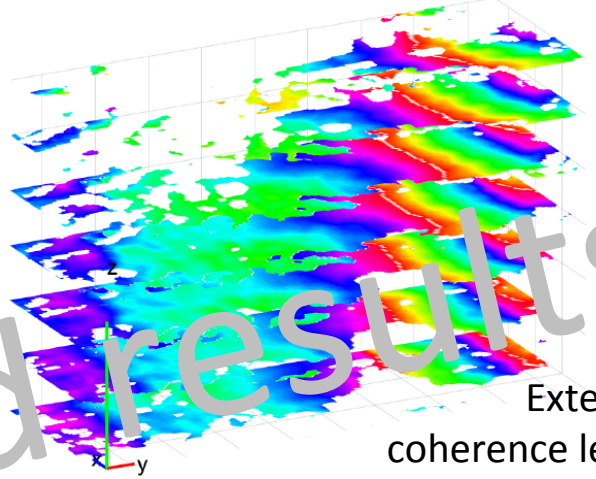
→ Different crystallisation pathways present different BP fingerprints

Solid / solid transition



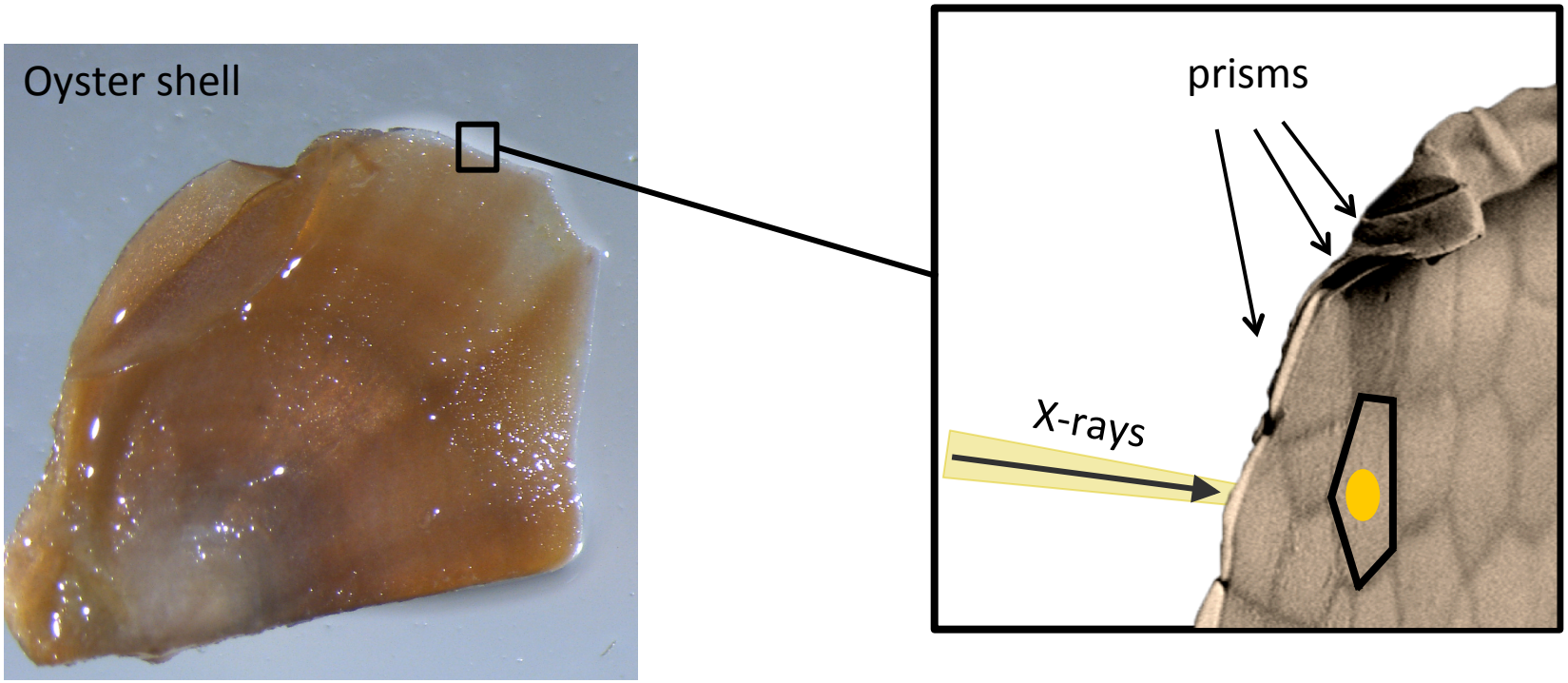
Limited coherence length (50 x 200 nm^2)

