Bragg Coherent Diffraction Imaging for Nano-Materials Investigation

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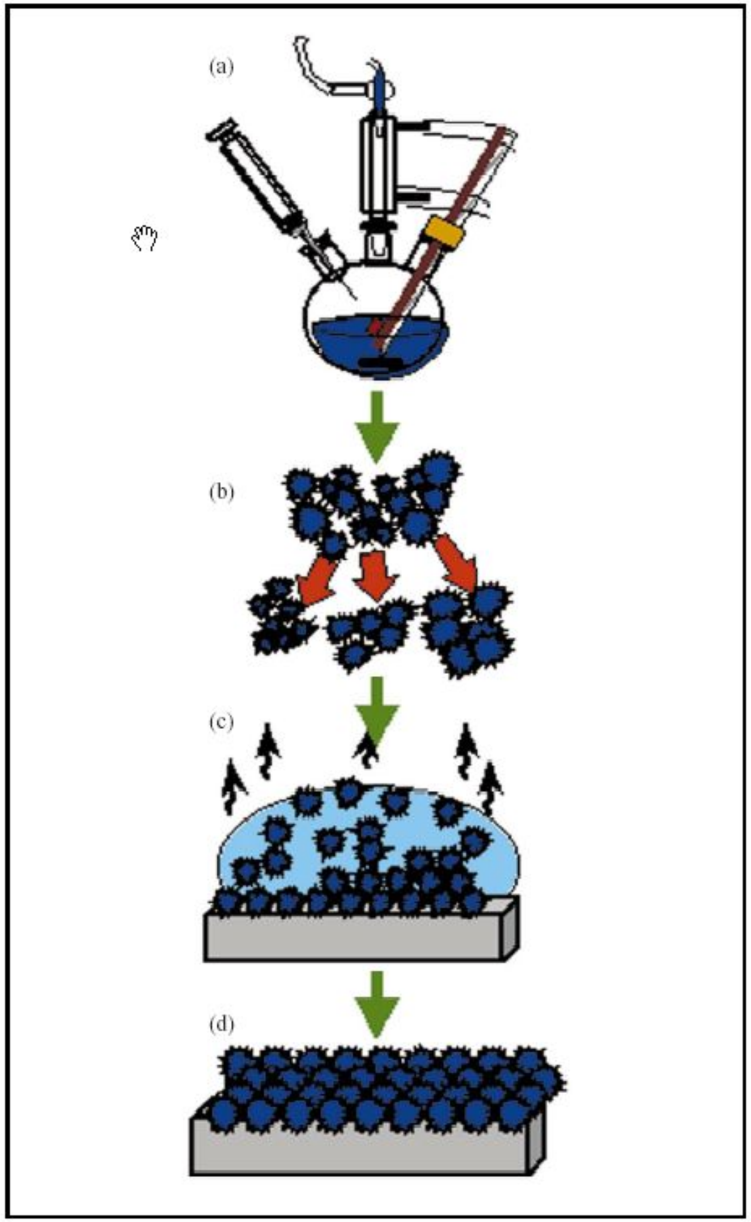
Outline

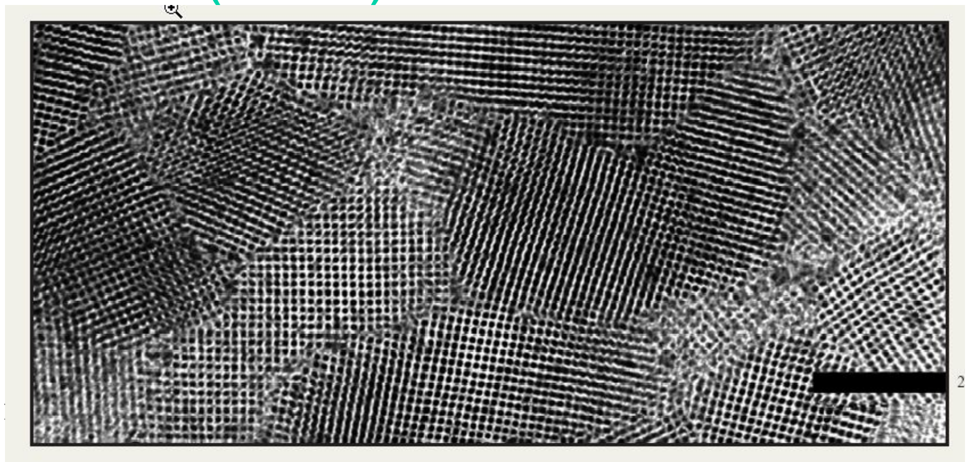
- Nanocrystal structures
- Coherent X-ray diffraction
- Crystal strain as complex density
- Nanoscale alloying
- Ultrafast snapshots of moving matter
- Crystallographic phase determination

Chemical Synthesis of Nanocrystals



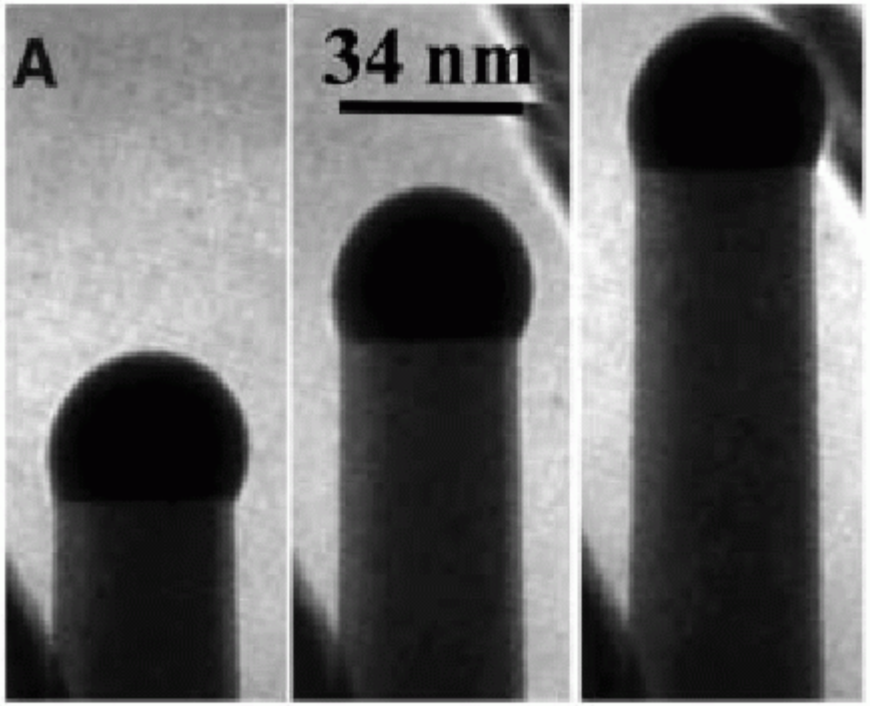
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

