Introduction to Coherent Diffraction Imaging

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APS 34-ID-C

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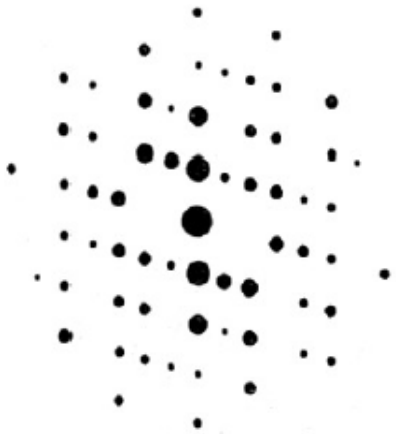
Workshop on Round Beams
SOLEIL
June 2017

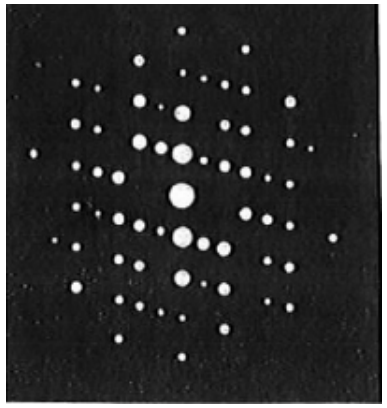
Outline

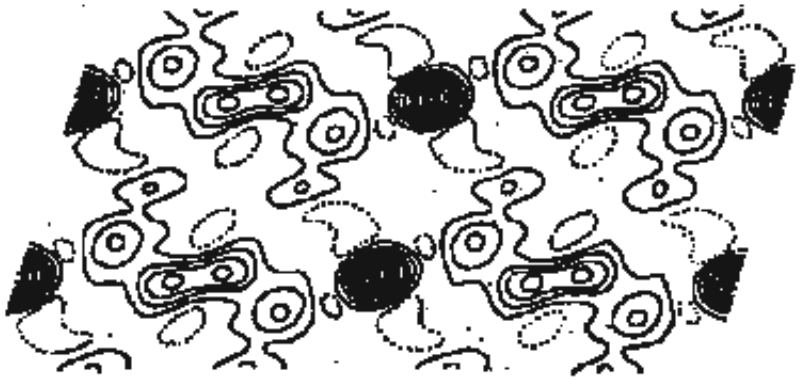
- Bragg Coherent Diffraction Imaging
- Crystal strain as complex density
- Dislocations Visualised
- Nanoparticle Alloying
- Bragg Projection Ptychography

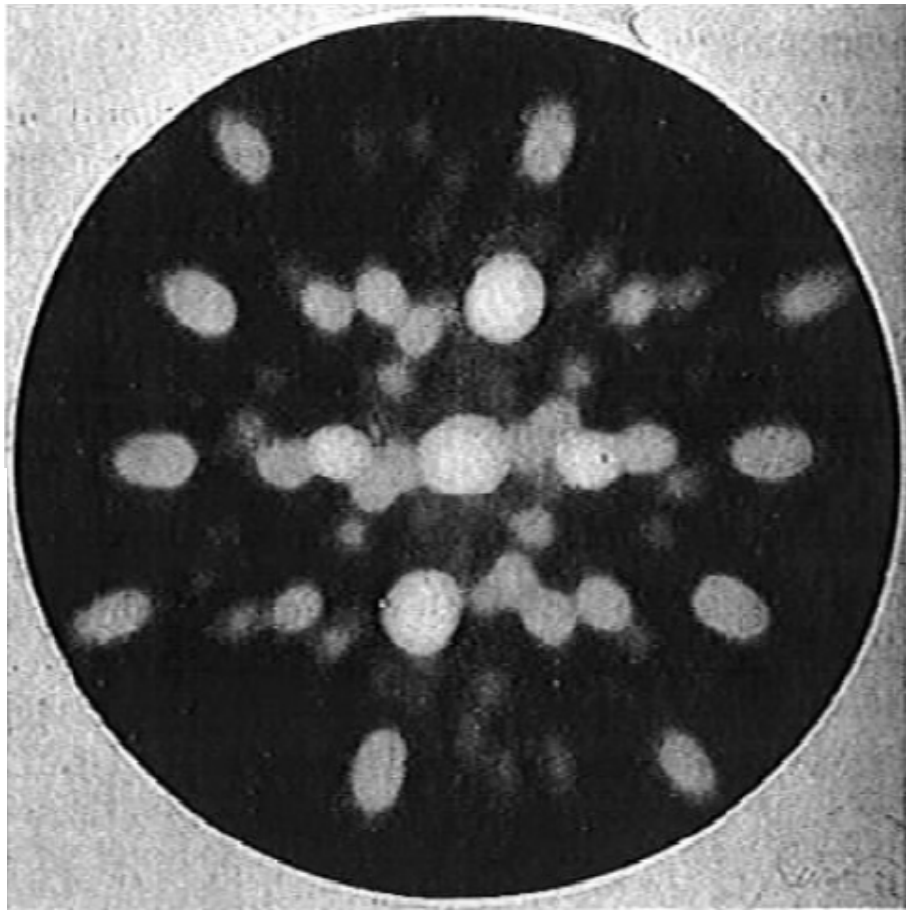
Bragg's "X-ray Microscope"