Localized dissolution / reprecipitation

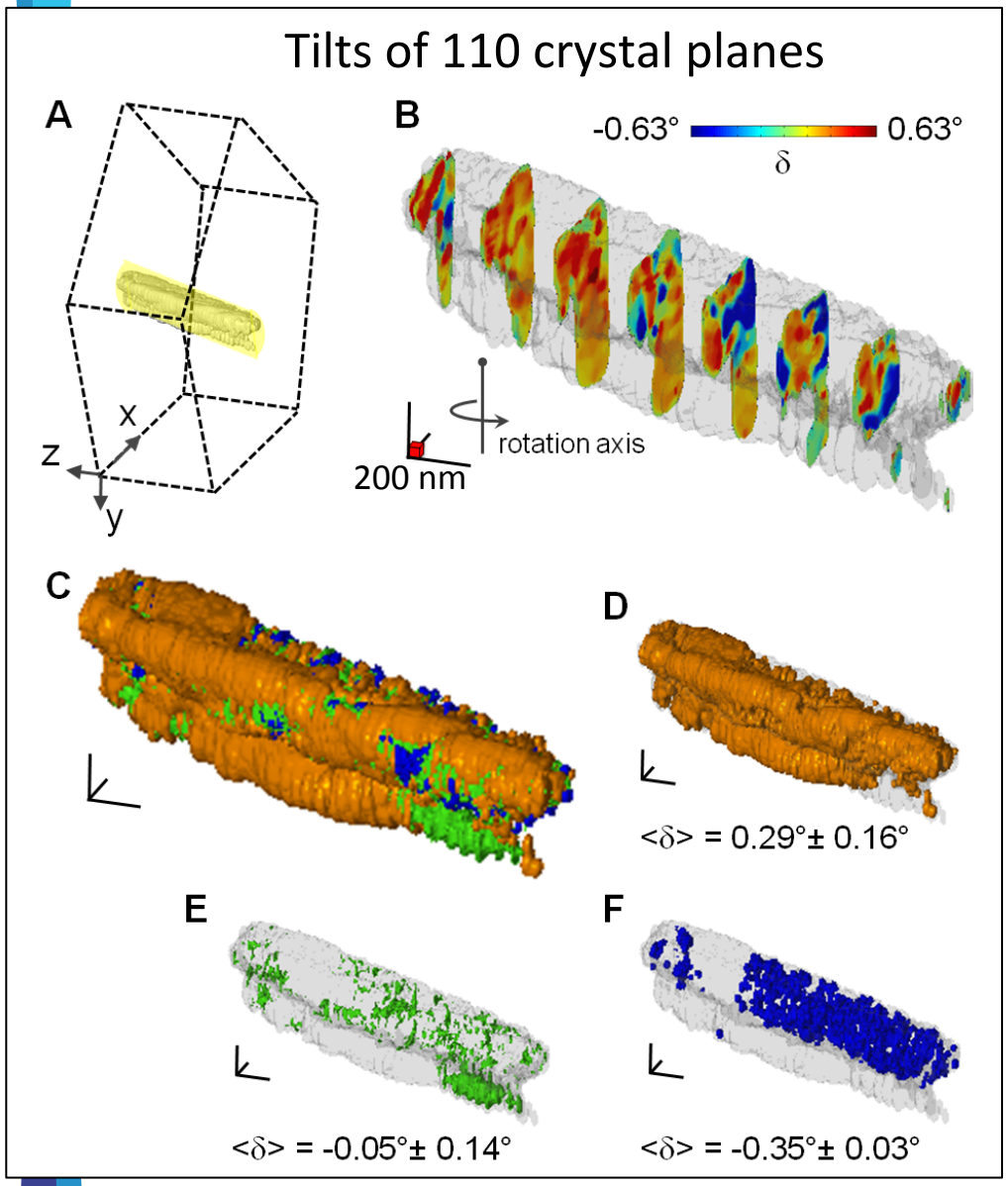


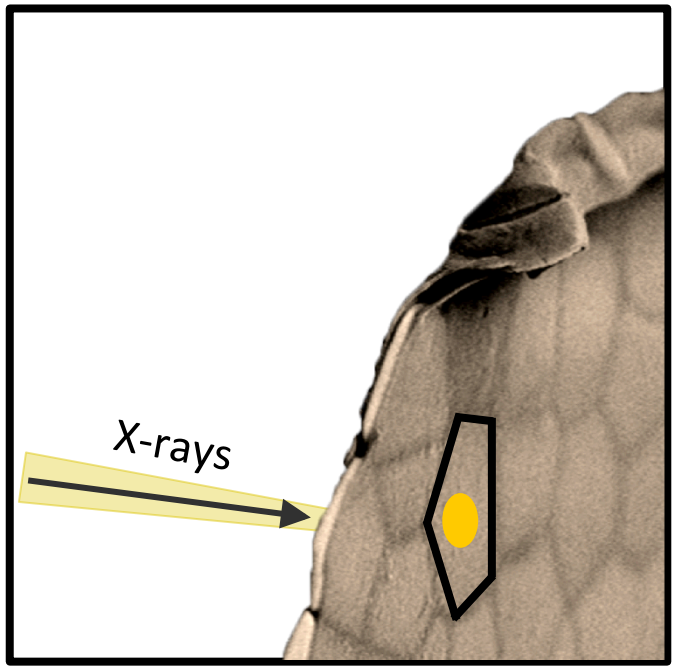
Extended coherence length (700 x 250 nm^2)