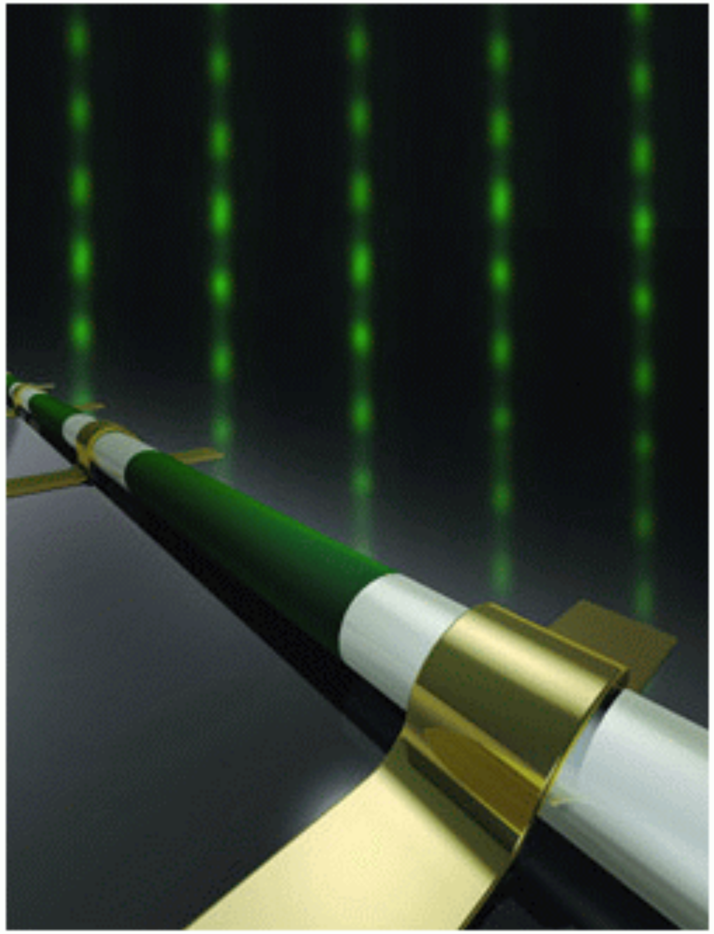
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



VLS growth of nanowires

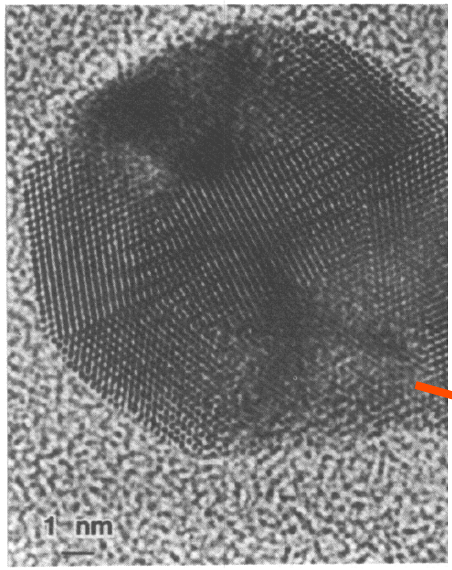
S. Kodambaka et al., Science 316 729 (2007)



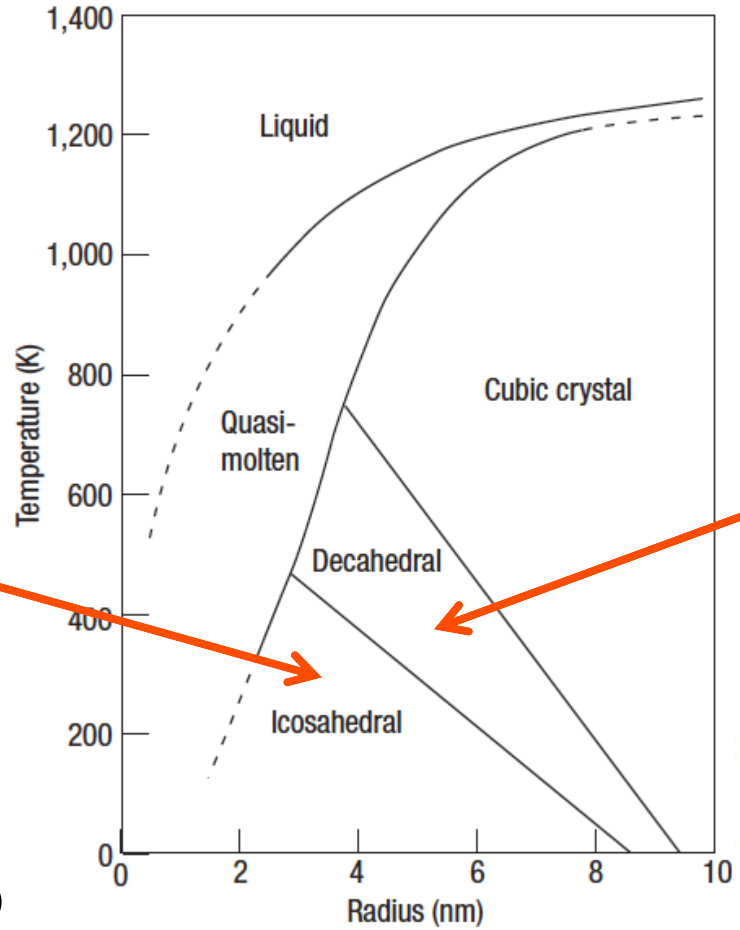


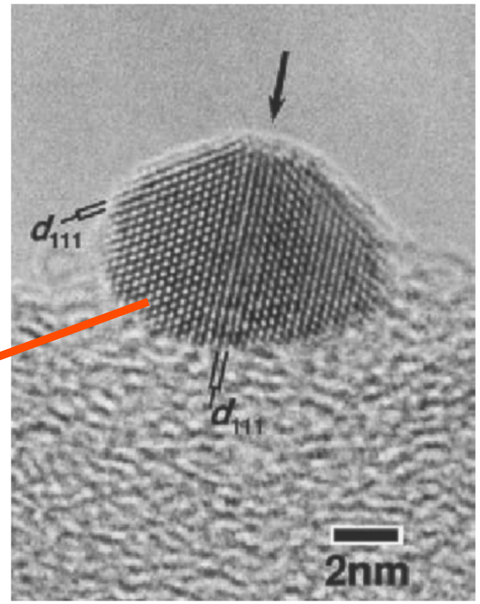
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