W.L.Bragg Nature, 143, 678 (1939): diopside, $CaMg(SiO_3)_2$



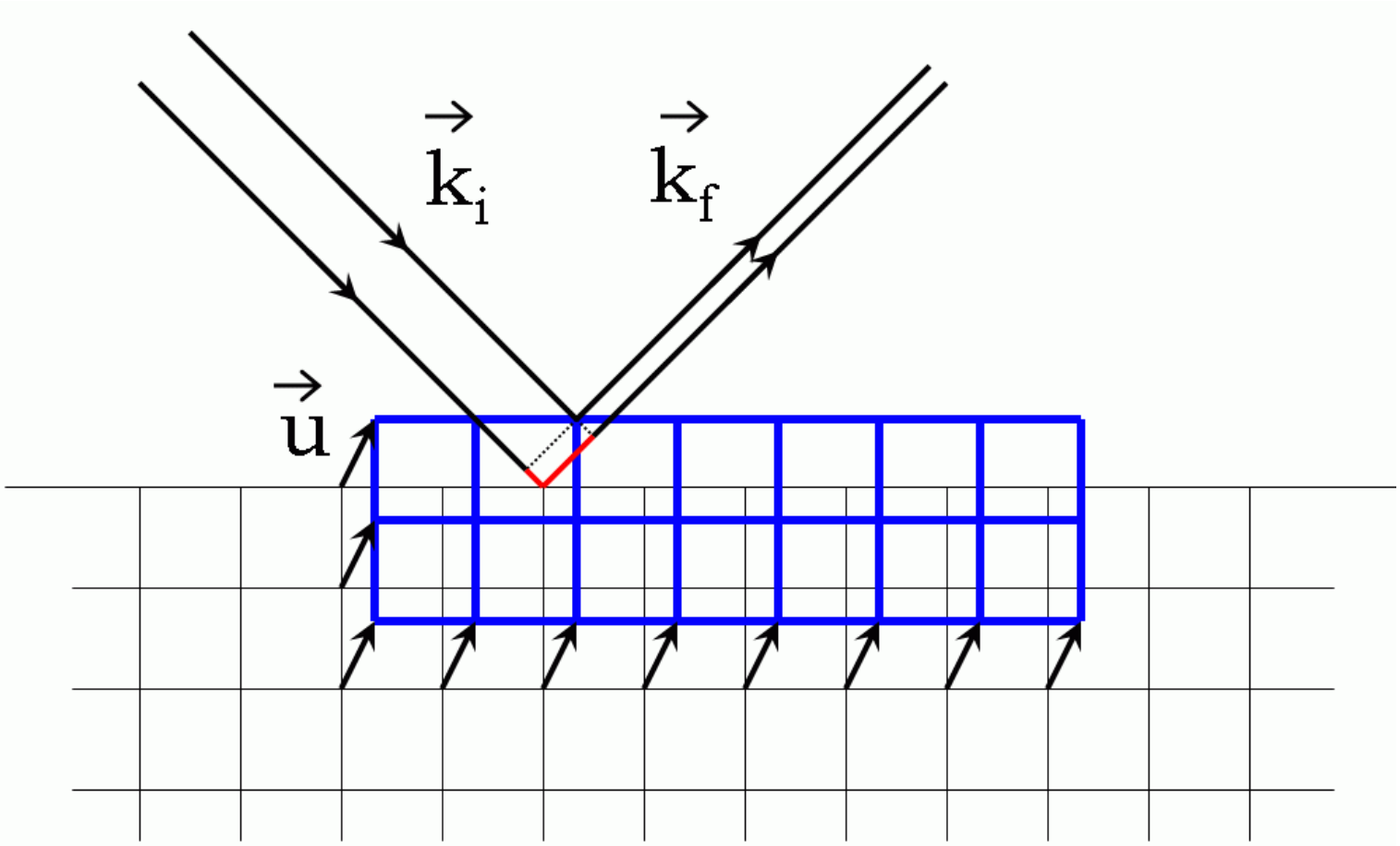




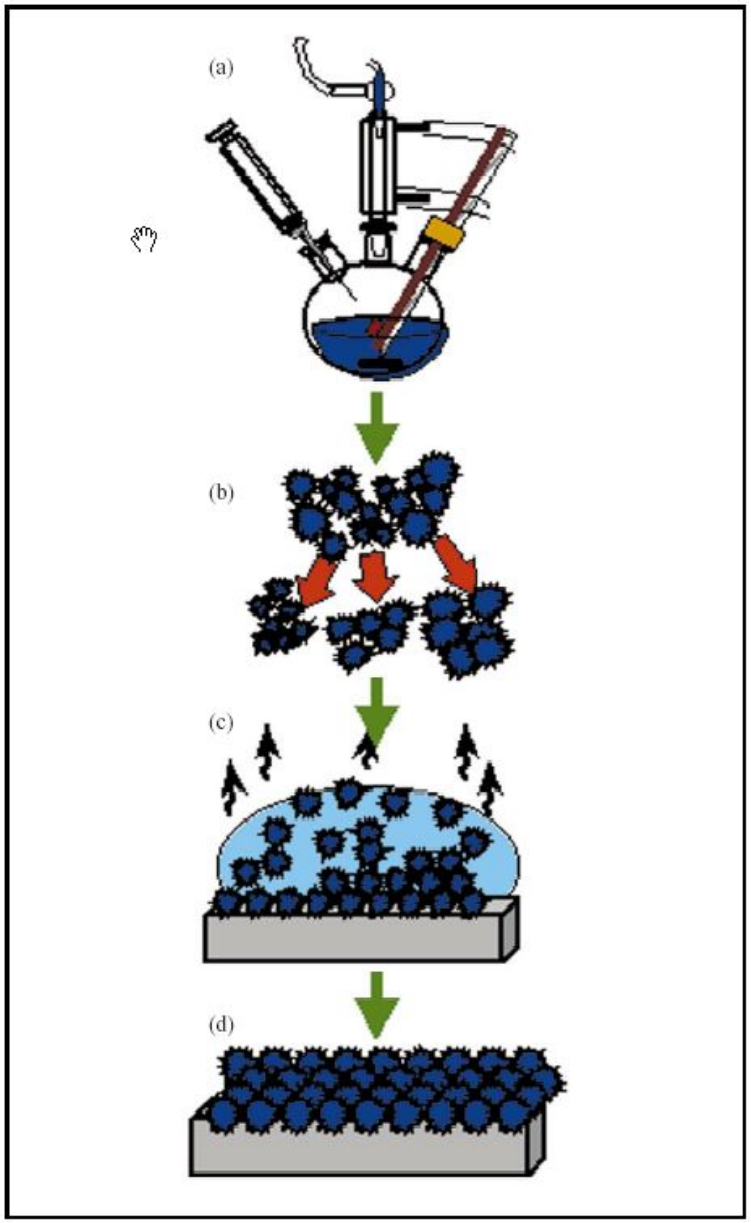


Sensitivity to strain

$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$

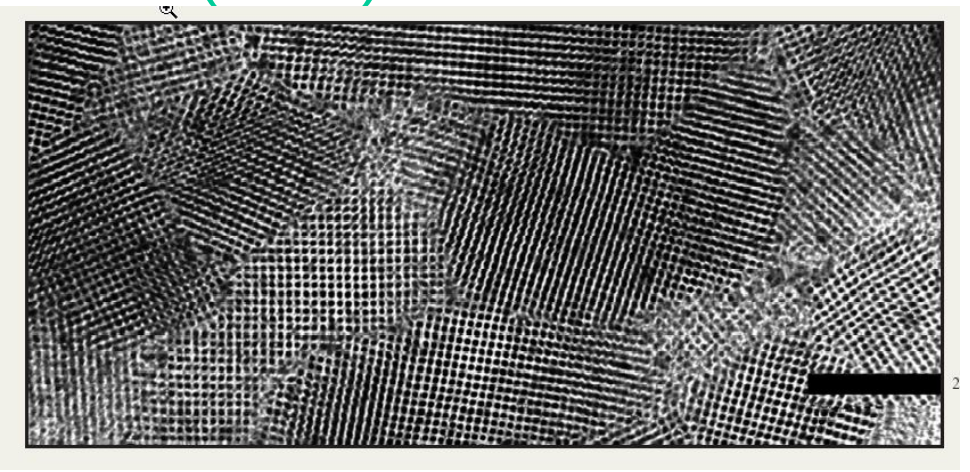


Chemical Synthesis of Nanocrystals

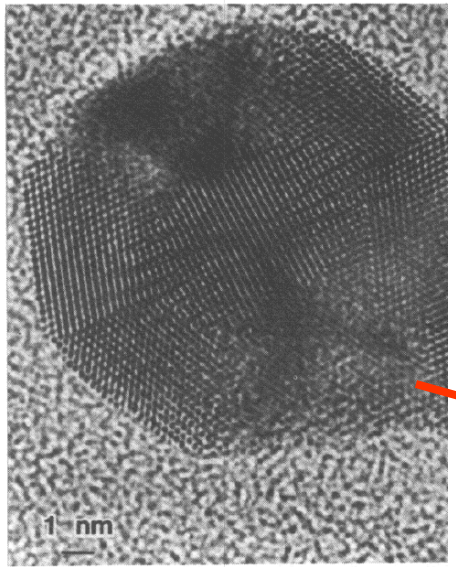


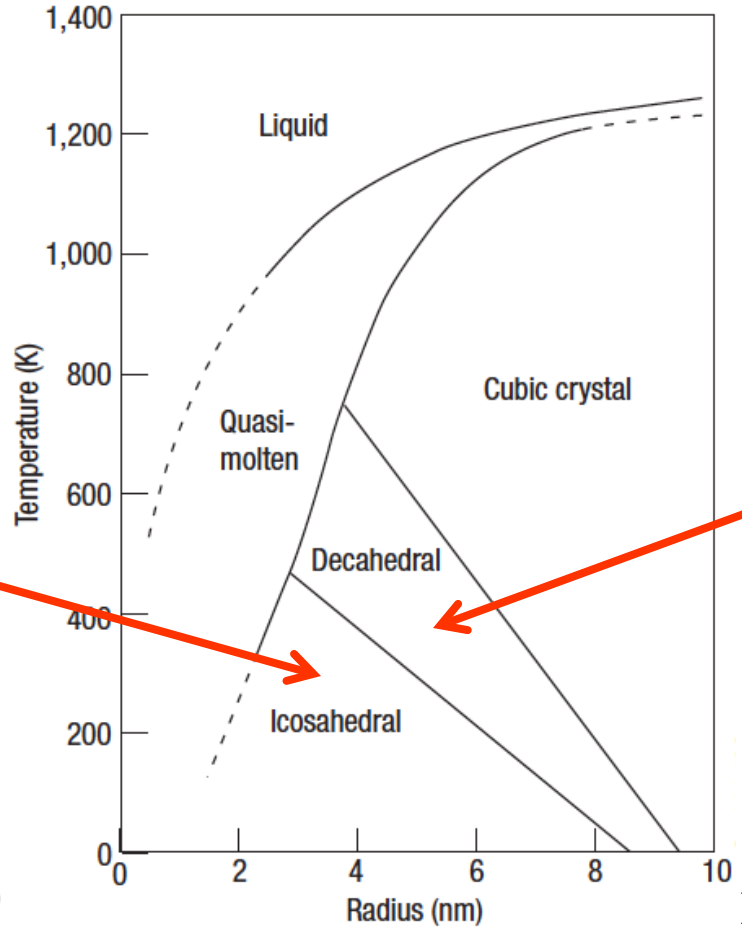
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

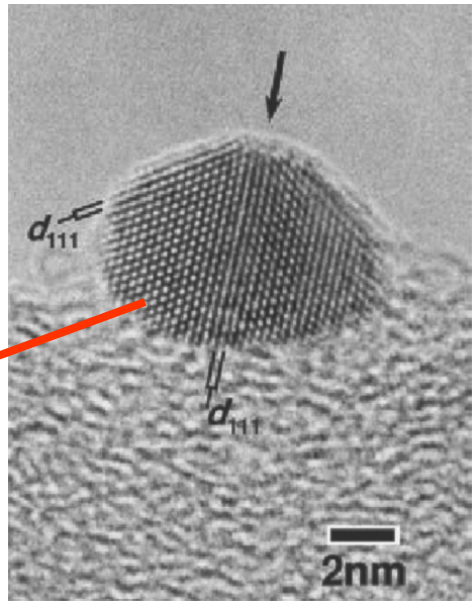
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