Biomineral mesoscale structure: biogenic calcite



Biomineral mesoscale structure: biogenic calcite



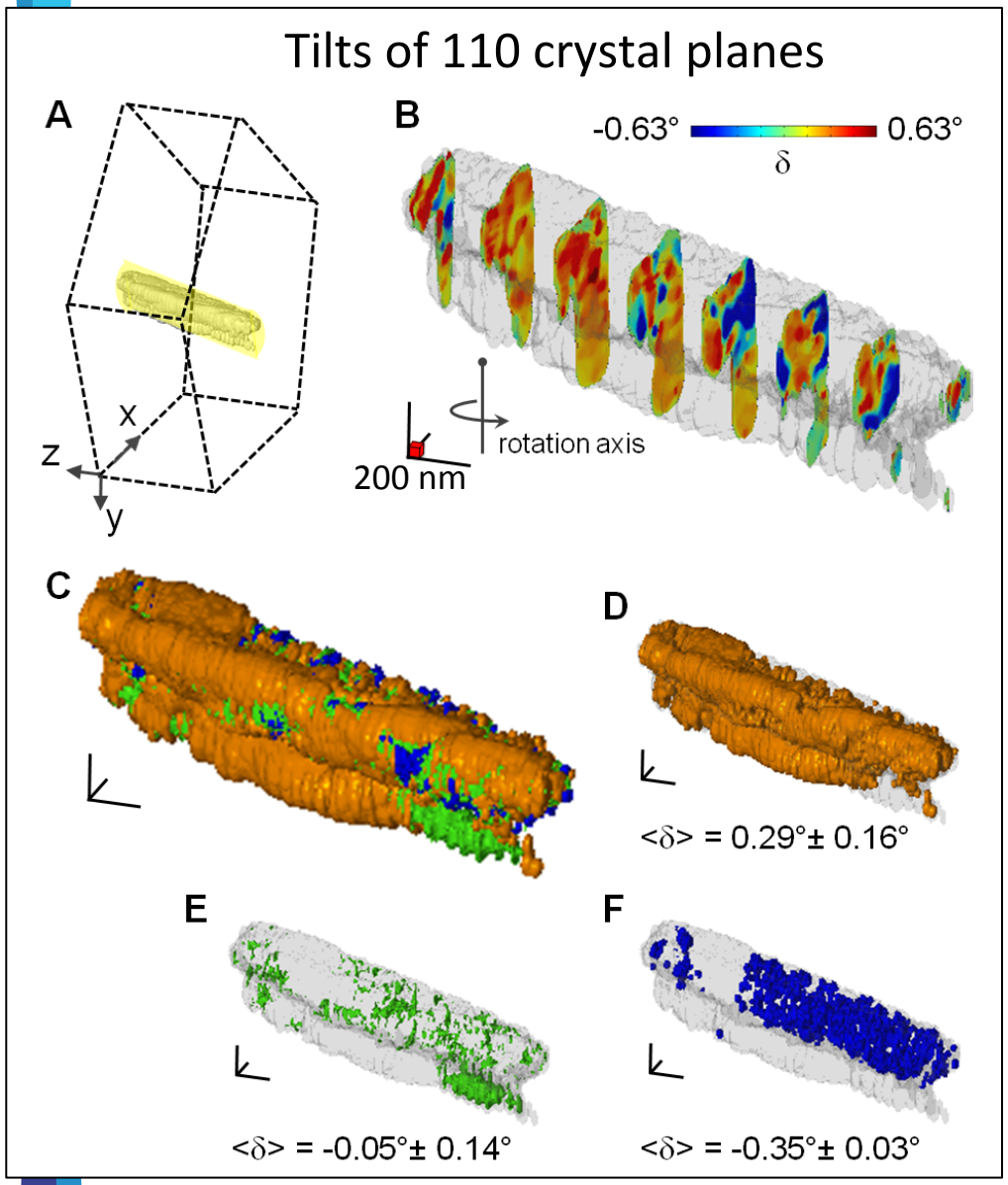


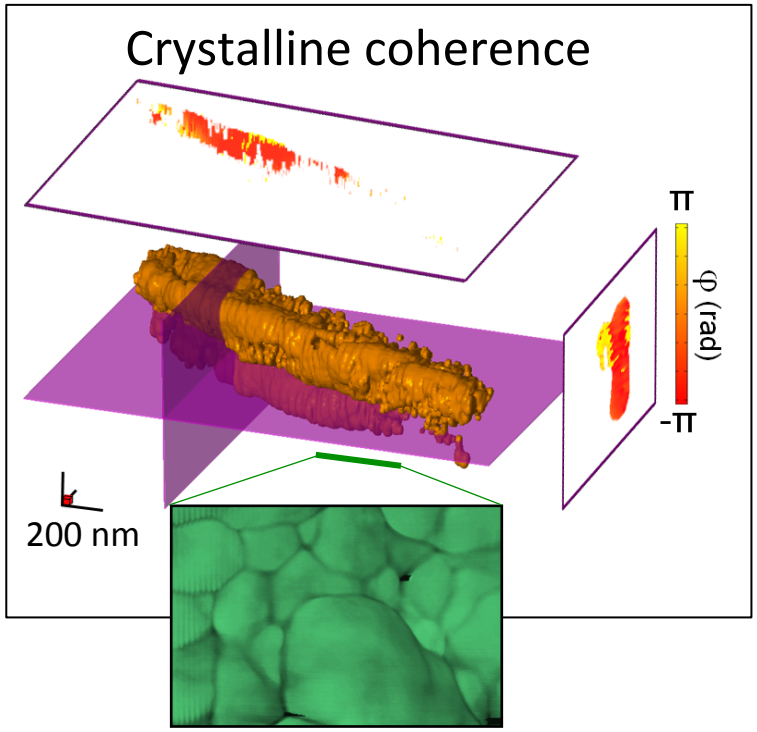
Limit of the single-crystal description is reached

→ The prism is composed of several slightly mis-orientated crystalline domains

Nature Materials (2017)

Biomineral mesoscale structure: biogenic calcite





Limit of the single-crystal description is reached

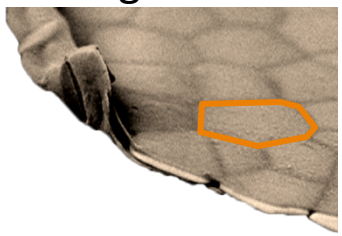
→ The prism is composed of several slightly mis-orientated crystalline domains

→ Each iso-oriented domain contains several coherent crystals larger than a granule

Nature Materials (2017)

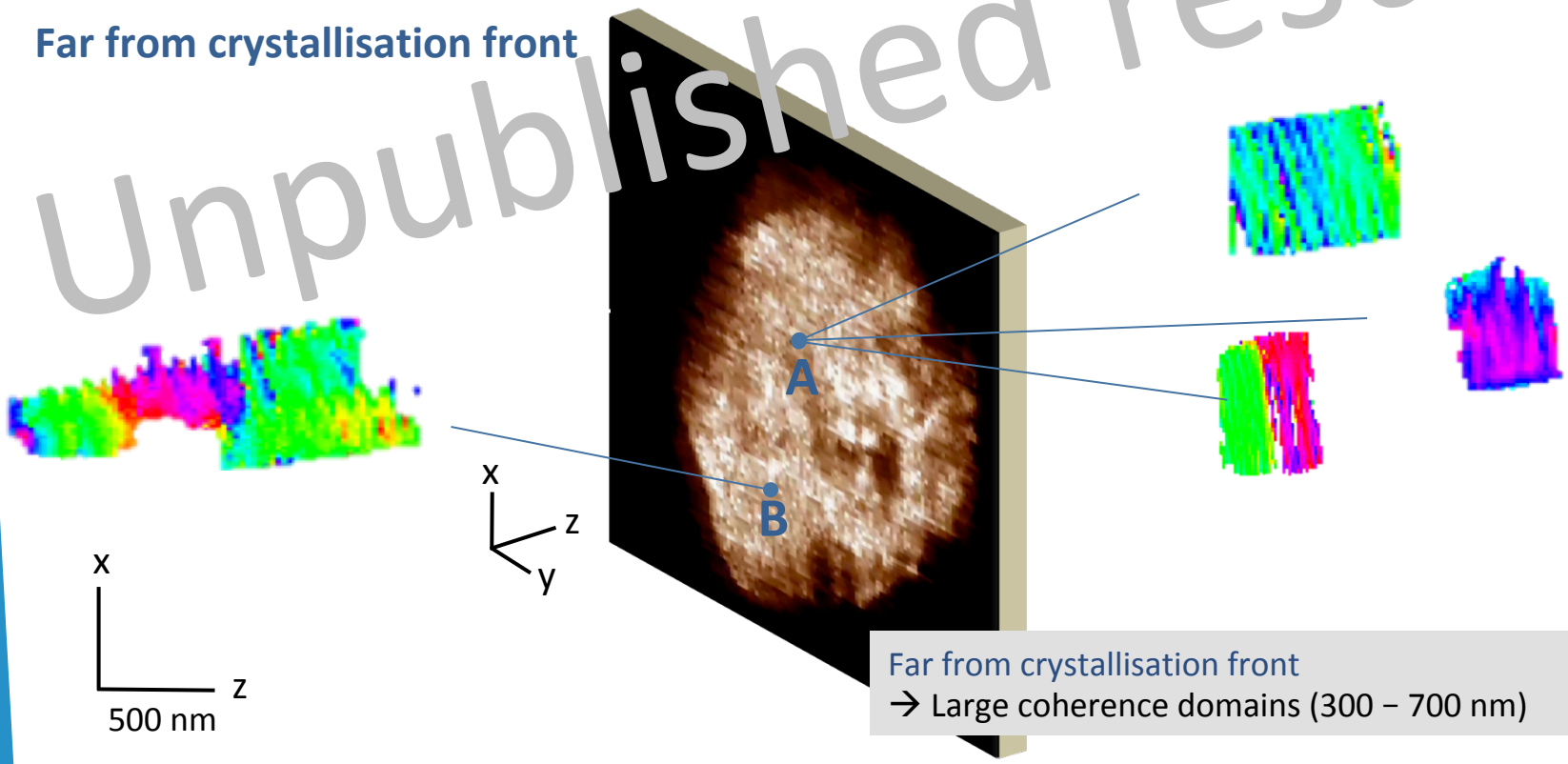
A closer look to the crystalline coherence