Structure of Gold vs Size



L. D. Marks, RPP (1994)





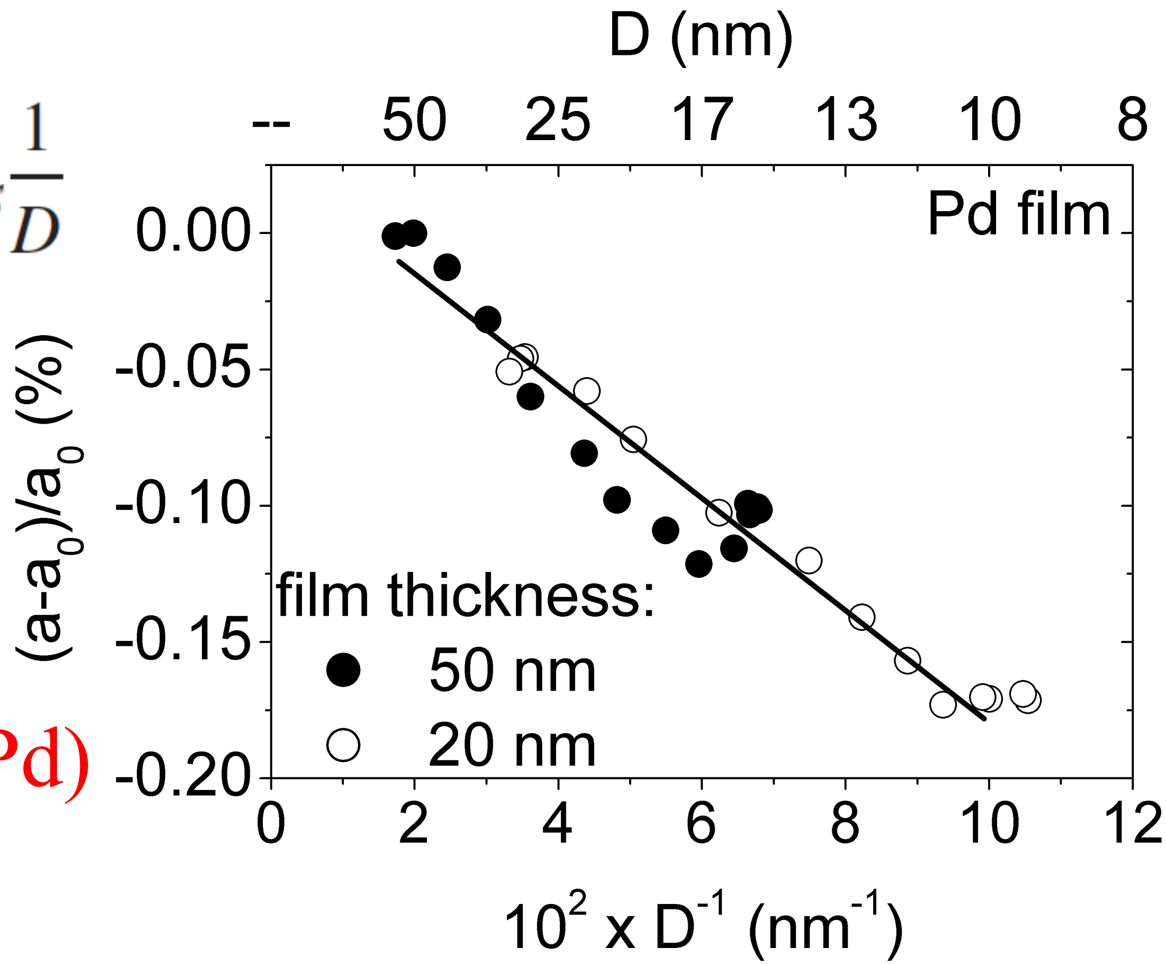
Koga and Sugawara (2003)

Contraction of Small Particles

Gibbs Thomson pressure + Bulk modulus

Sheng, Welzel & Mittemeijer, APL 97 153109 (2010)

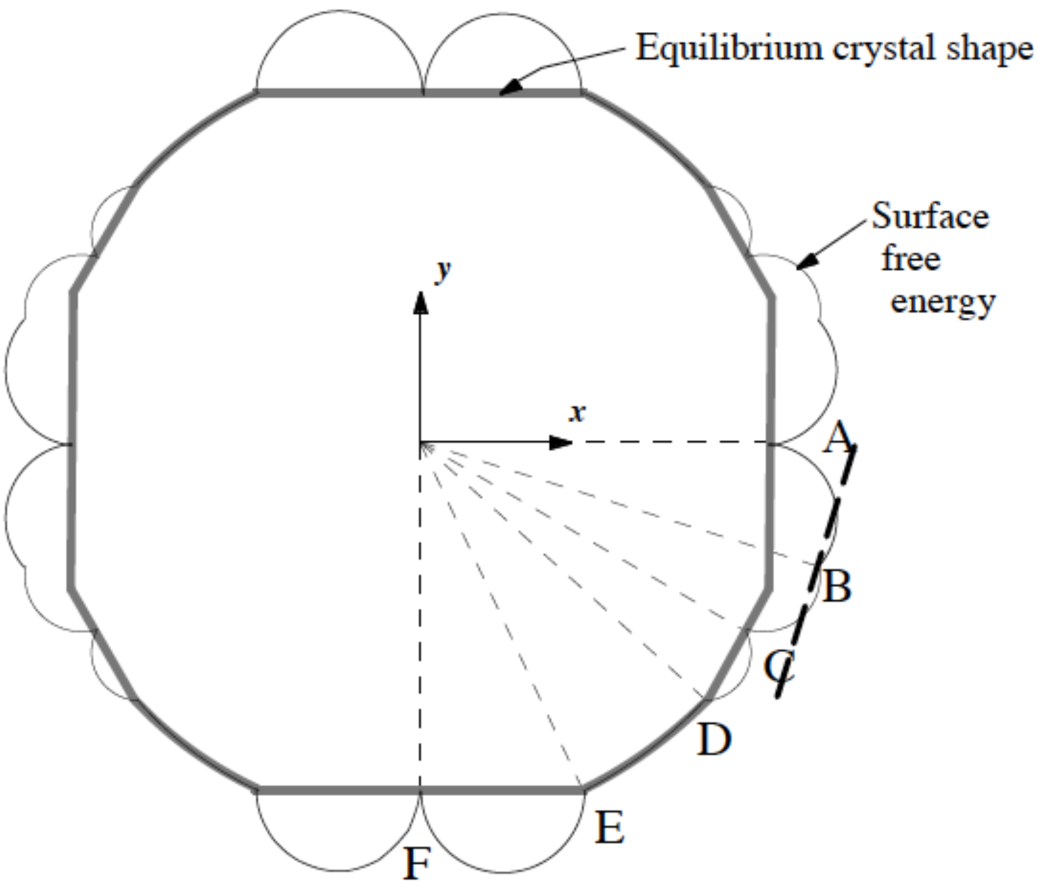
$$\frac{a-a_0}{a_0} = -\frac{4}{3K}\sigma_S\frac{1}{D}$$