Structure of Gold vs Size



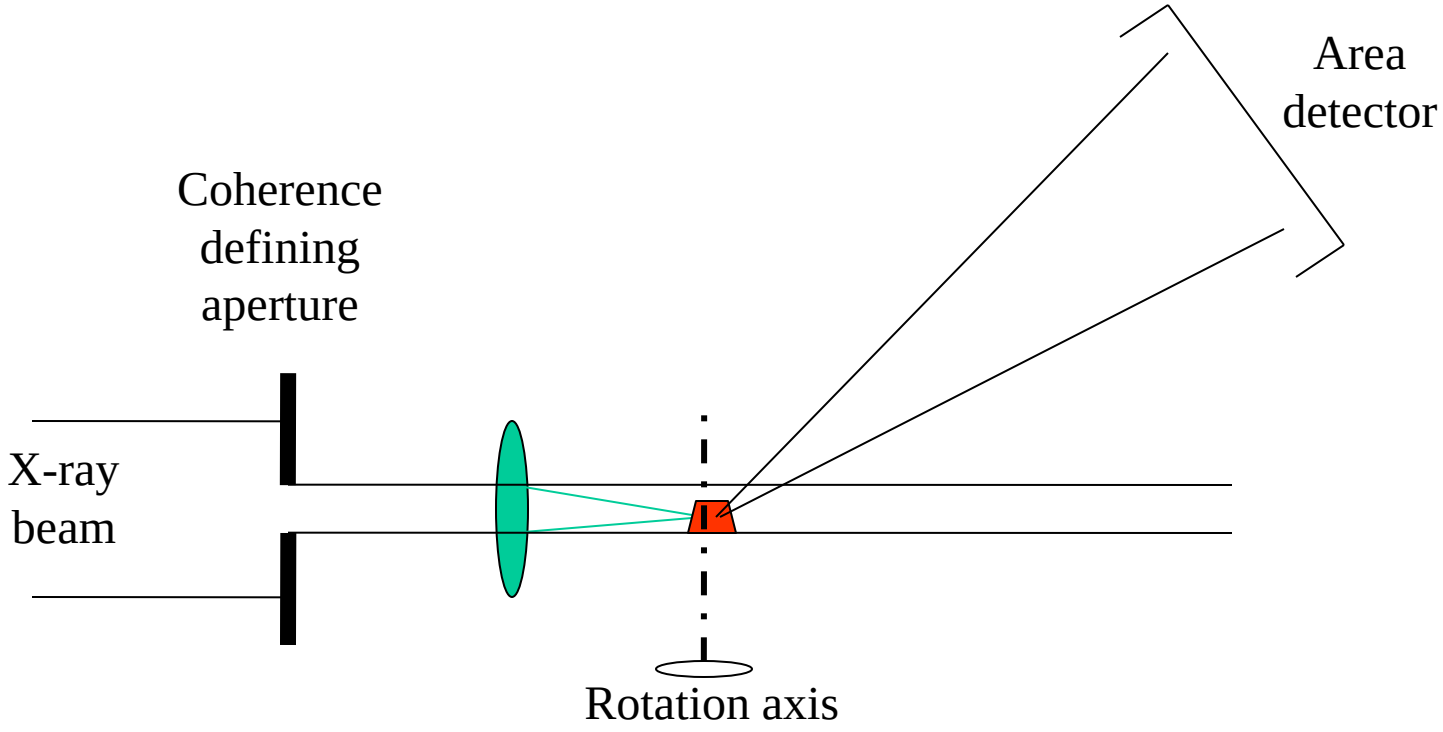


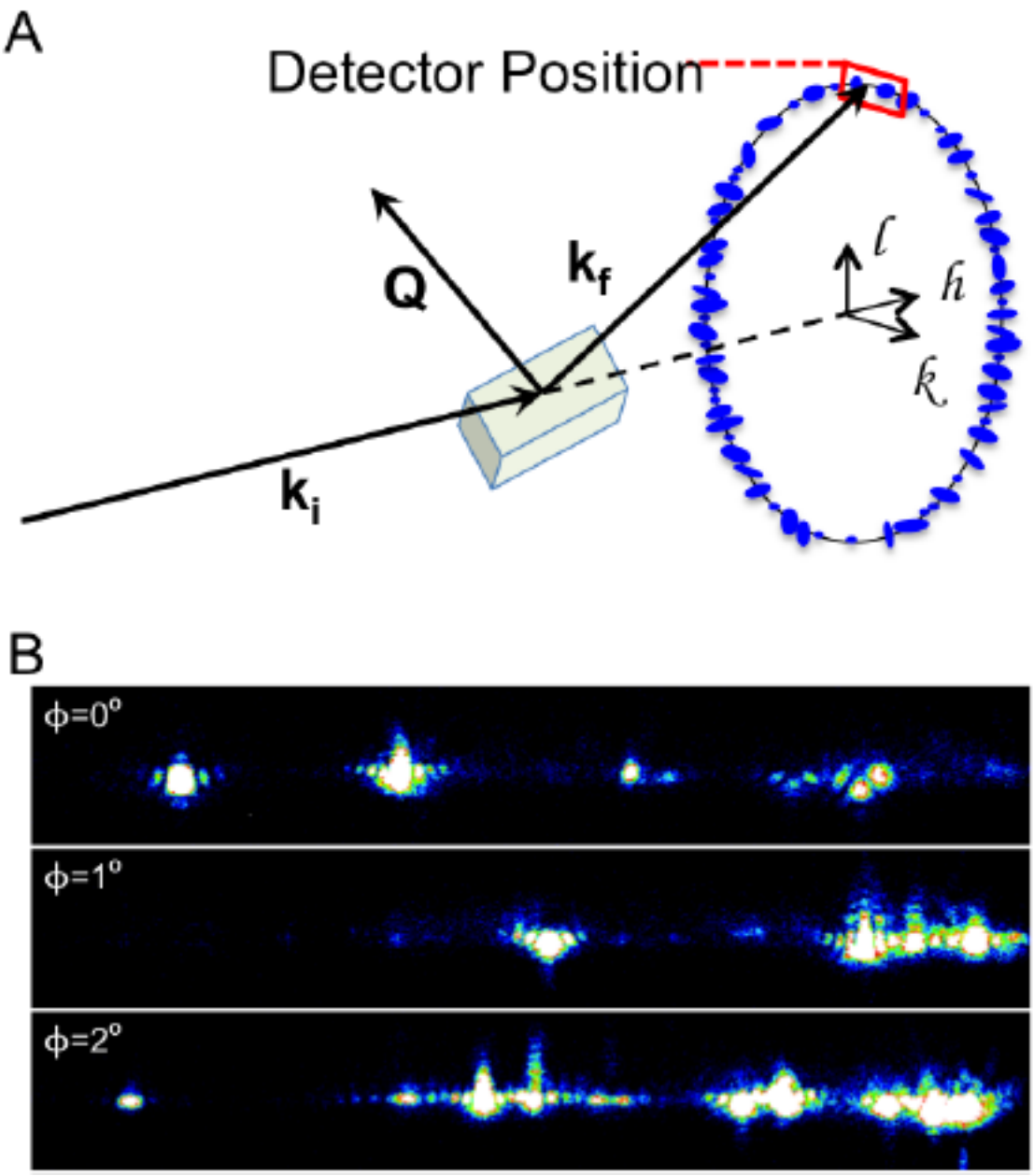


L. D. Marks, RPP (1994)

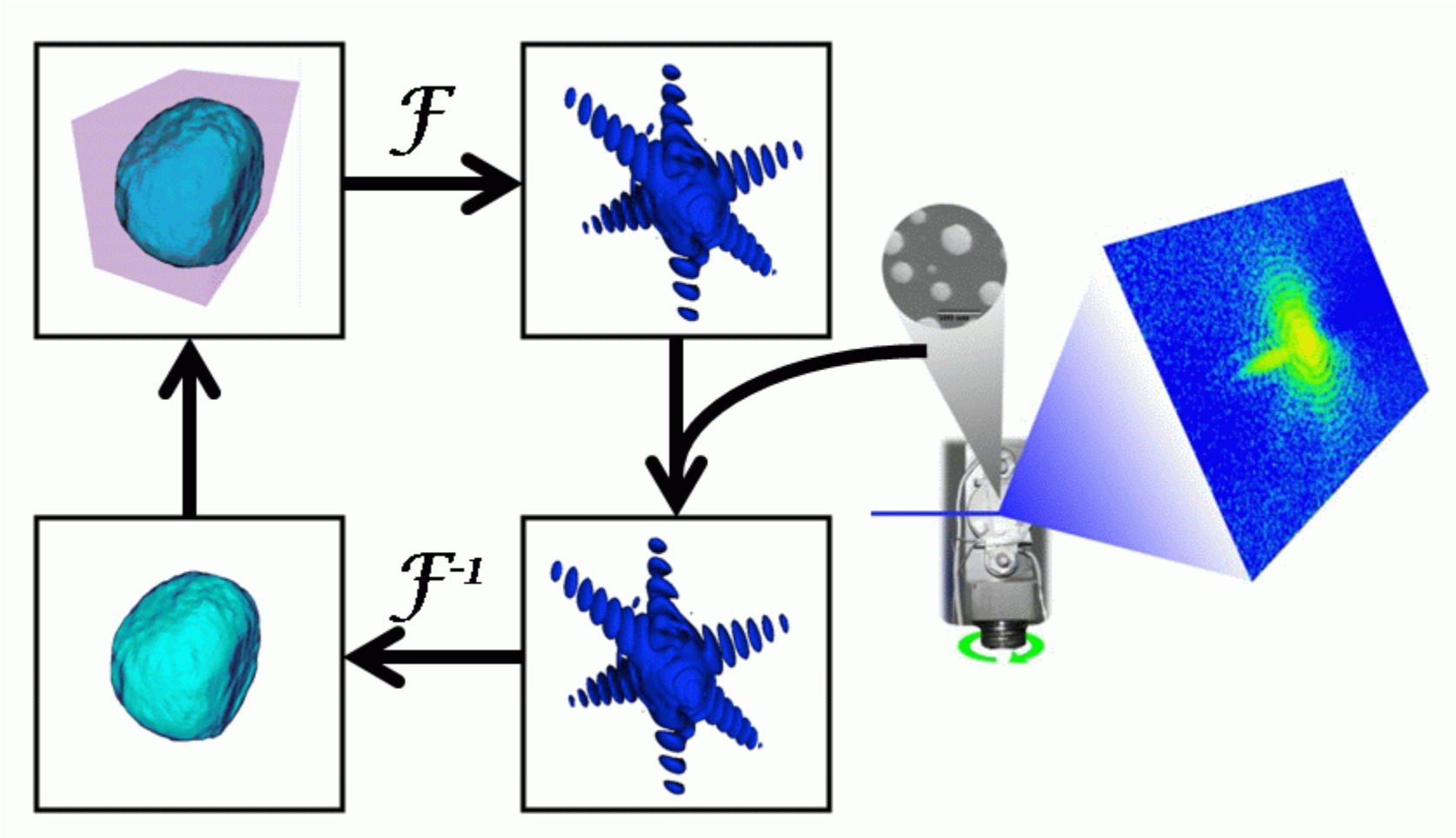
Koga and Sugawara (2003)

Lensless X-ray Microscope, 2003




A
Detector Position
Q
k_f
k_i
l
h
k
B
ϕ=0°
ϕ=1°
ϕ=2°

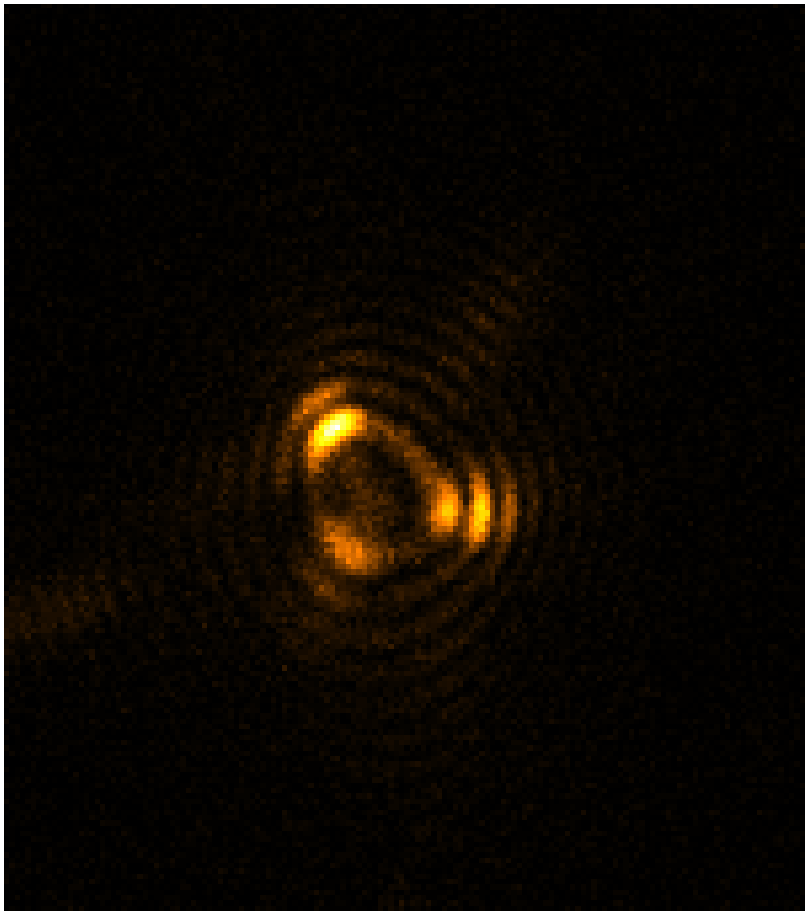
Generic “Error Reduction” method

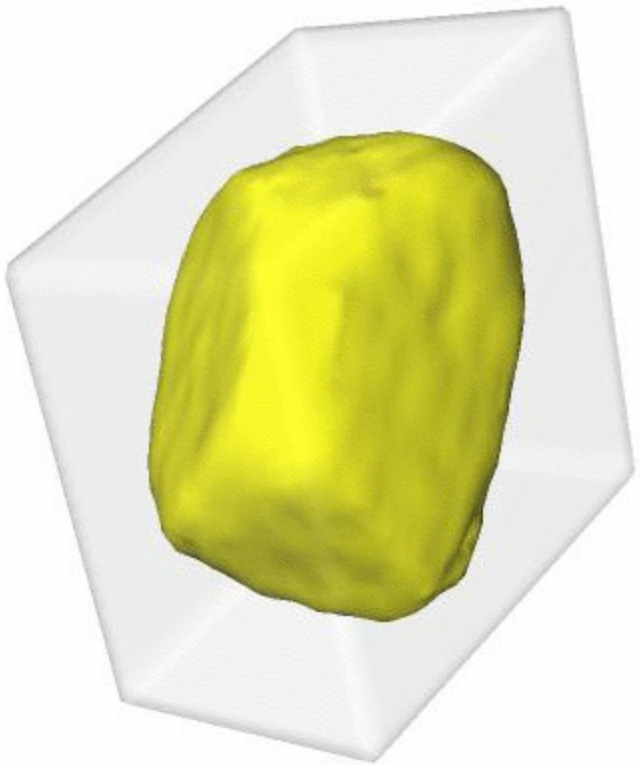


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

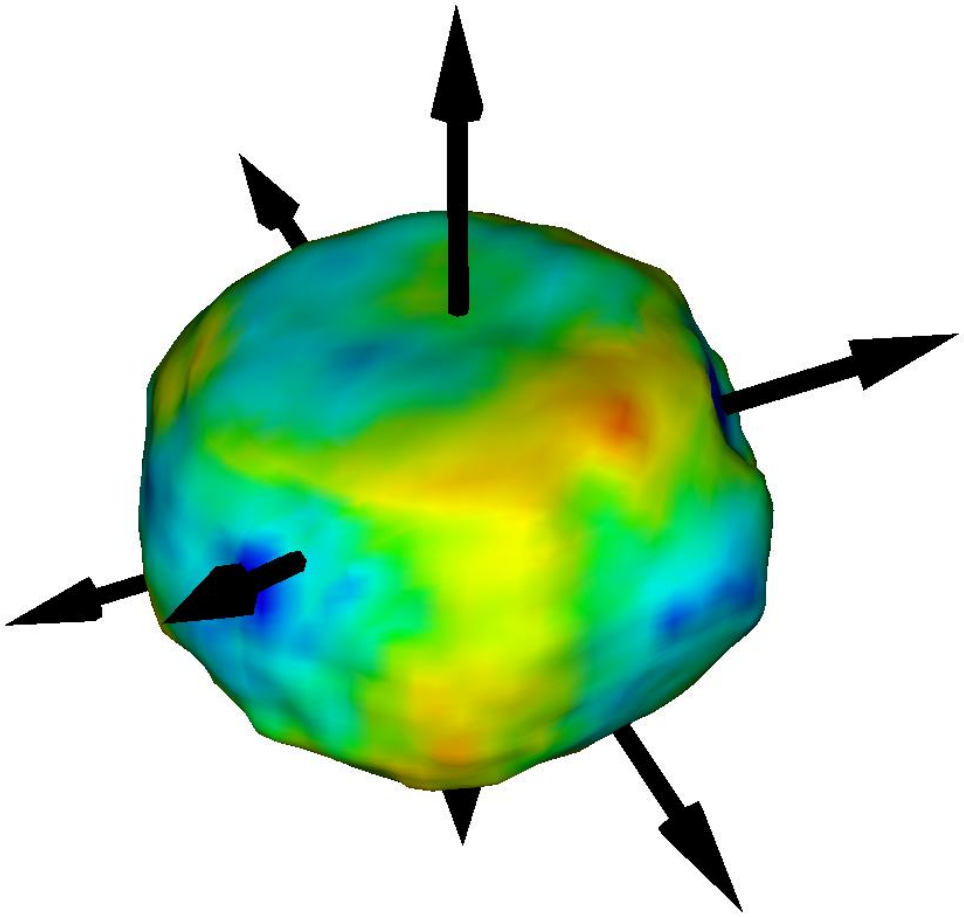
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