Comparison of different crystalline regions within a prism



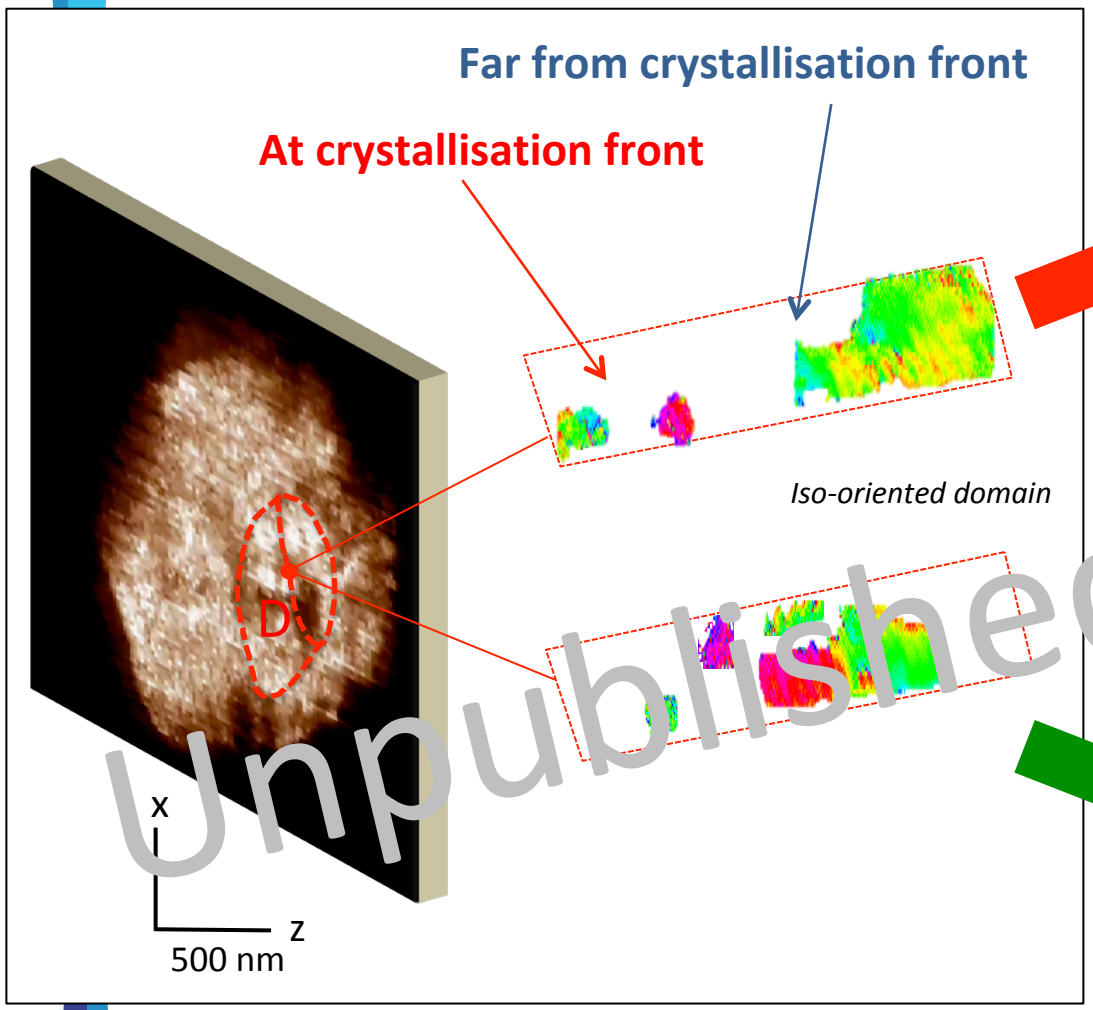
Thickness of about 1.5 µm

Far from crystallisation front

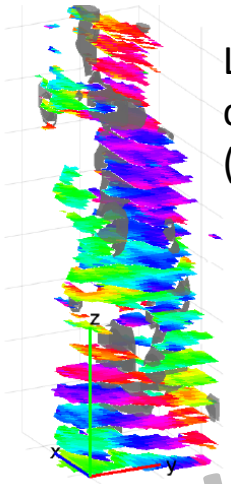


Far from crystallisation front
→ Large coherence domains (300 – 700 nm)

Comparison with non-classical crystallization pathways



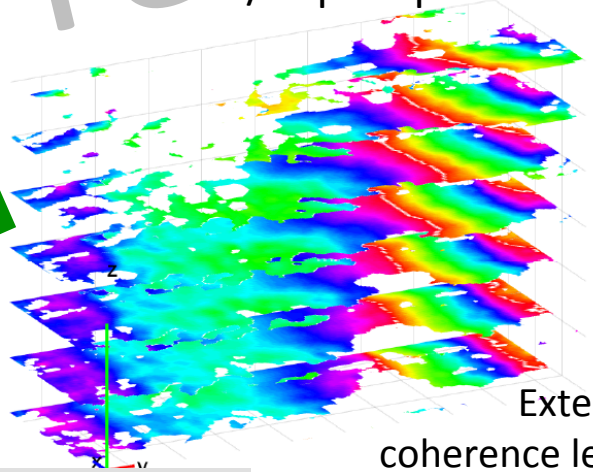
Solid / solid transition



Limited coherence length (50 x 200 nm²)

?

Dissolution / reprecipitation



Extended coherence length (700 x 250 nm²)

→ Biomineral crystallisation would involve ionic transfert

Concluding remarks

Inversion based microscopy methods are valuable tools for 3D x-ray microscopy

- CDI for isolated particles
- Ptychography for extended samples
- Combined with Bragg geometry for crystalline properties

→ These are mature techniques, available worldwide
Easy to implement and analyse, compatible with complex sample environment

→ Bragg ptychography is recent, available at some synchrotrons worldwide
Set-up uses nano-diffraction approach, analysis is non-trivial
Inversion is robust

4th generation synchrotron sources are expected to revolutionize the field

- Faster and smarter data acquisition schemes
- Leading to dynamical study of material-science related questions

→ Wider use of Bragg ptychography is expected

The EasyBragg project

Bragg ptychography for a wider community of users

Axis I - Development of a 3DBP **<u>user-friendly open-source suite and implementation</u>**

- at four beamlines (ID01/ID13/ESRF, I13-1/Diamond and NanoMAX/MAX IV),
- online analysis of 3DBP data acquired at these instruments,
- code freely available to synchrotrons and their user community, for further implementation at other beamlines.

Axis II - Development of a full **<u>dissemination suite</u>**

- to train and teach the BP users

→ Interested by the first tutorial? Please express our interest!

Acknowledgements

Bragg ptychography developments

M. Allain
P. Li (now in UST China)
T. Gruenewald
J. Garriga Ferrer
P. Godard (now in Poitiers)
F. Mastropietro (now in Bordeaux)