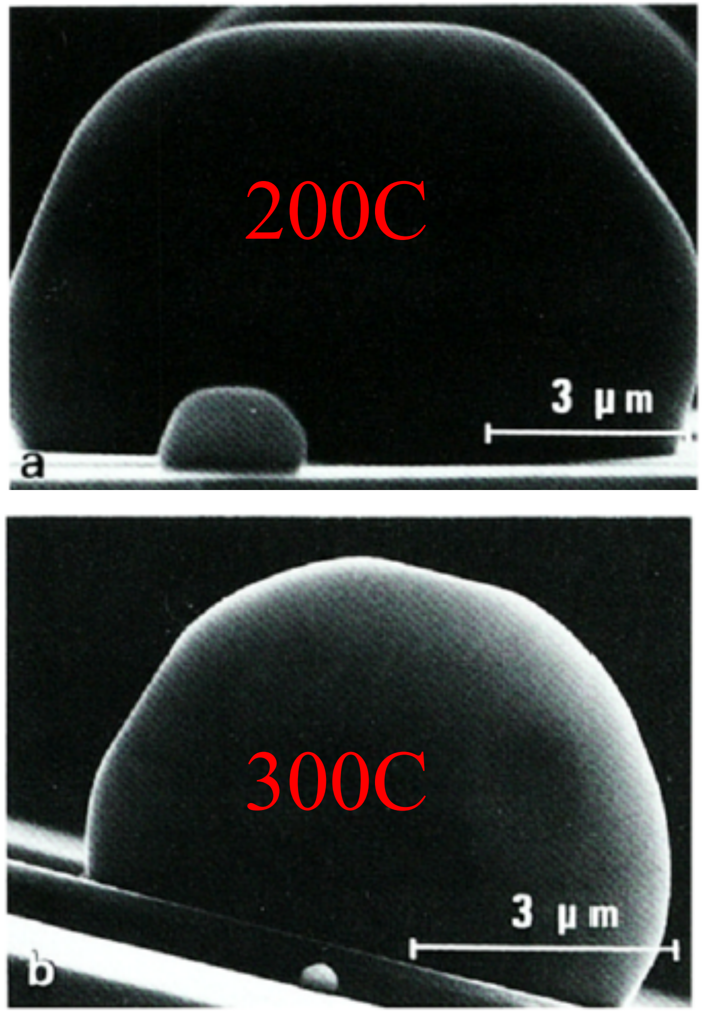


$\sigma_S = 2\text{N/m}$ (Pd)

Equilibrium crystal shape

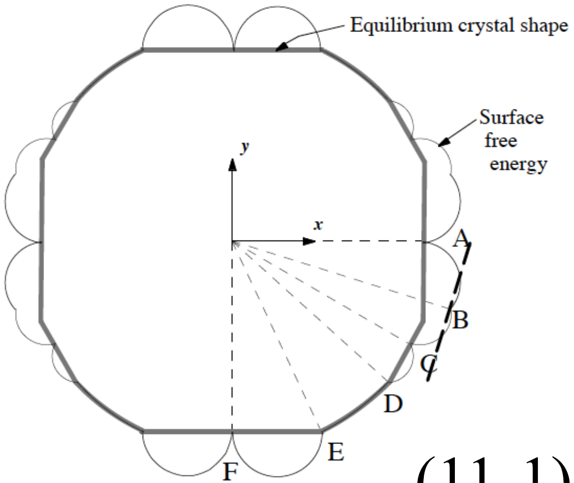
Wulff construction; Heyraud & Metois, Surf Sci 128 334 (1983)





Equilibrium crystal shape

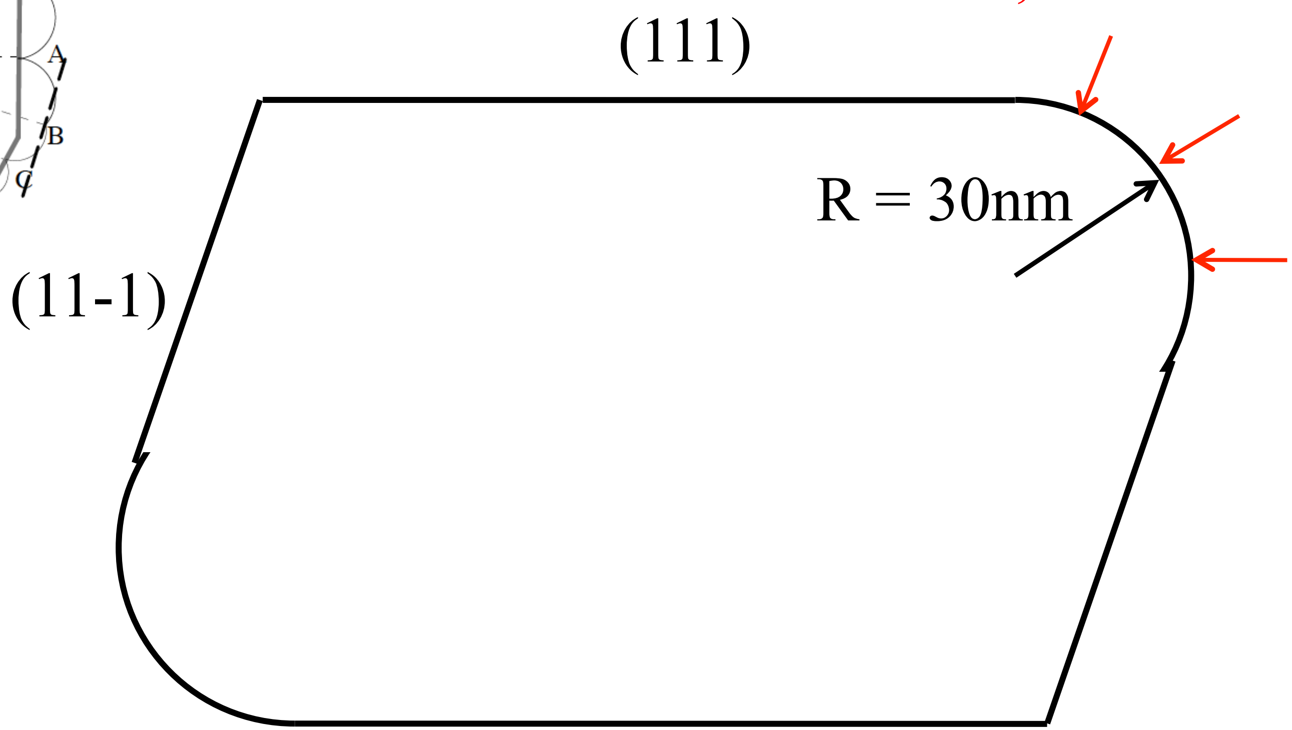
Wulff construction + Gibbs Thomson (Young-Laplace) pressure