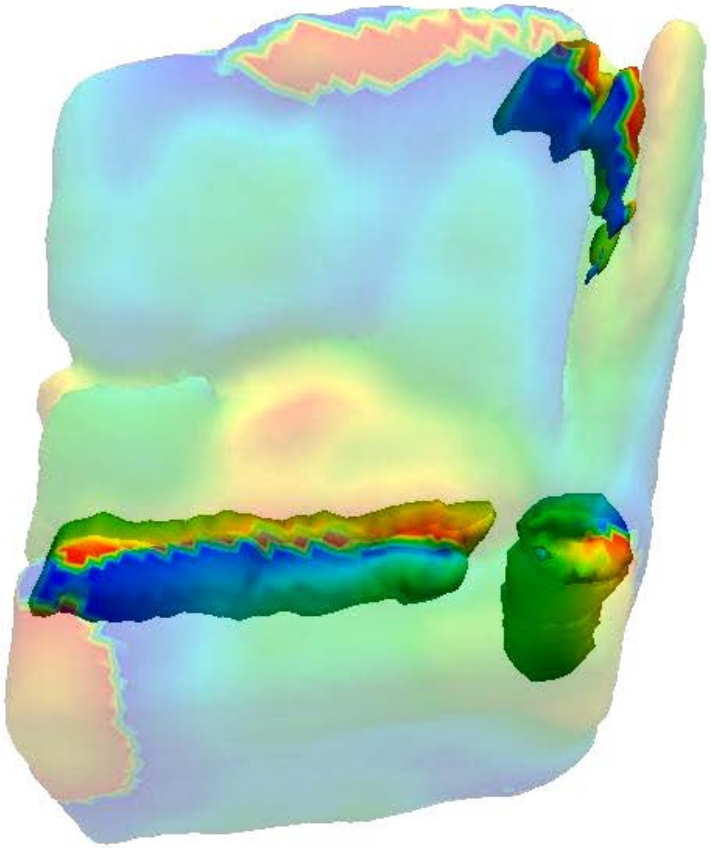


Phase isosurface of residual strain



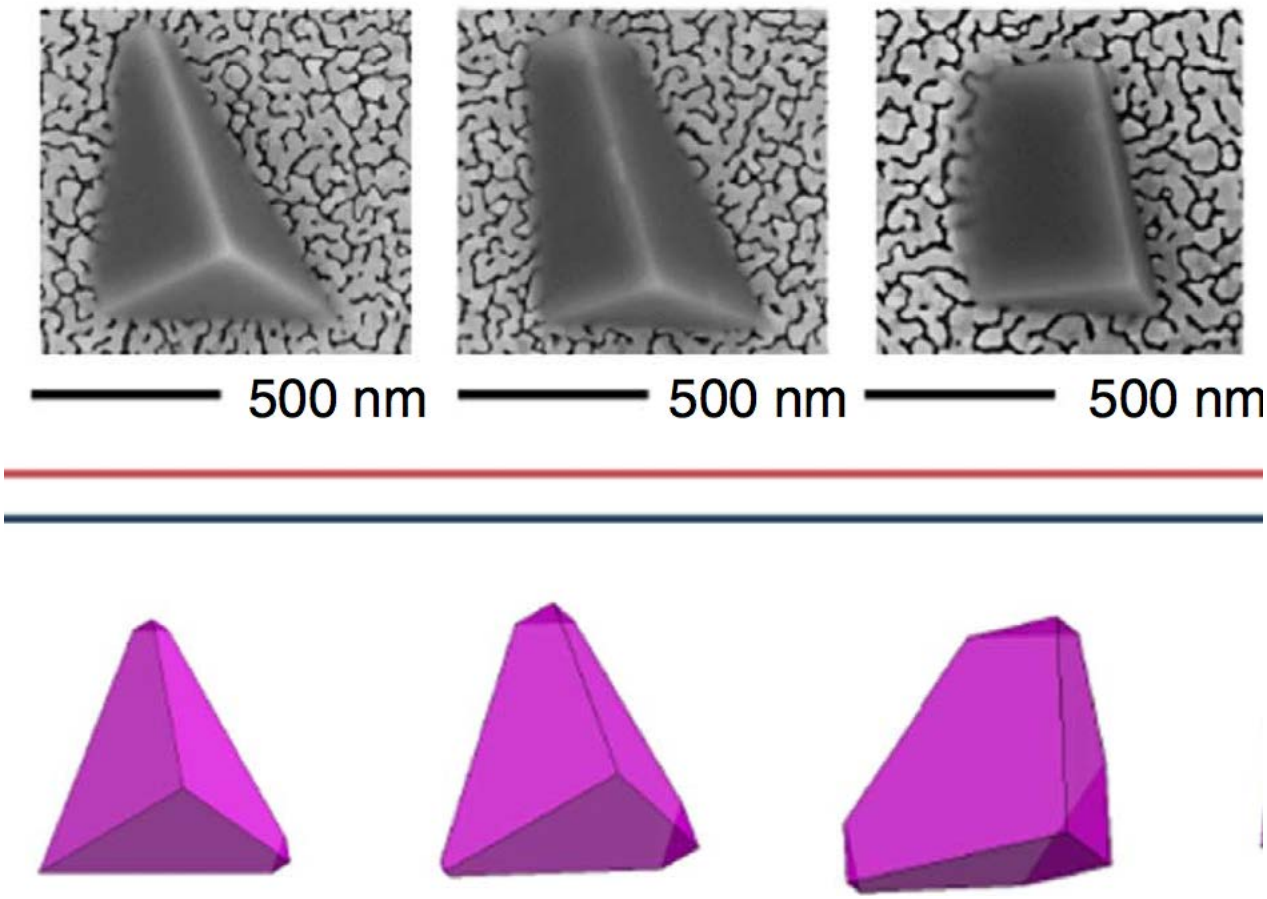
Screw dislocations in Calcite

Jesse Clark, Johannes Ihli et al, PNAS (2015)



Calcite growth on SAM/Au(111)

J. Ihli, J. N. Clark, et al, N. Comms **7** 11878 (2016)



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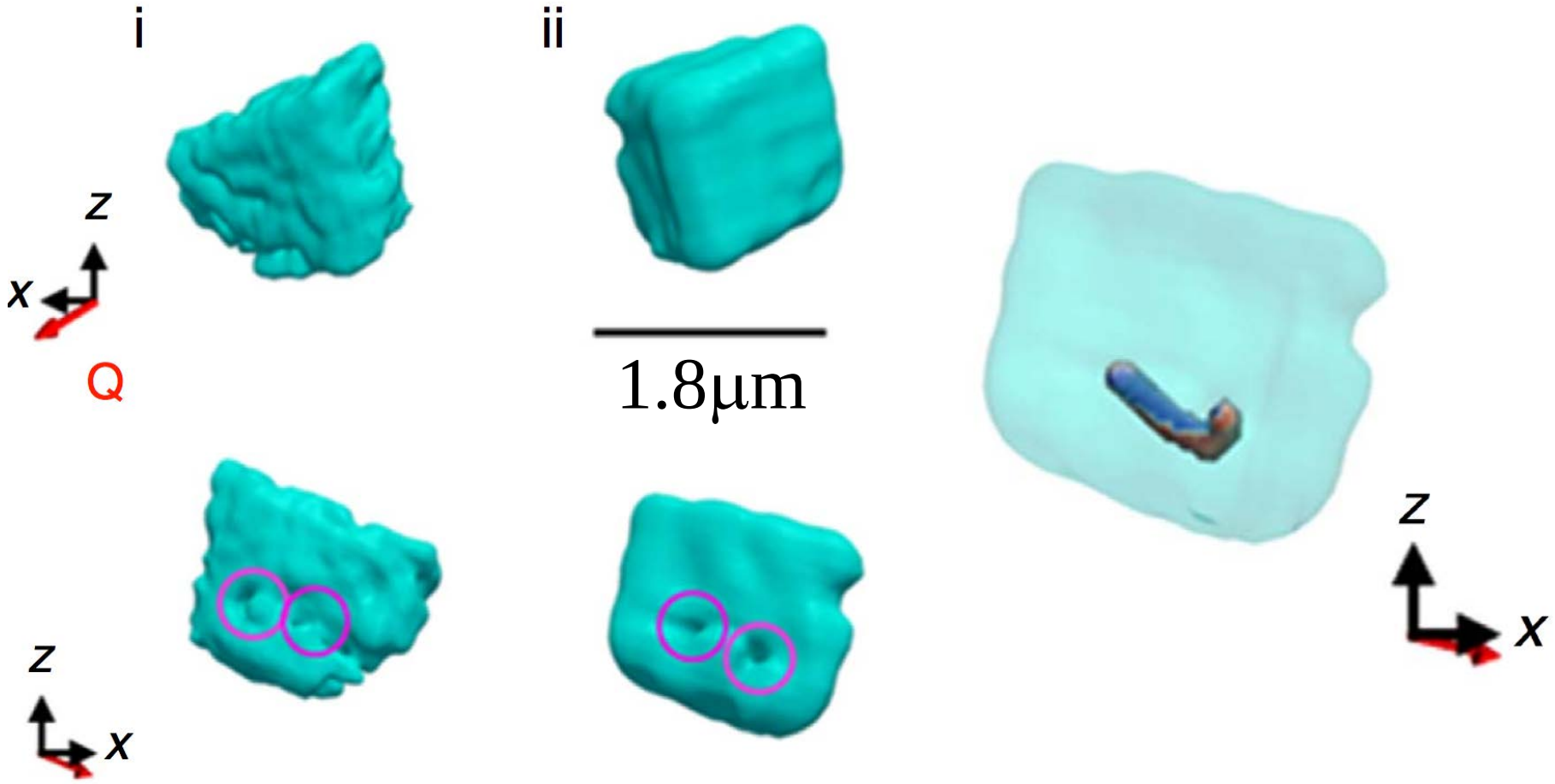