D. Carbone

M. Burghammer
S. Leake
V. Favre Nicolin
T. Metzger

Universidad Zaragoza

I. Calvo-Almazan

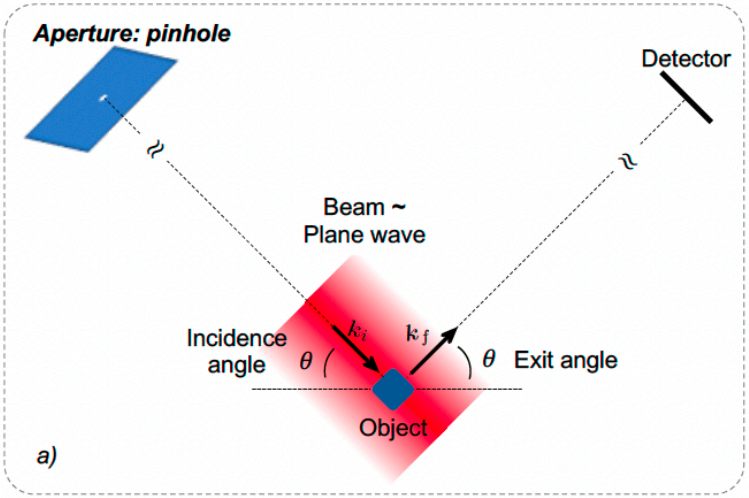
Bragg ptychography applications

F. Hofmann
N. Phillips

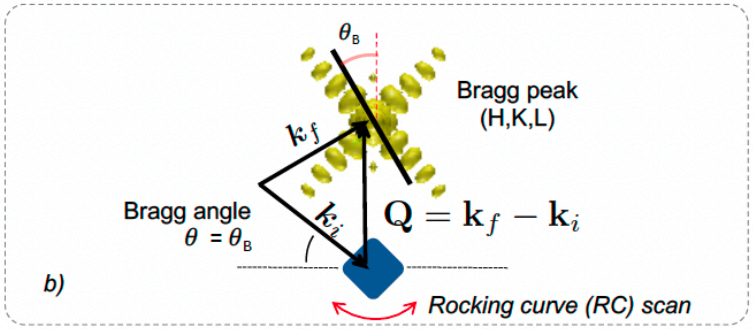
C. Chevallard
C. Colas

www.fresnel.fr/comix

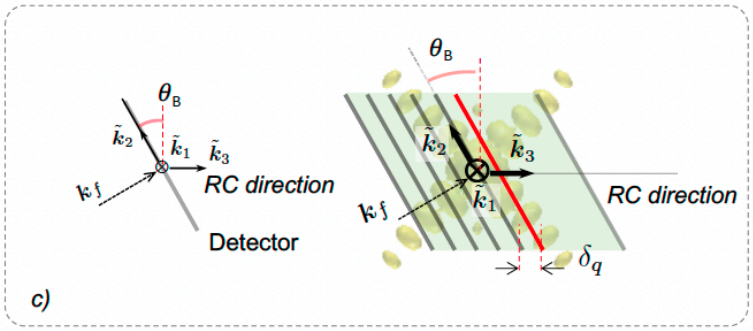
Experimental geometry



Coherent illumination (plane wave-like)
of the particle in Bragg condition



Use of a 2D detector
to finely sample the diffraction pattern



Angular exploration along the rocking curve
to acquire 3D information