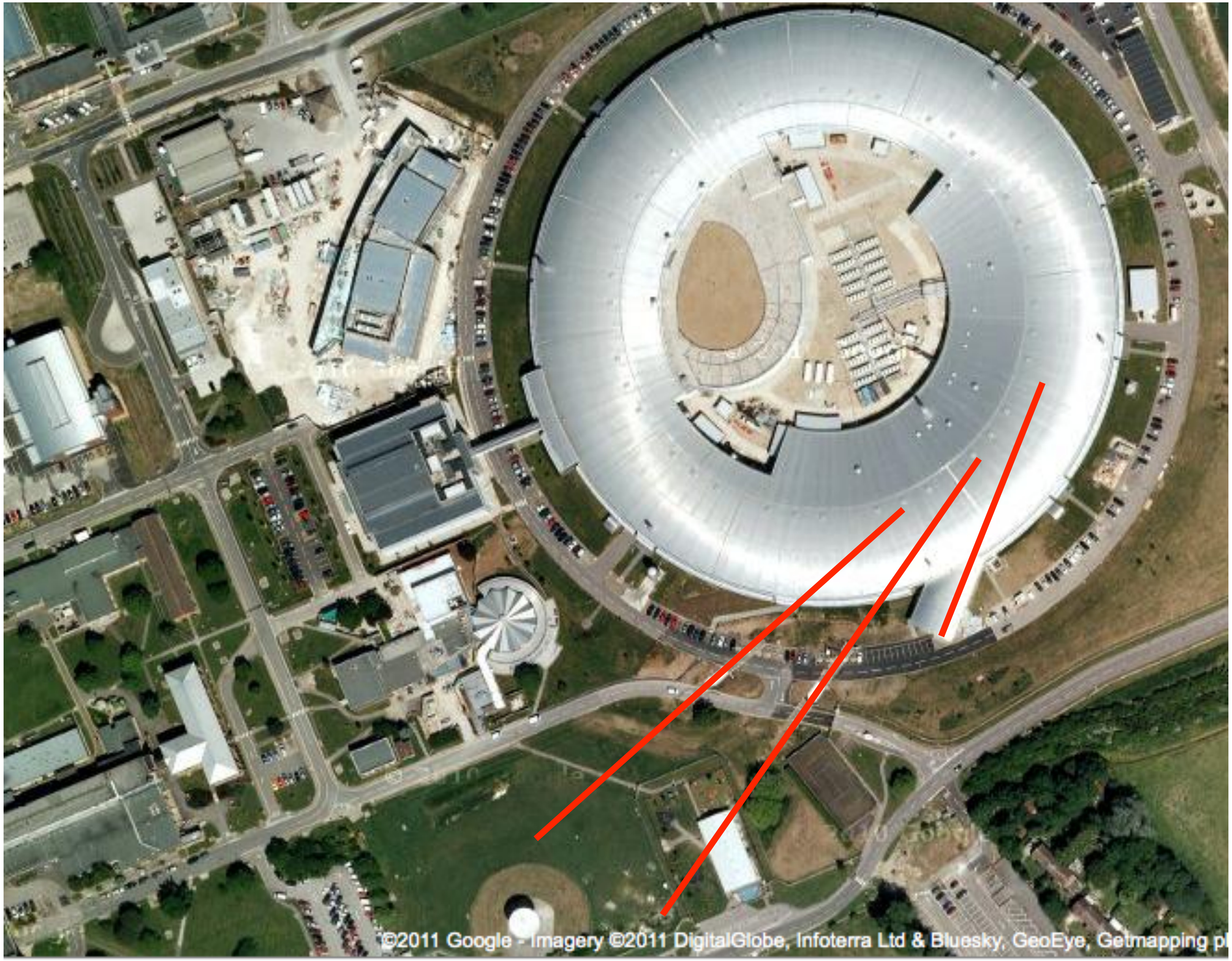
$\gamma = 2\text{N/m}$

$P = 2\gamma/R = 70\text{MPa}$

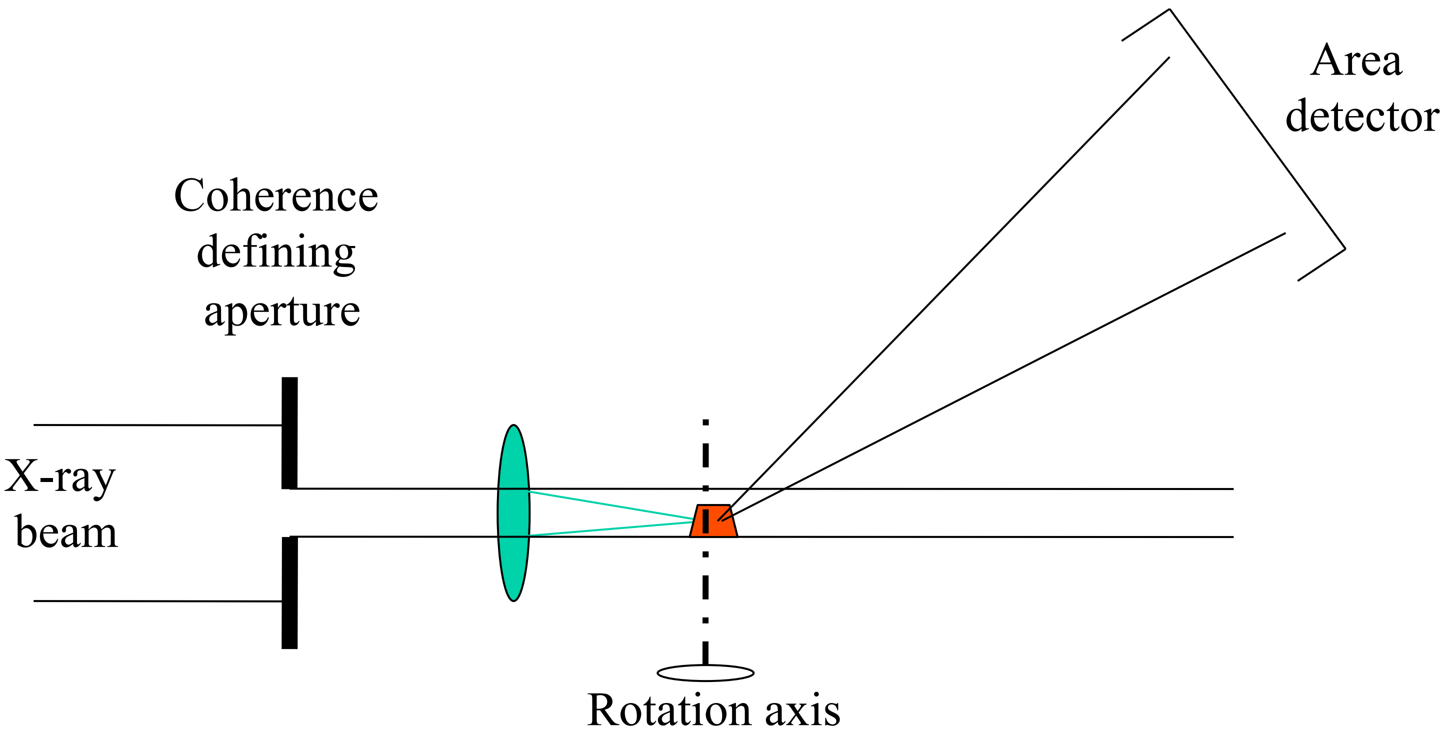
$\varepsilon = 0.1\%,\ \ \Phi = 0.6\ \text{rad}$