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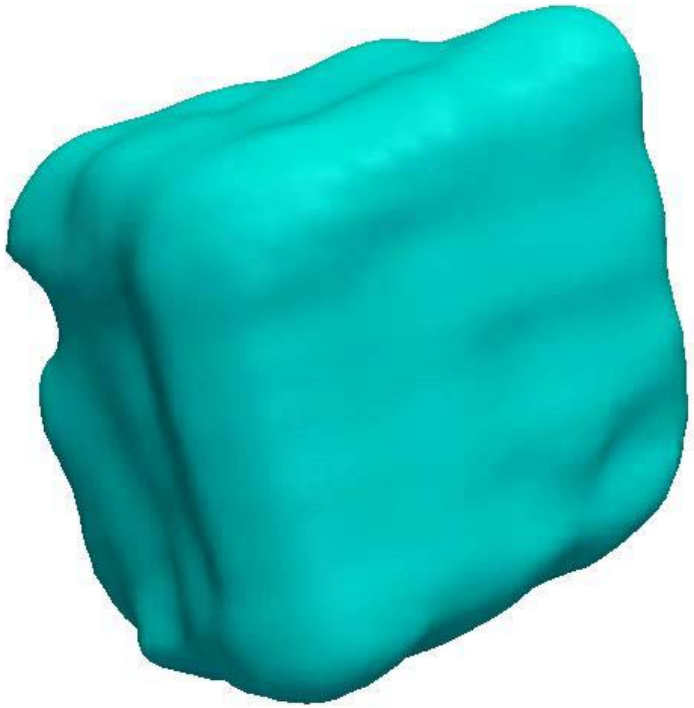
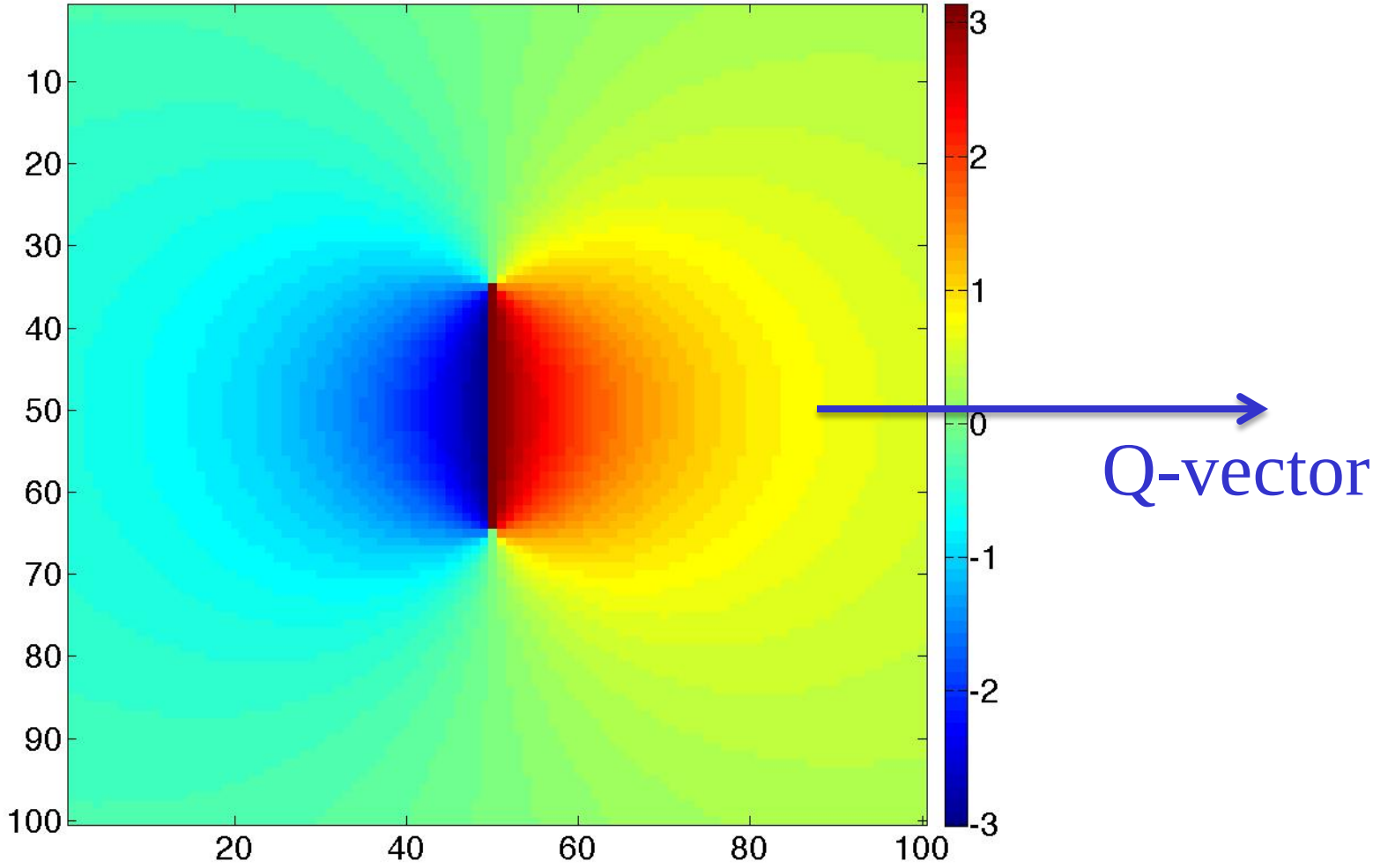
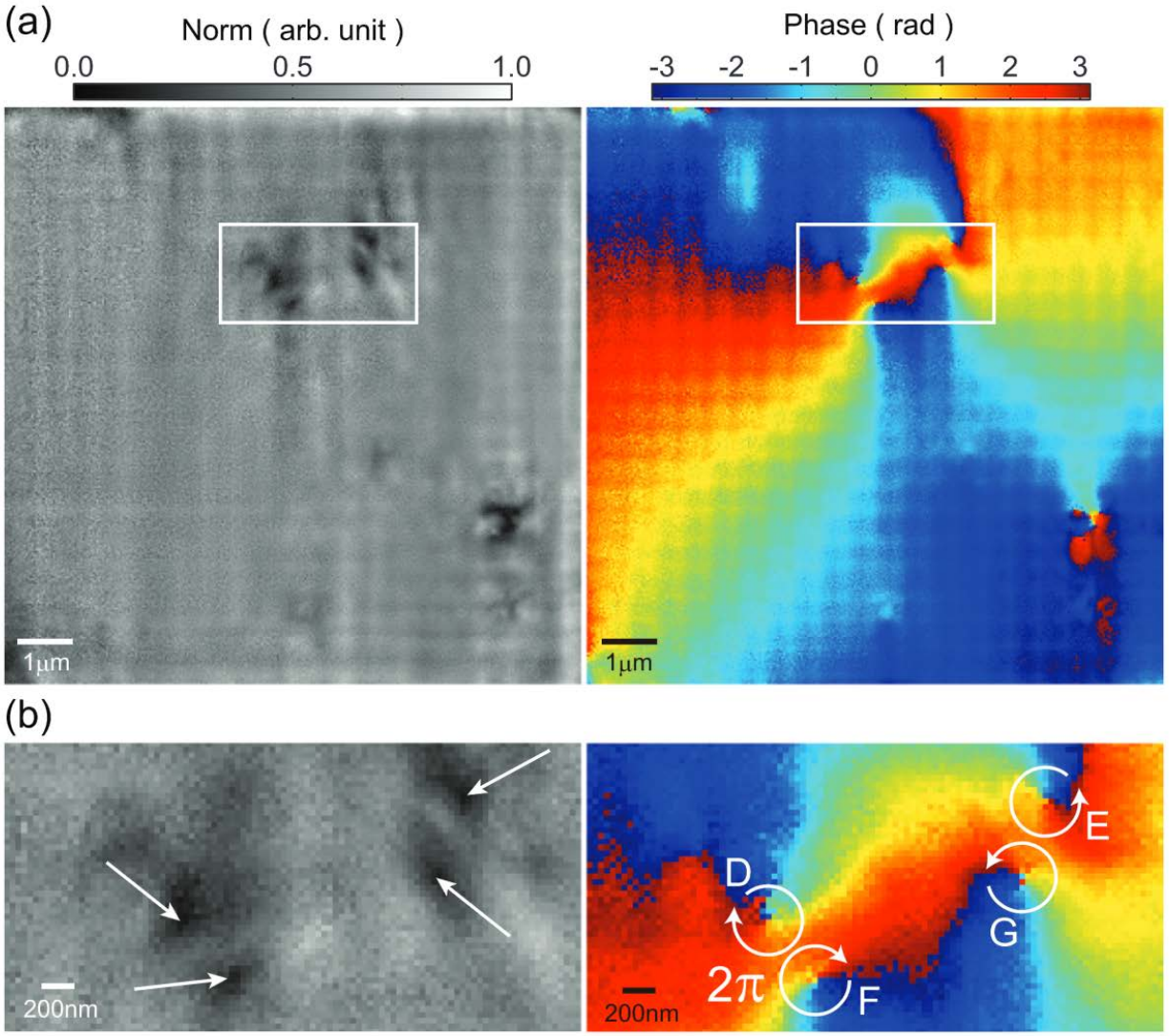


Strain field of Edge Dislocation Loop



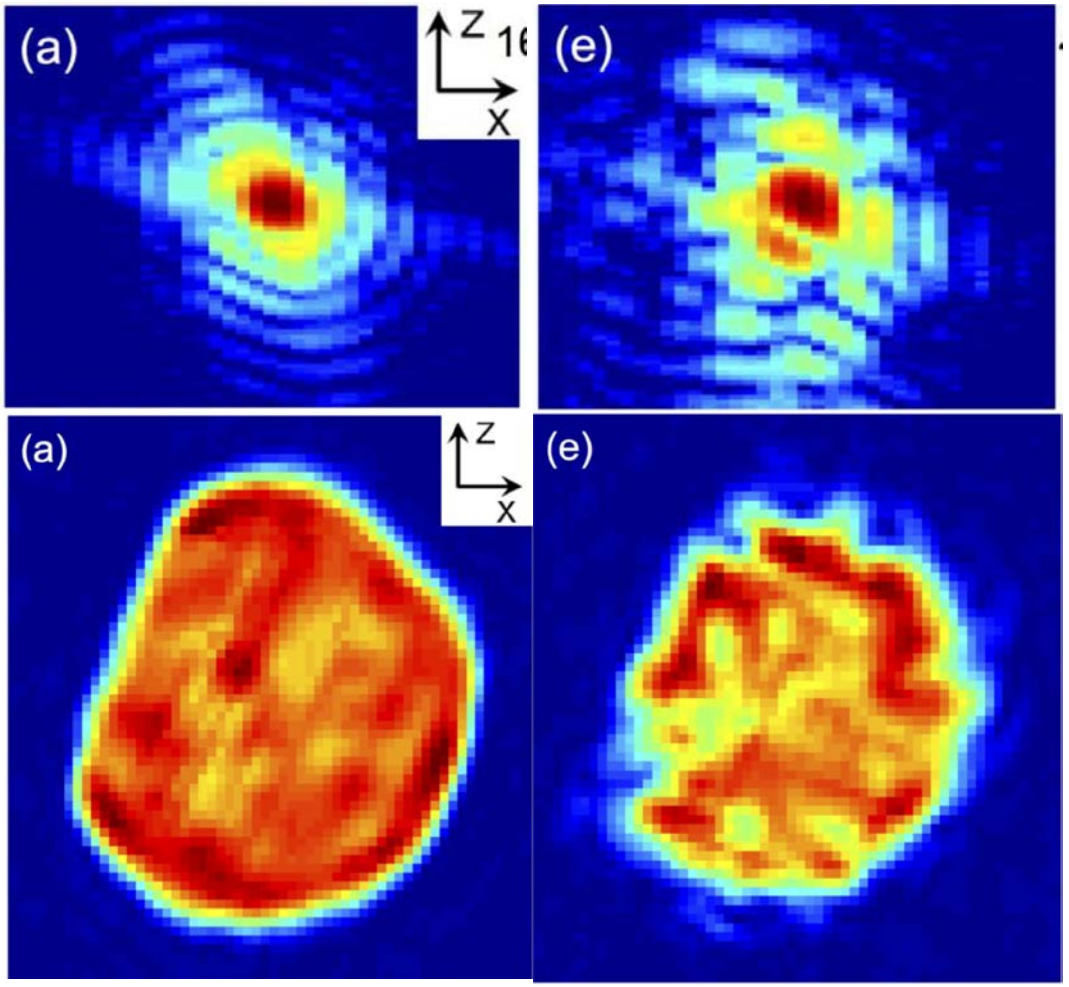
Ptychography of Dislocation Loops

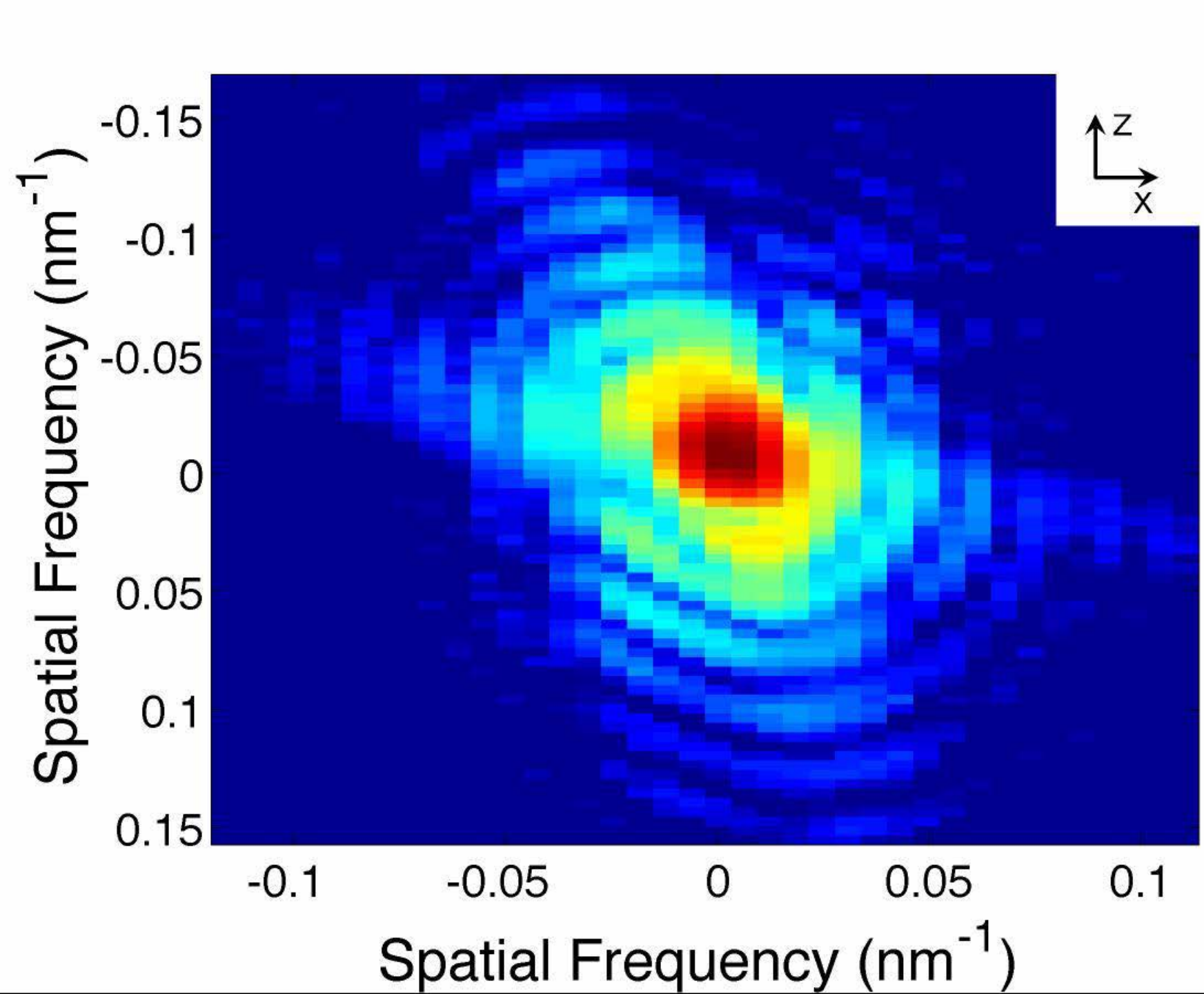
Y. Takahashi et al Phys Rev B **87** 121201 (2013)