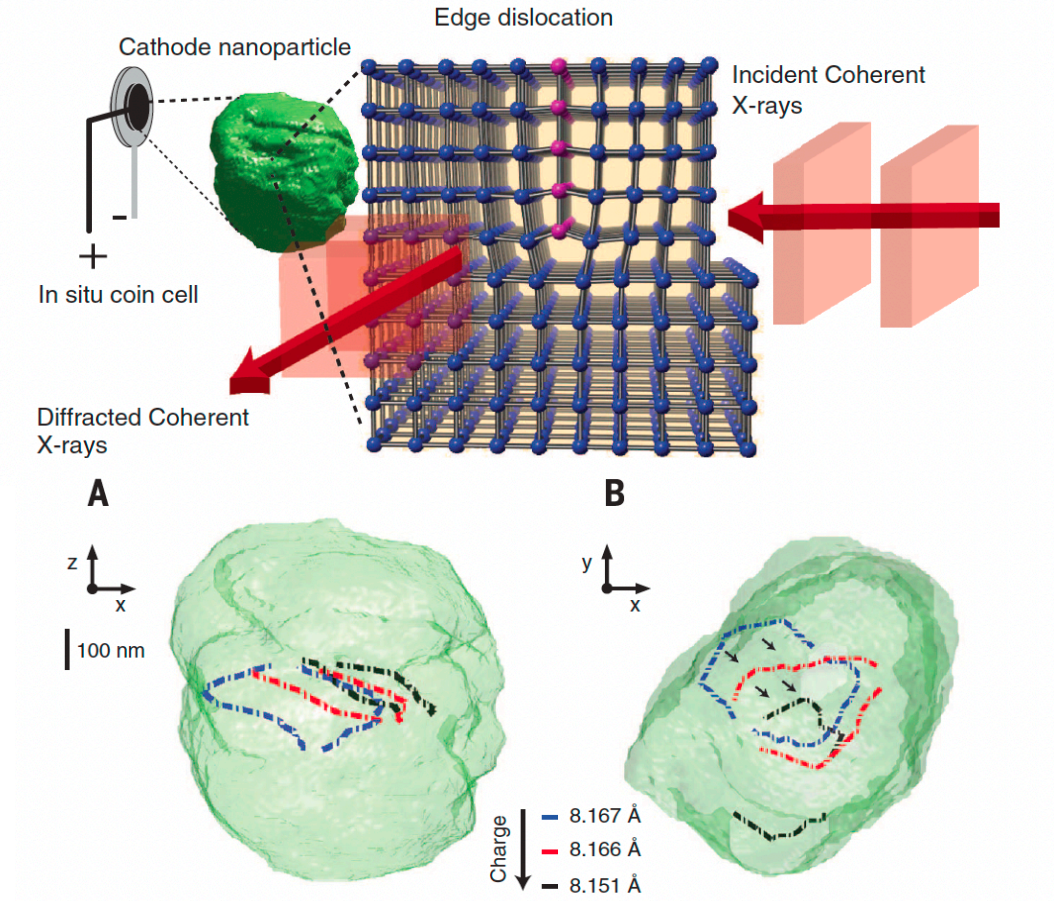
Calvo-Almazan et al., under revision

BCDI – a mature technique

Dislocation dynamics under external stimuli

Operando battery nanoparticles

Ulvestad et al., Science 2015



See also, mechanical loading, *e.g.*,

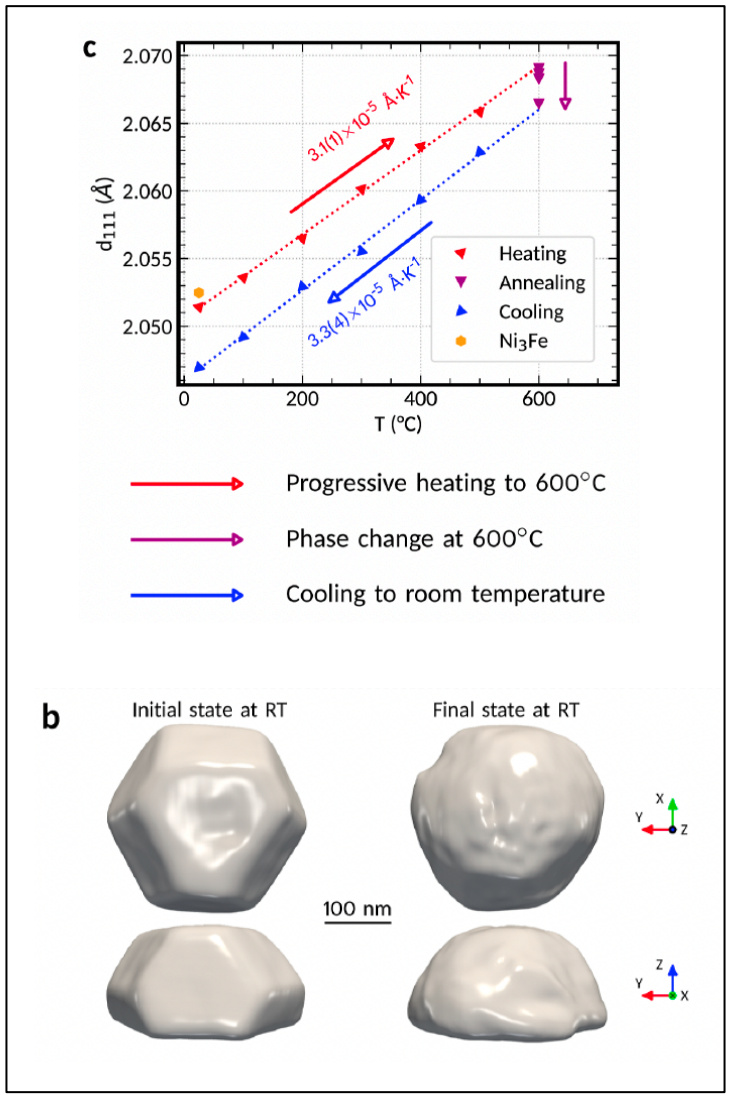
Dupraz et al., Nano Lett. 2017

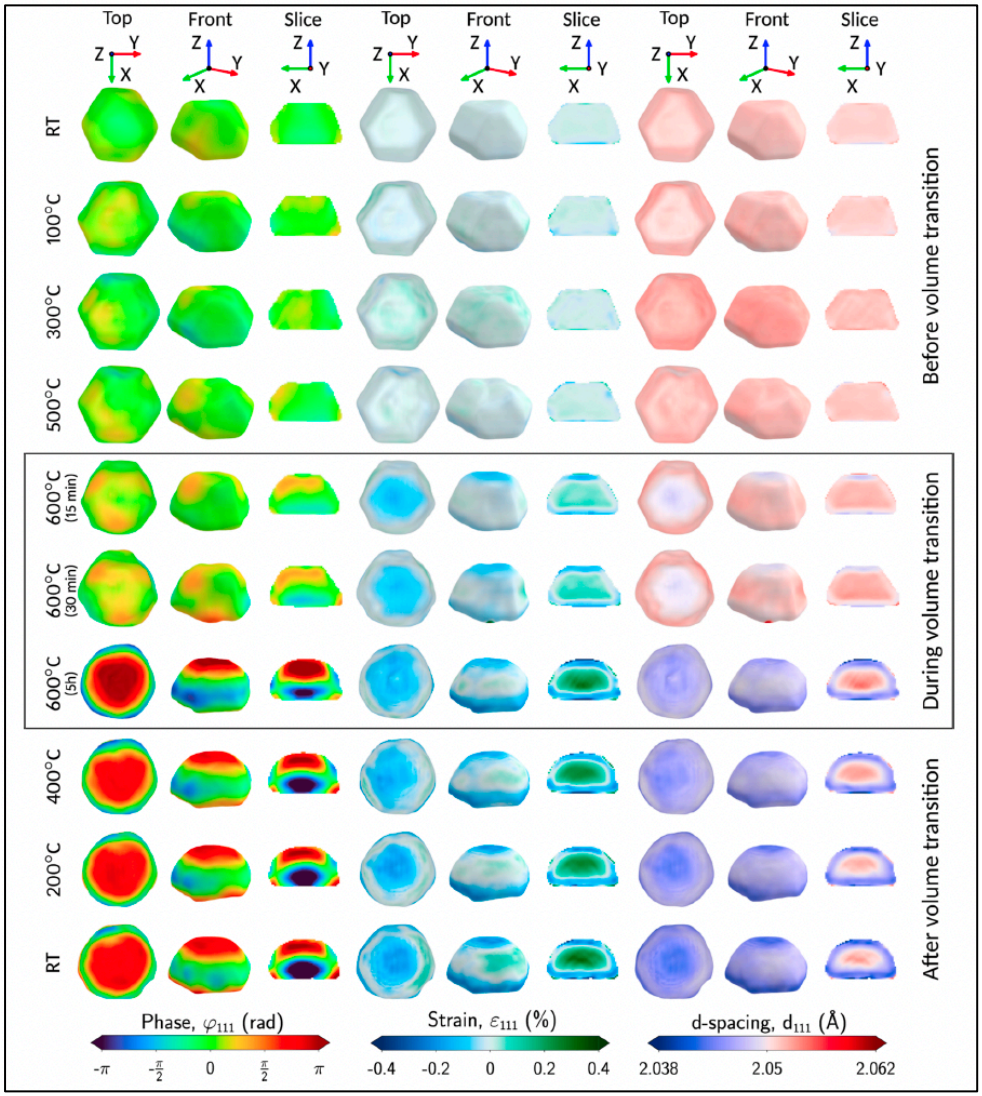
BCDI – a mature technique

Phase transition / phase separation

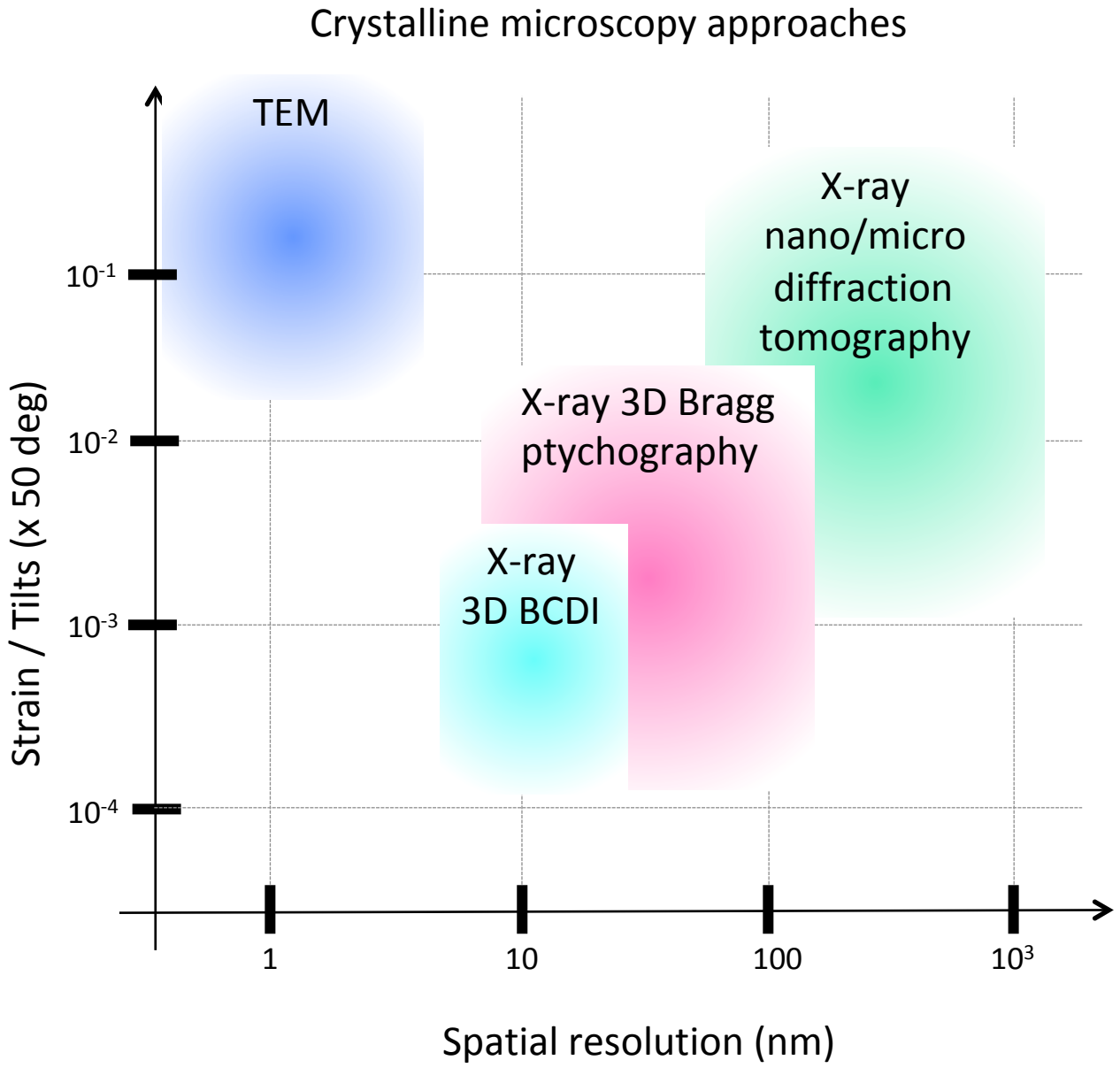
Solid-state transition of a Ni_3Fe nanoparticule towards a Ni_3Fe –Ni core-shell particles