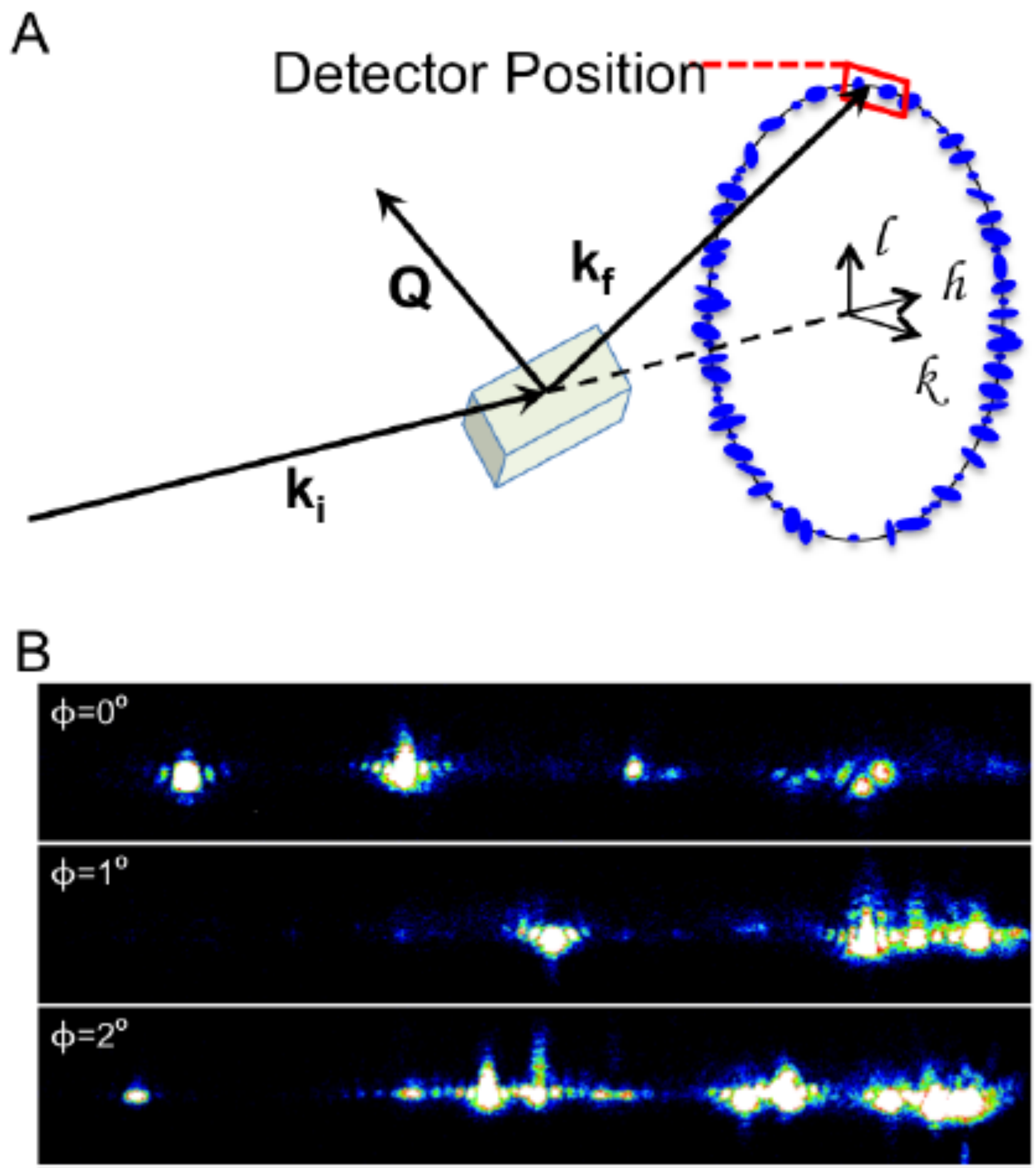


Diamond Light Source, 2009

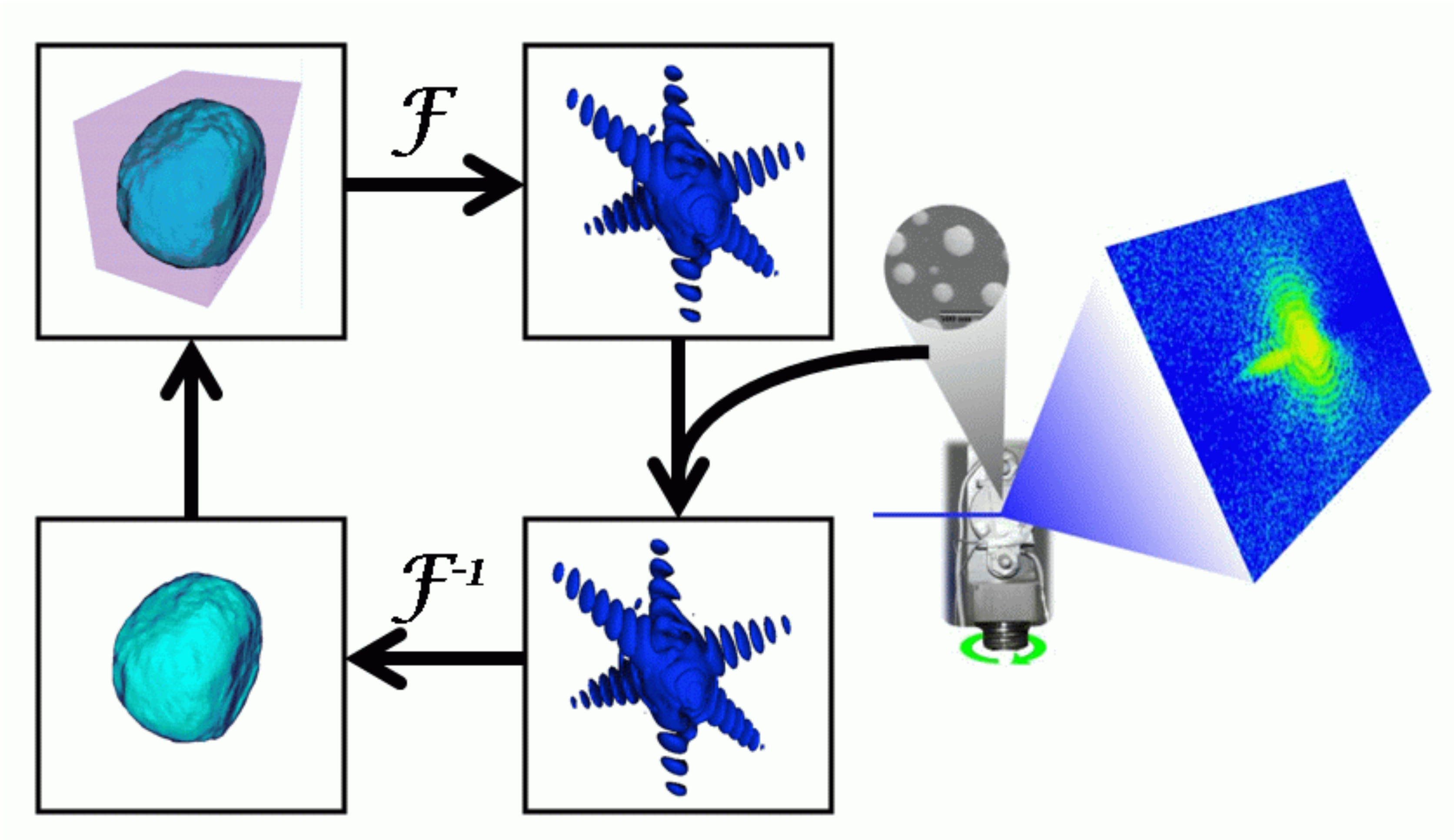


Lensless X-ray Microscope, 2003




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

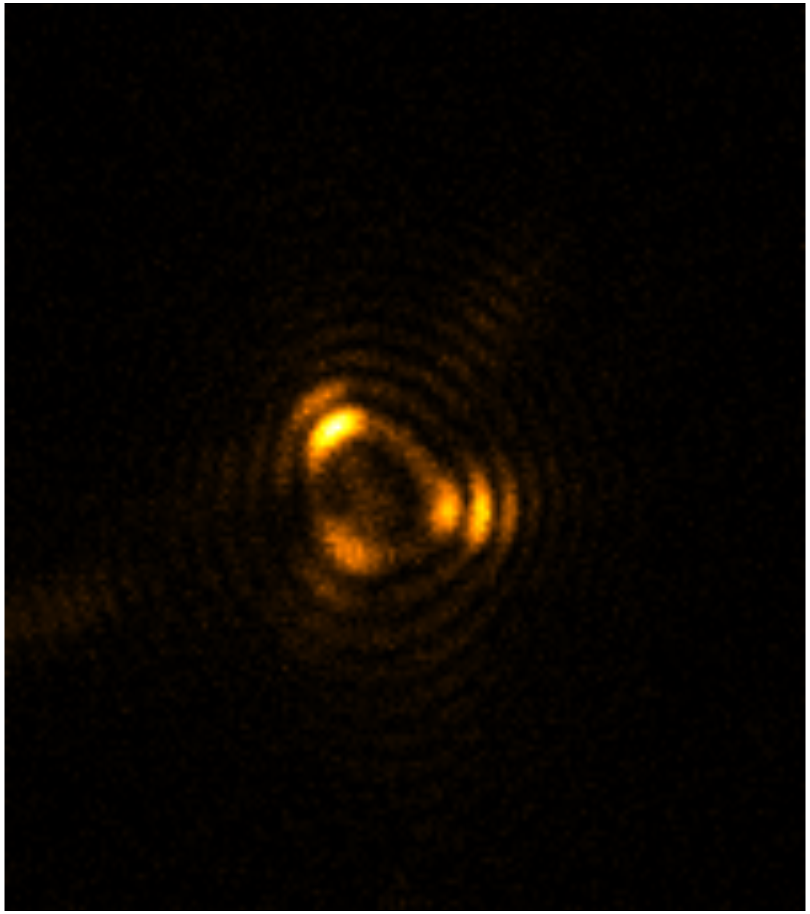