Copper Diffusion into Gold Nanocrystal

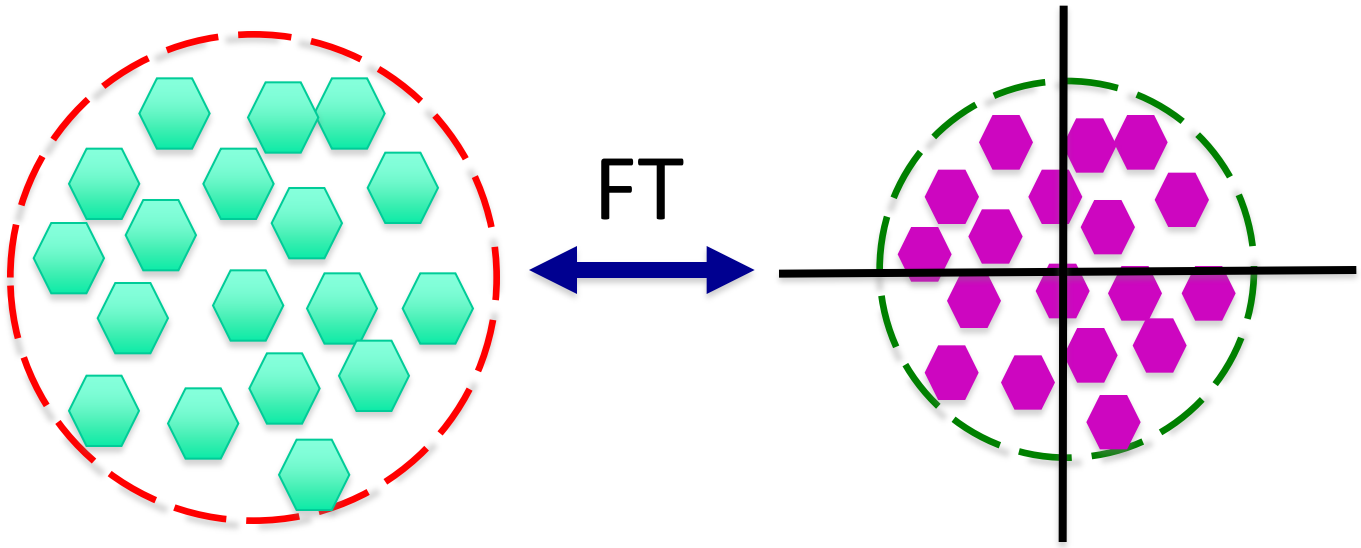
Gang Xiong, et al, Sci Rep 4 6765 (2013)

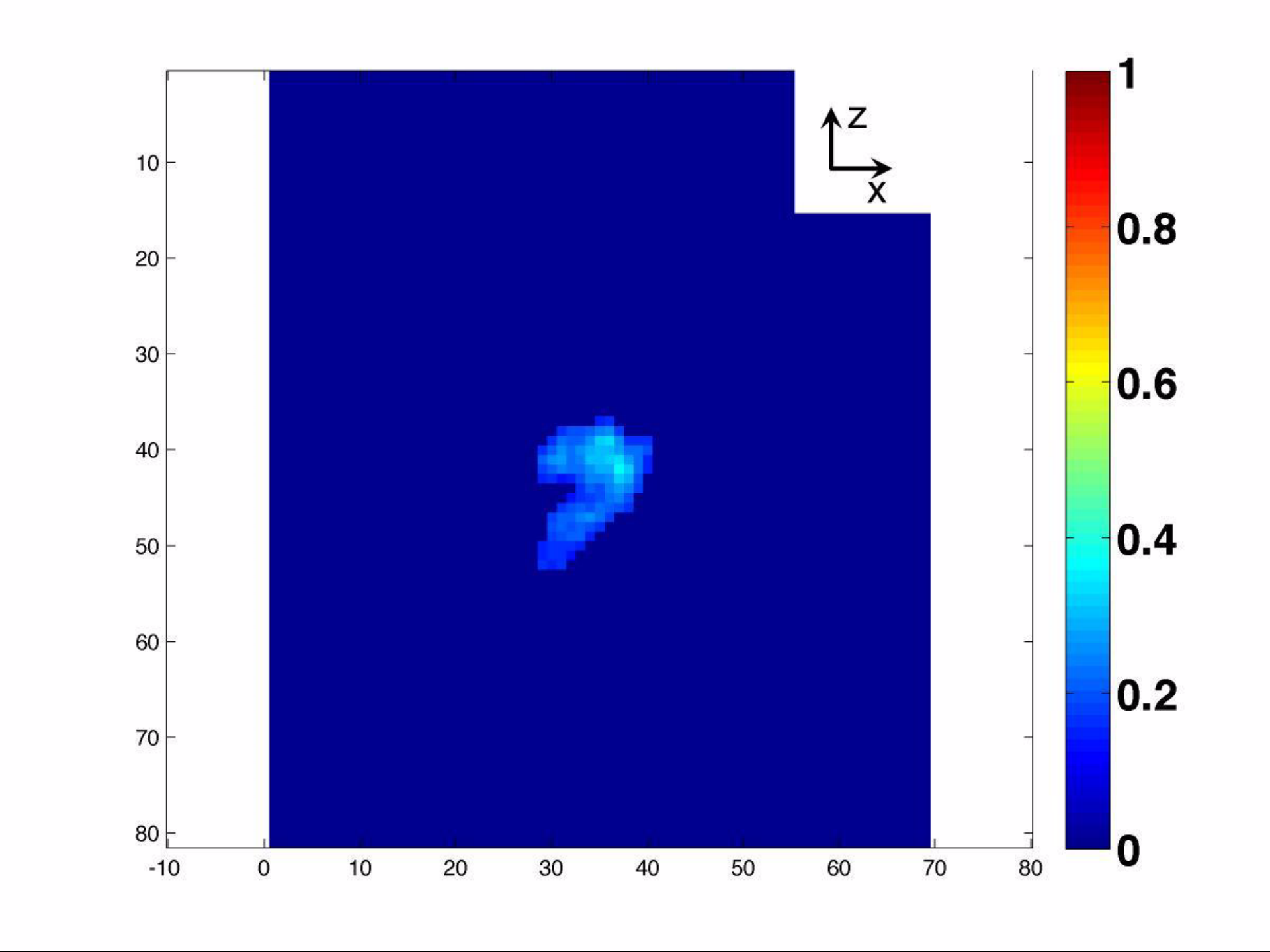


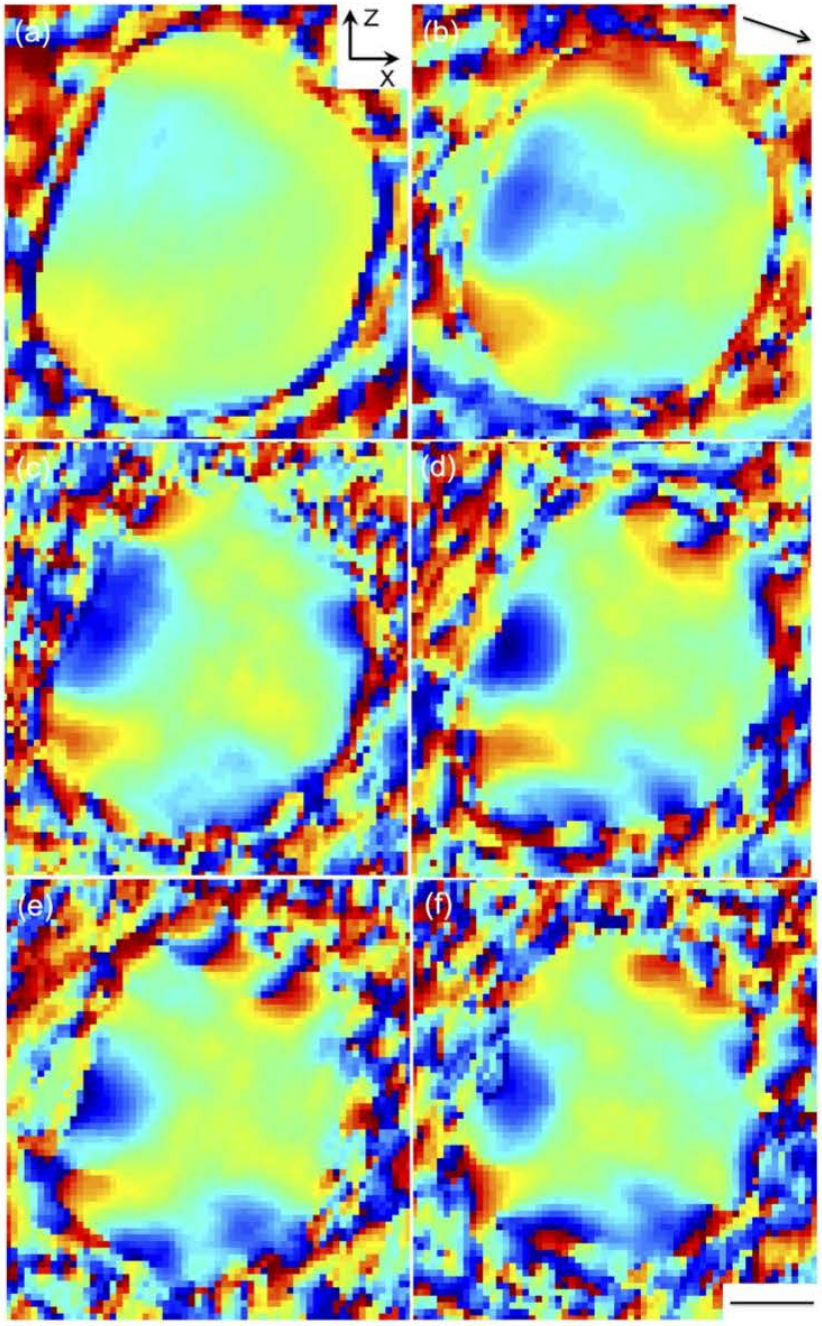

-0.15
-0.1
-0.05
0
0.05
0.1
0.15
Spatial Frequency (nm-1)
-0.1
-0.05
0
0.05
0.1
Spatial Frequency (nm-1)
z
x