Chatelier et al., ACS Nano 2024





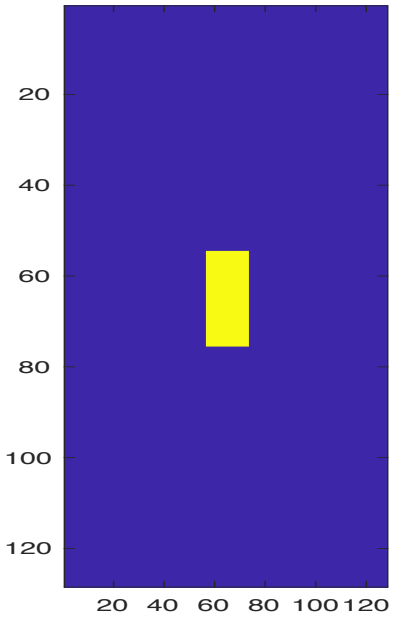
Positioning of inversion microscopy wrt to other techniques



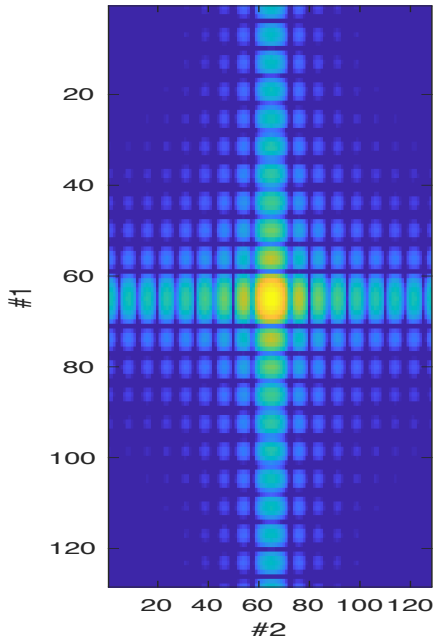
Introducing oversampling

In other words: It is possible to retrieve the phase of the measured intensity if intensity signal is **oversampled**

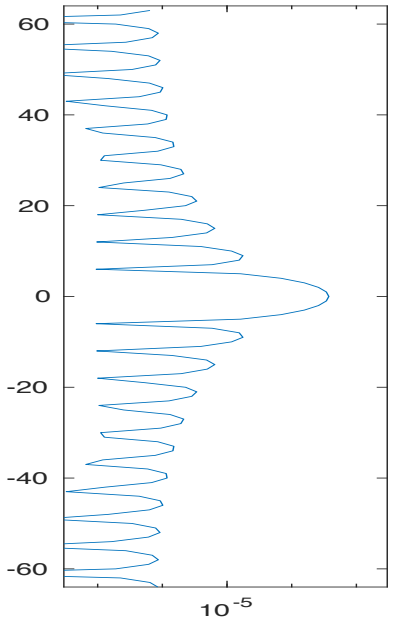
Object



Intensity



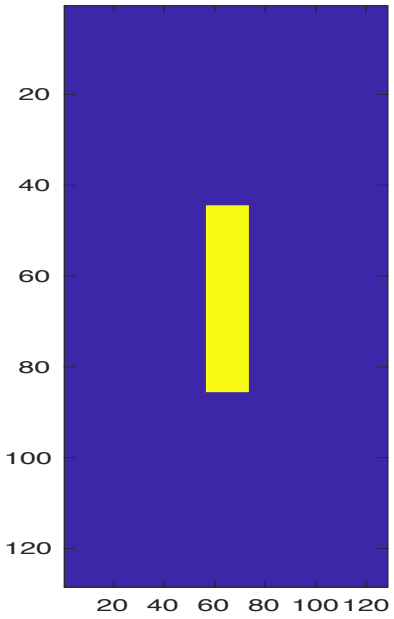
Intensity (cut)



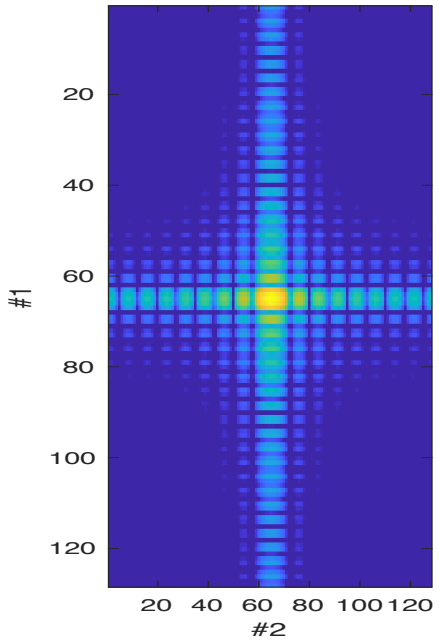
Introducing oversampling

In other words: It is possible to retrieve the phase of the measured intensity if intensity signal is **oversampled**

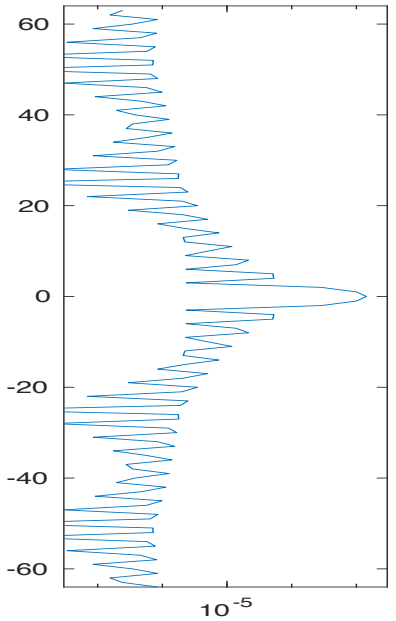
Object



Intensity



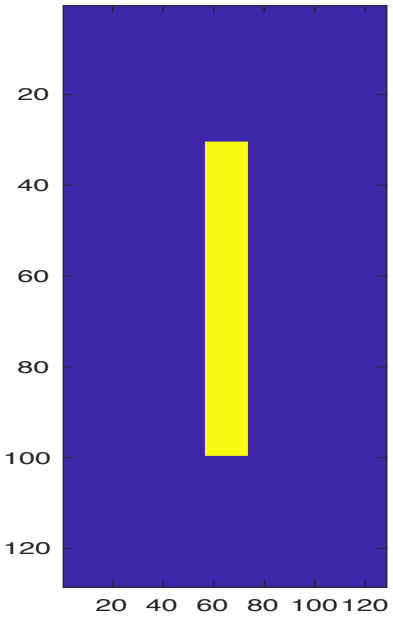
Intensity (cut)