Generic "Error Reduction" method

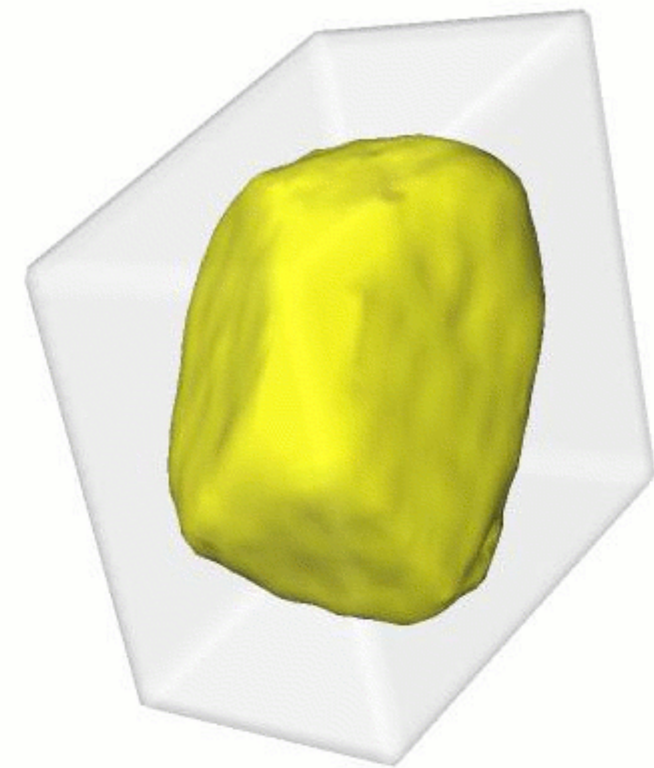


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

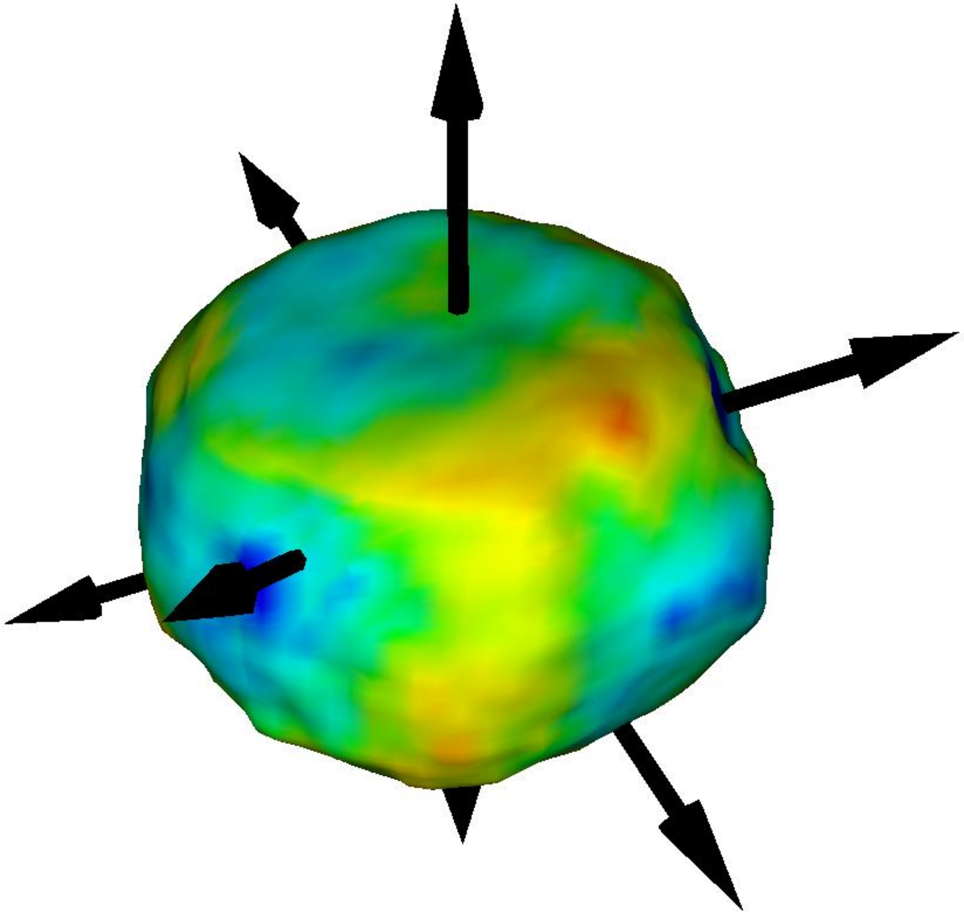
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