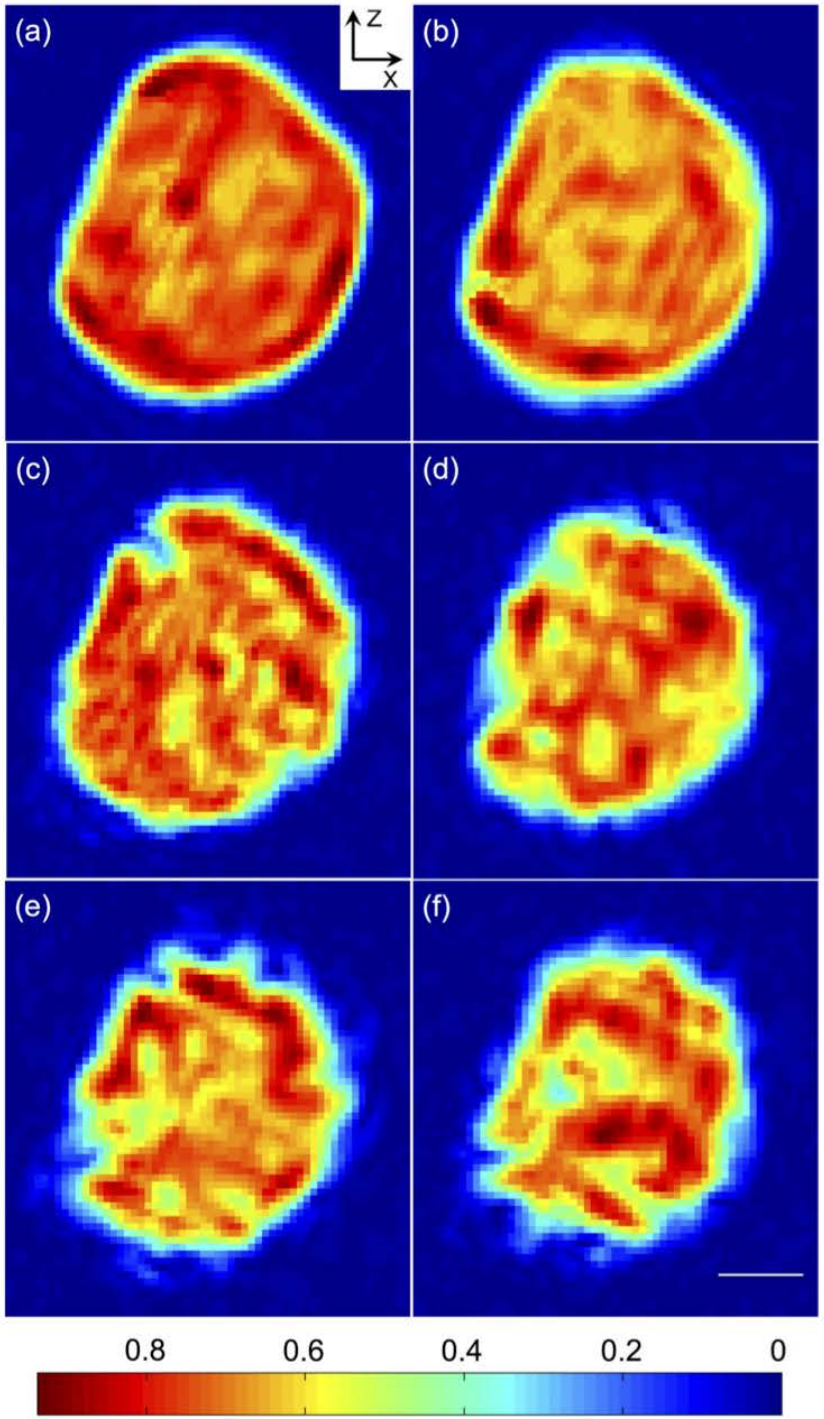
Domain structures give speckled diffraction

Real Space Reciprocal Space




Z
X
10
20
30
40
50
60
70
80
-10
0
10
20
30
40
50
60
70
80
1
0.8
0.6
0.4
0.2
0

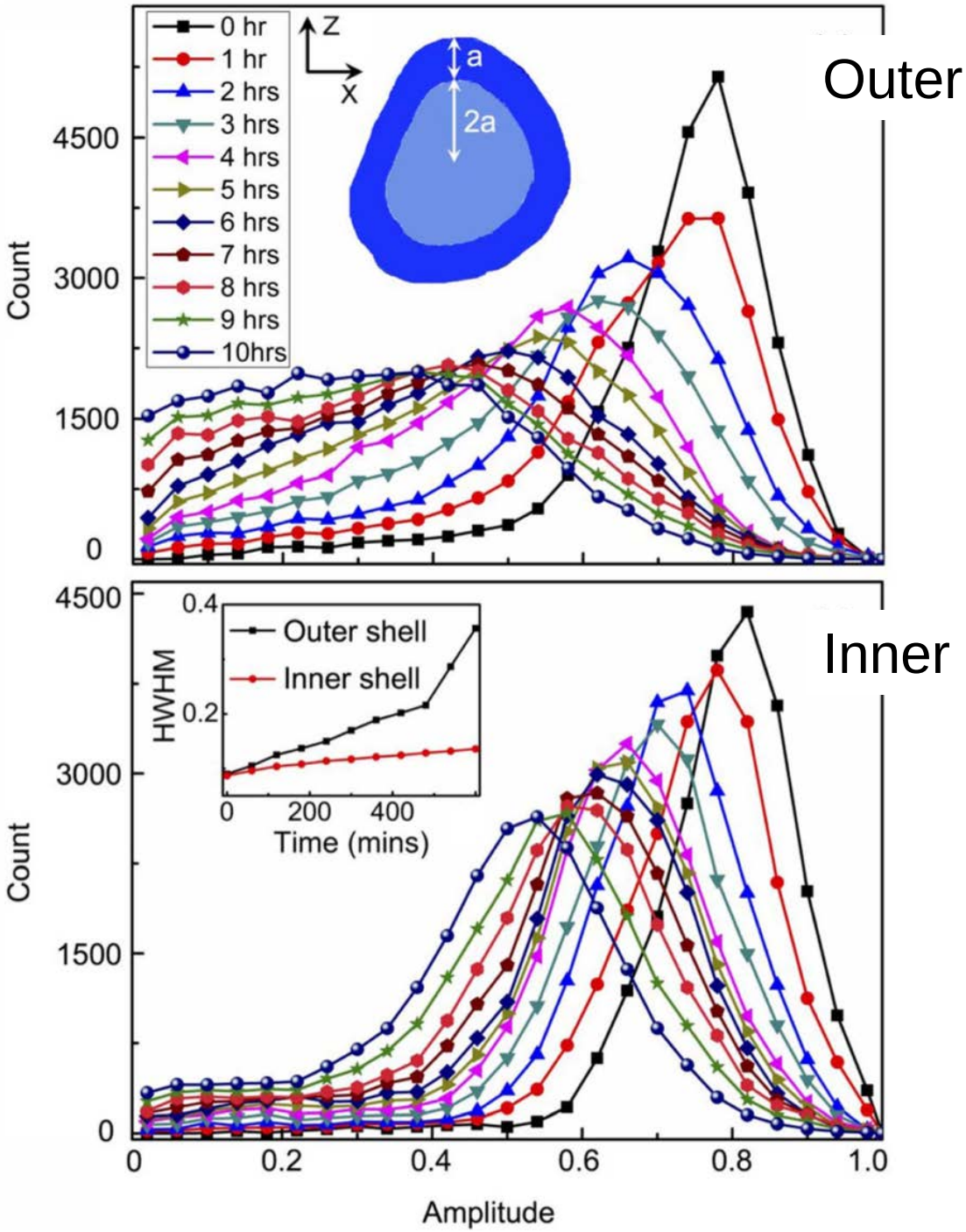

(a)
z
x
(b)
(c)
(d)
(e)
(f)
3
2
1
0
-1
-2
-3


(a)
z
x
(b)
(c)
(d)
(e)
(f)
0.8
0.6
0.4
0.2
0

Atomic Diffusion within Individual Gold Nanocrystal

Gang Xiong,
J. N. Clark,
C. Nicklin,
J. Rawle &
I. K. Robinson

Sci Rep **4** 6765 (2013)



ARTICLES
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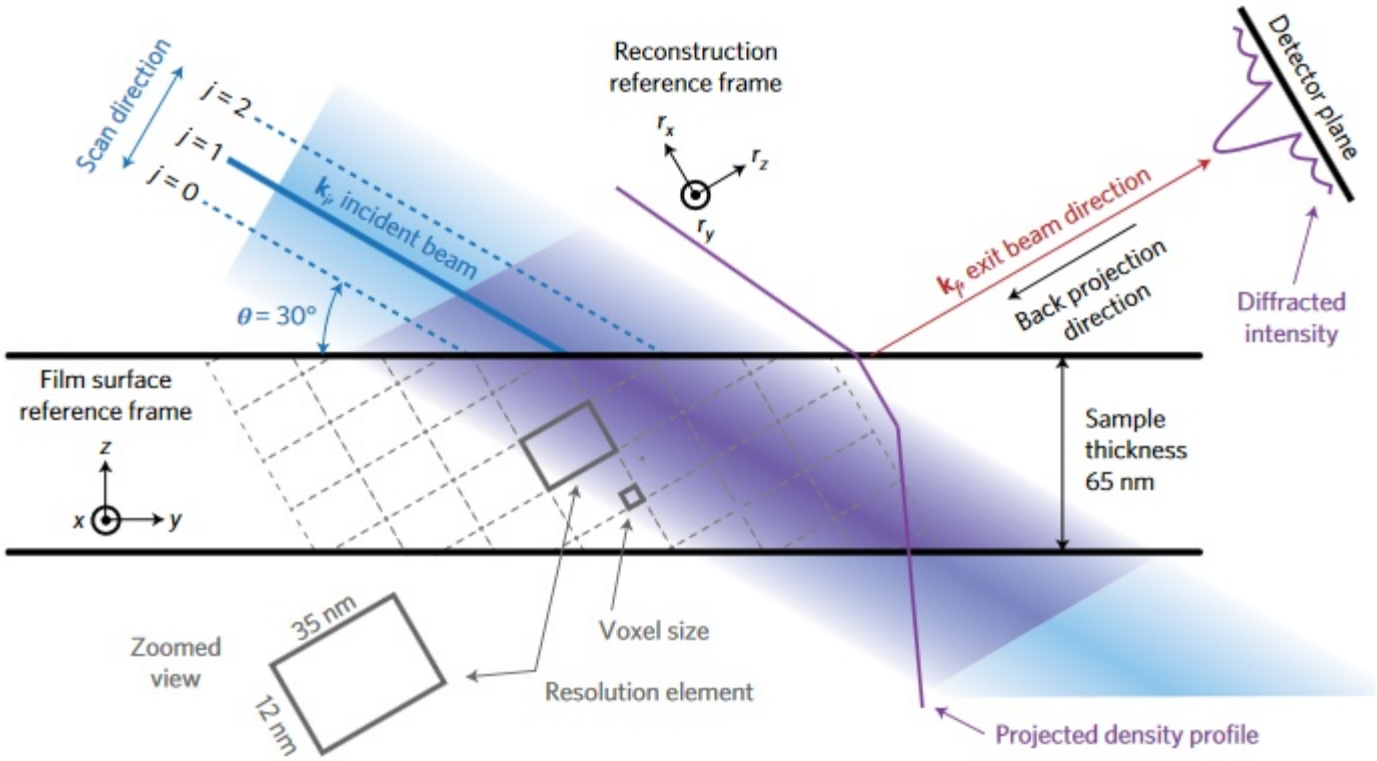
nature materials