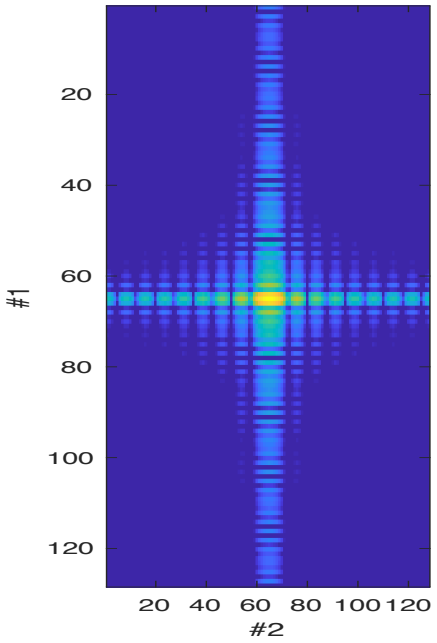
Introducing oversampling

In other words: It is possible to retrieve the phase of the measured intensity if intensity signal is **oversampled**

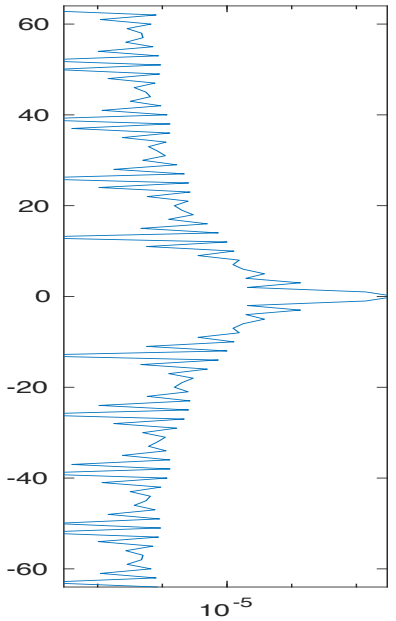
Object



Intensity



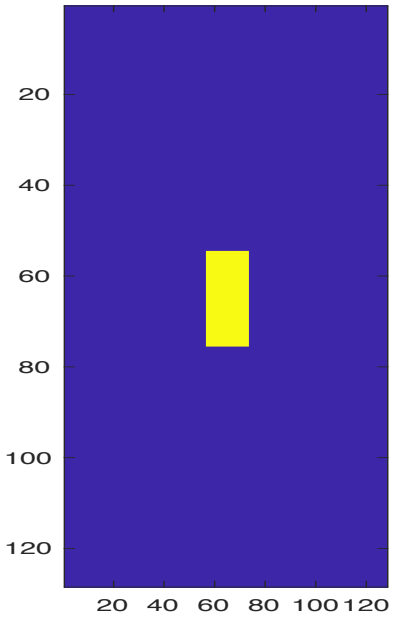
Intensity (cut)



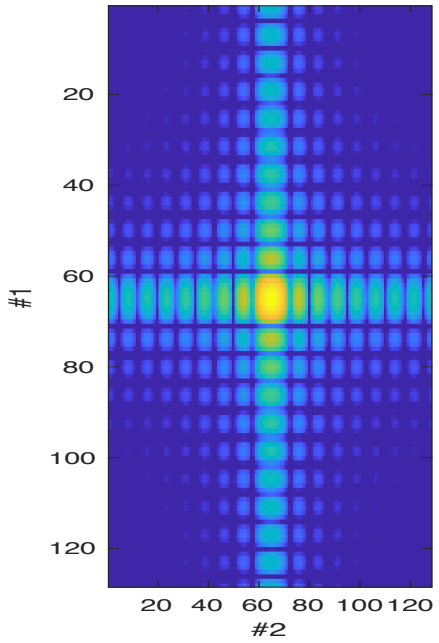
Introducing oversampling

In other words: It is possible to retrieve the phase of the measured intensity if intensity signal is **oversampled**

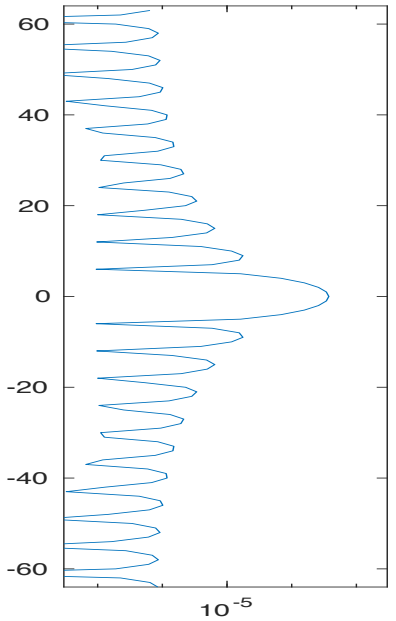
Object



Intensity

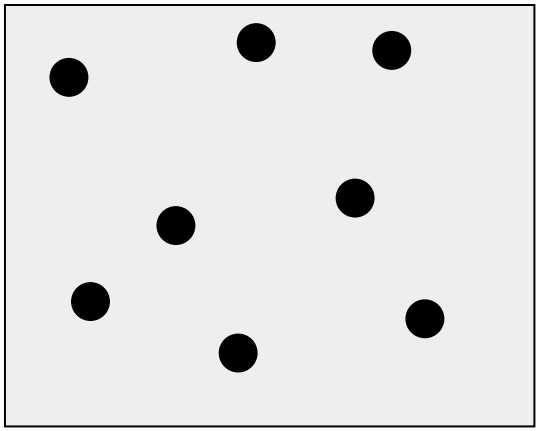


Intensity (cut)

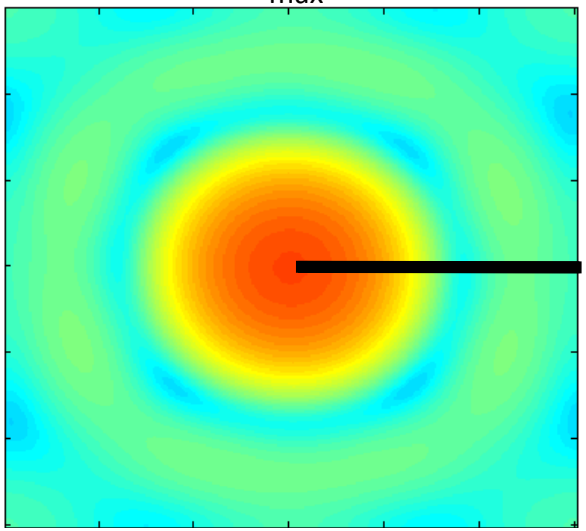


→ Increase sample to detector distance (1 m)
→ Decrease sample size (1 μm)

Information available in a diffraction pattern

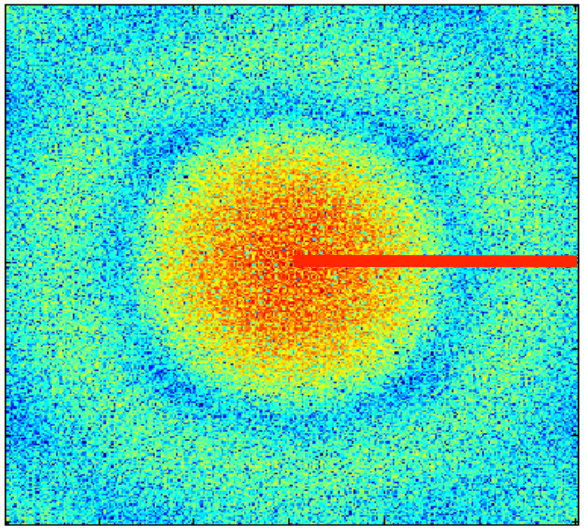


$\delta r = 2\pi/q_{max} \approx 5$ nm



incoherent scattering

δr + exact particle distribution



coherent scattering

Sensitivity to

- the particle shape
- the particle position