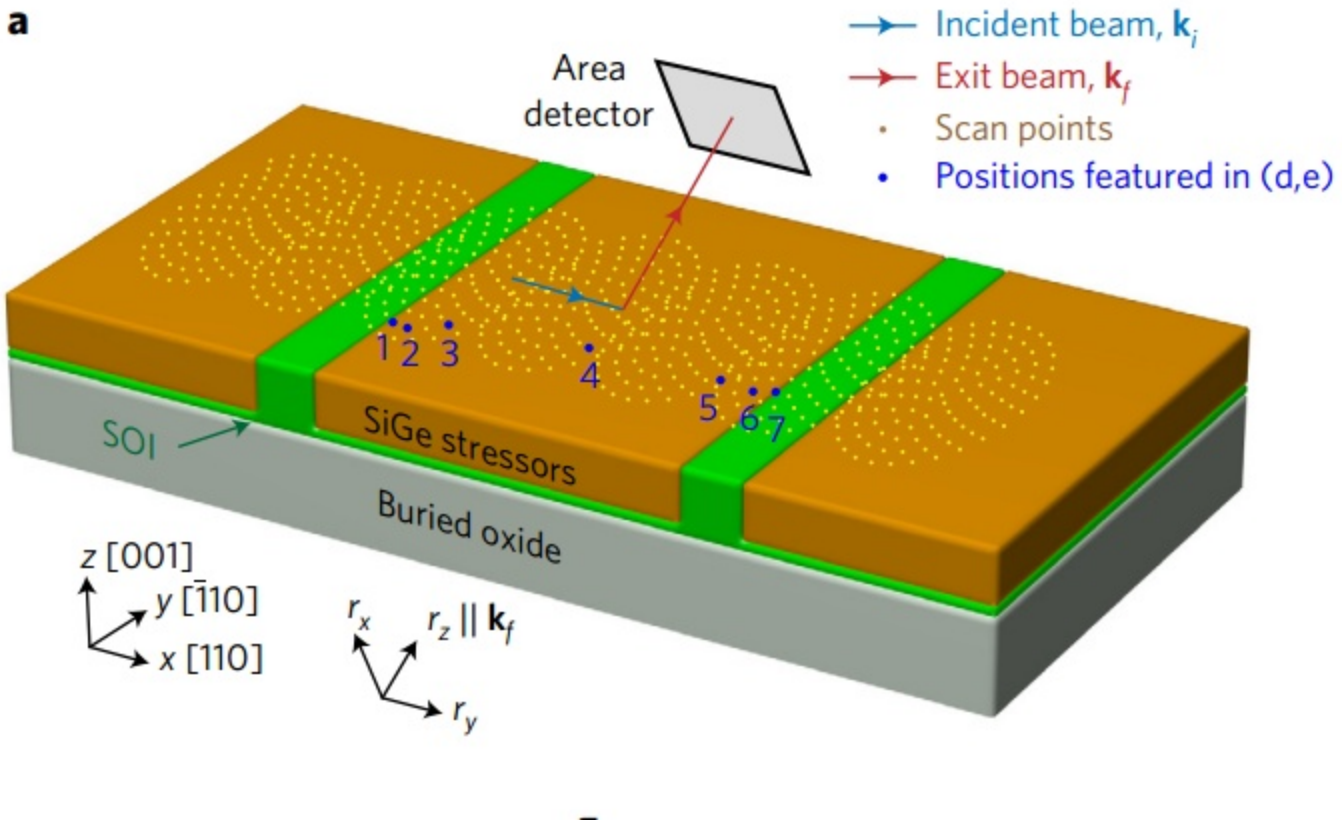
High-resolution three-dimensional structural microscopy by single-angle Bragg ptychography

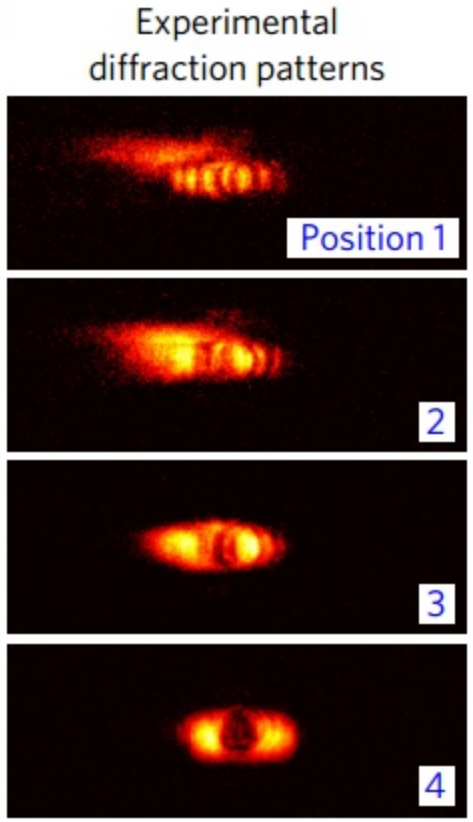
S. O. Hruszkewycz[1]*, M. Allain[2], M. V. Holt[3], C. E. Murray[4], J. R. Holt[5], P. H. Fuoss[1] and V. Chamard[2]



Bragg Projection Ptychography

Hruszkewycz et al Nat. Mat. **5** 026105 (2017)





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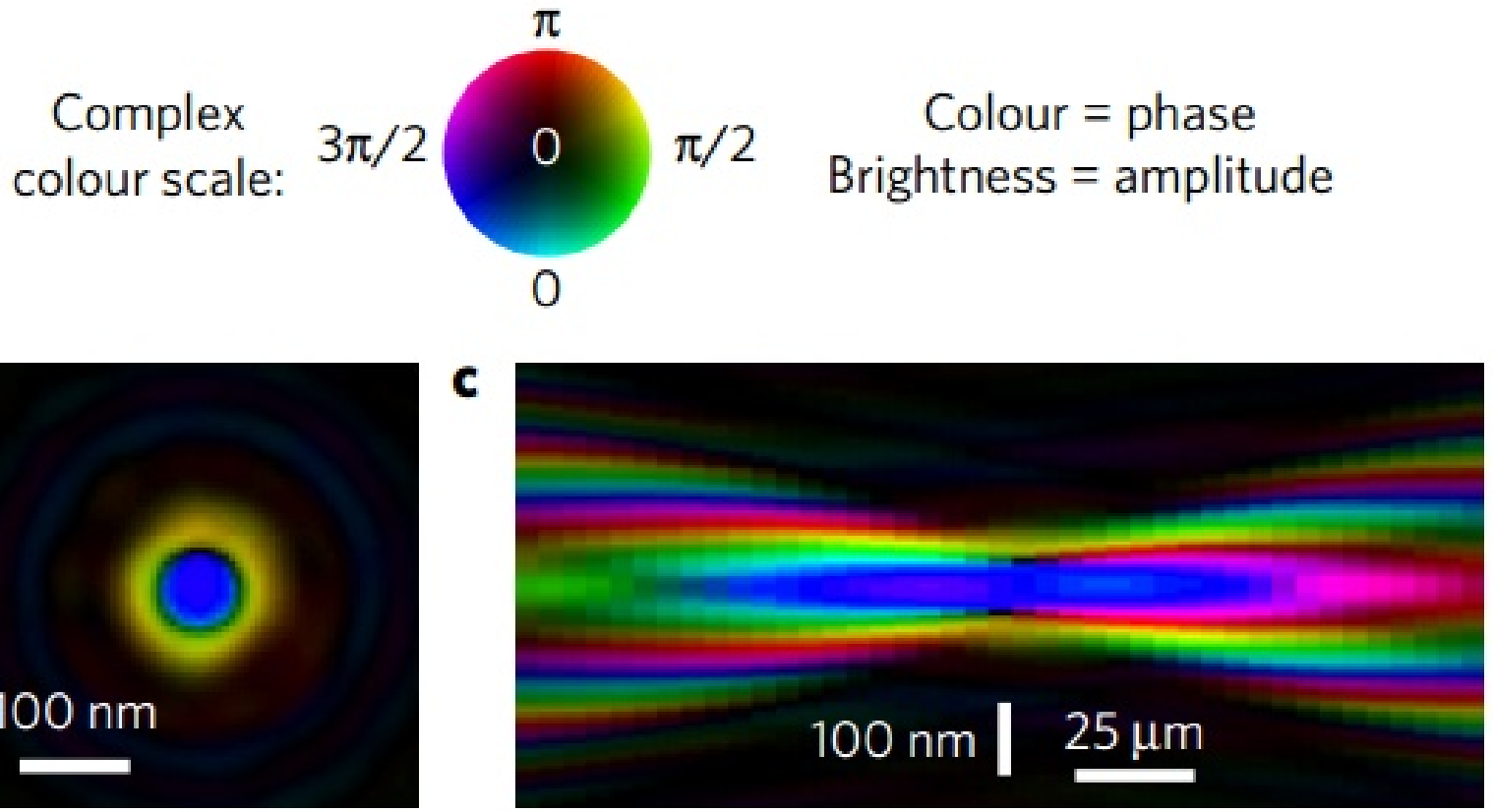

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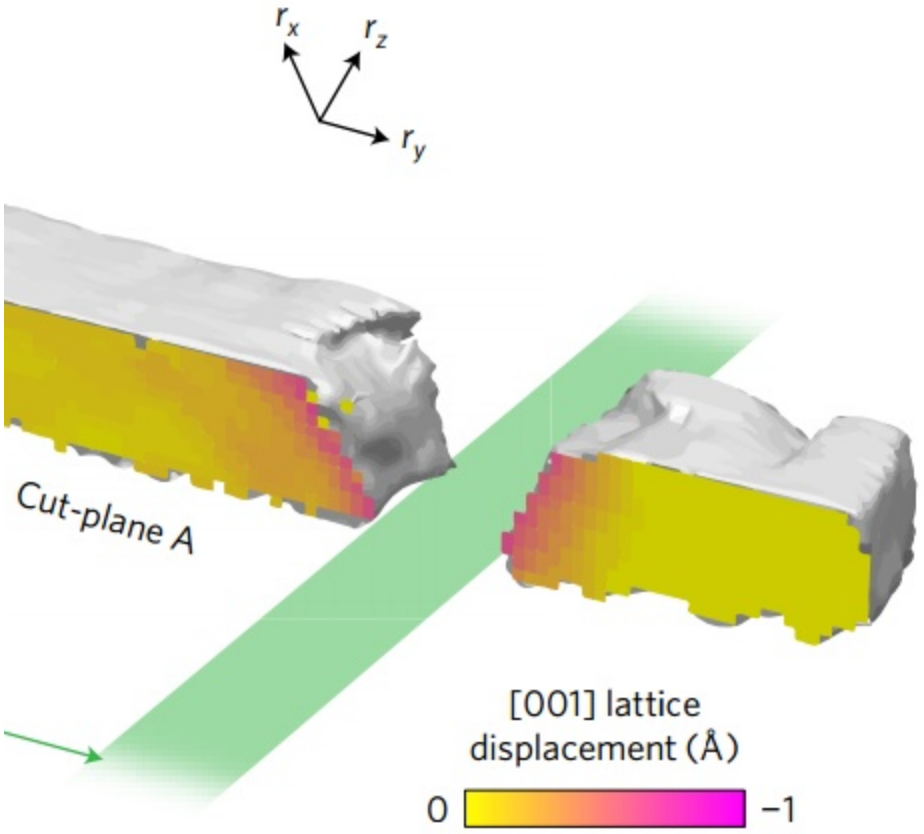

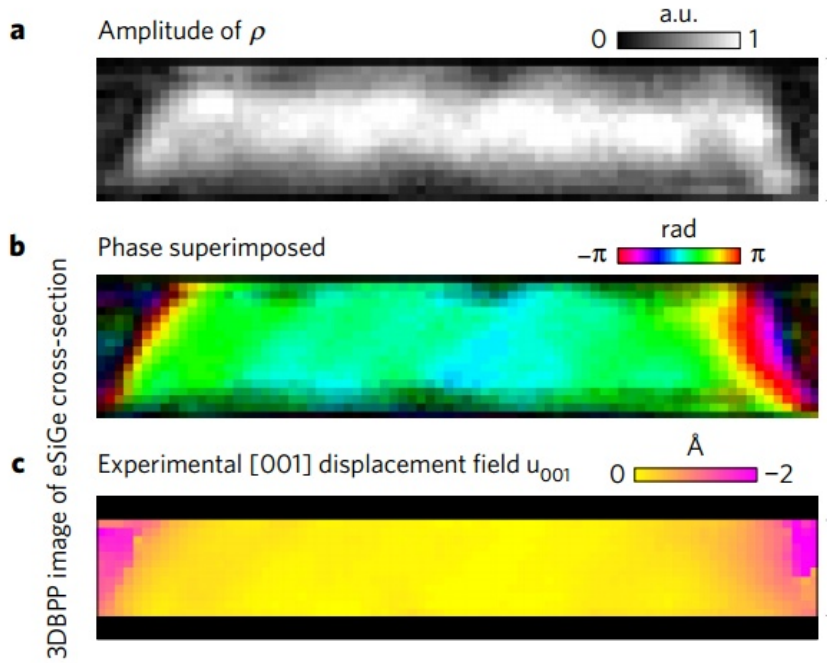

Bragg Coherent Diffraction Imaging

- Complex density can image strain
- Strain associated with nano-shape
  - Dislocations imaged
- Diffusion of Cu in Au nanoparticle
  - Porous structure generated
- Bragg Projection Ptychography
  - 3D imaging from 2D data