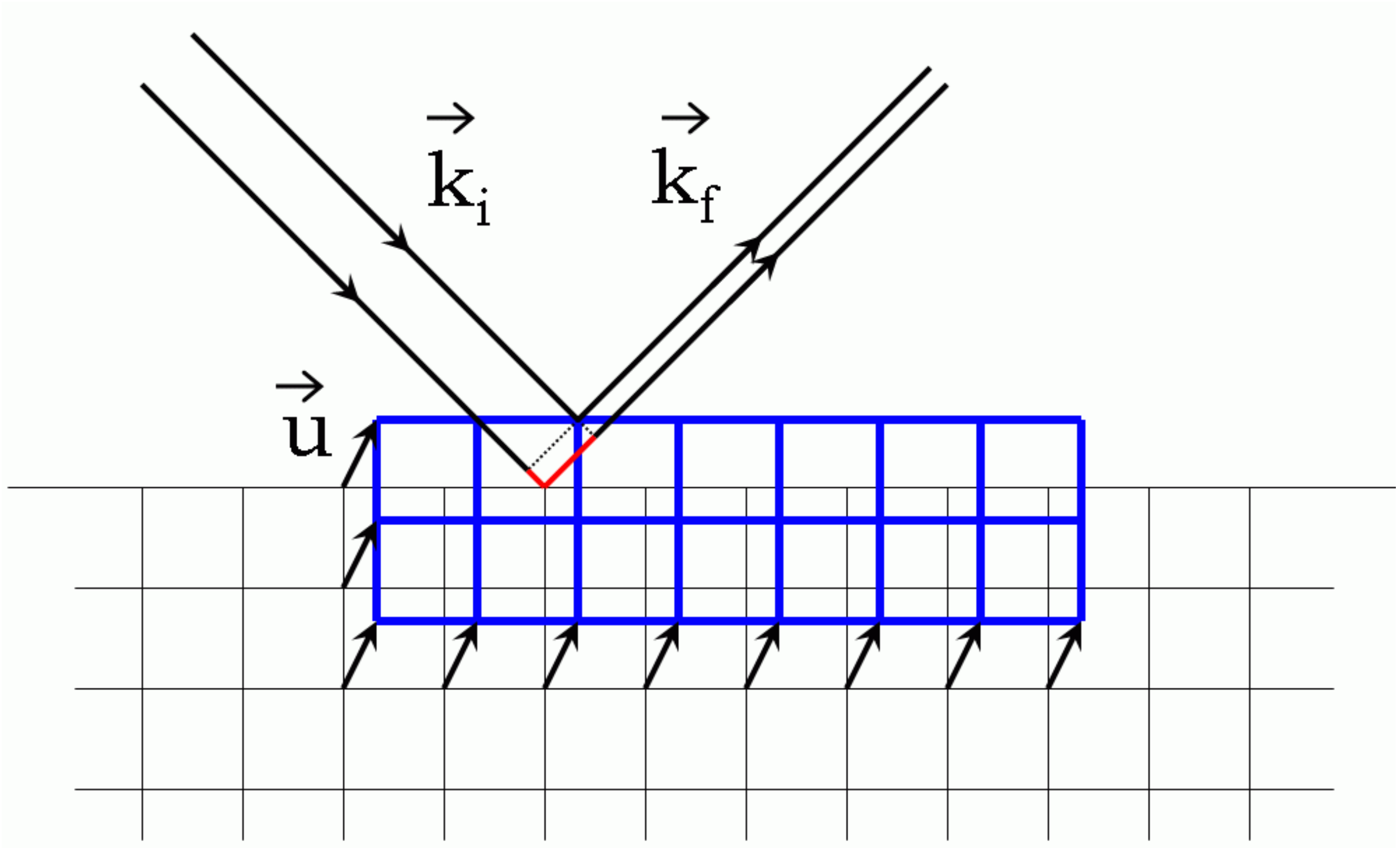


Phase isosurface of residual strain



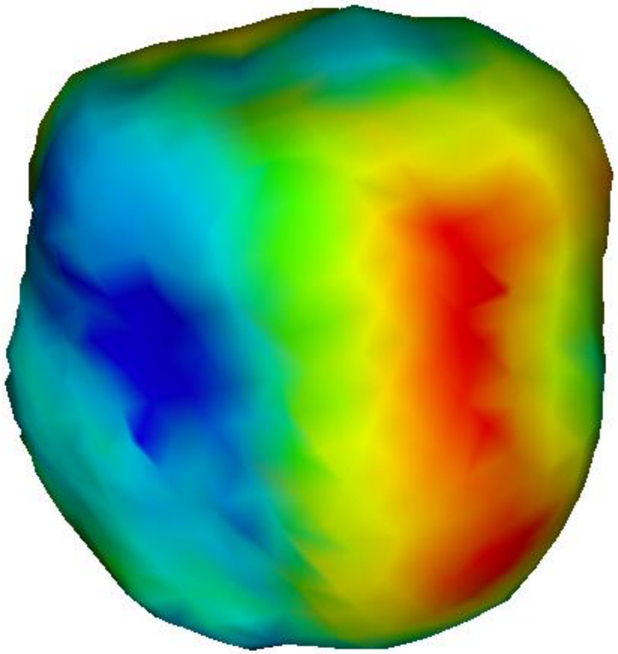
Sensitivity to strain

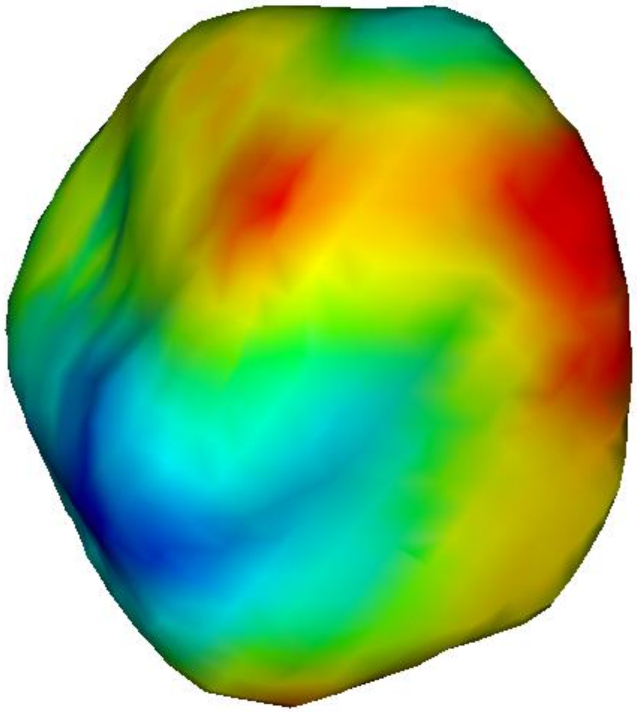
$\Delta\varphi = \mathbf{k_f \cdot u - k_i \cdot u = Q \cdot u}$



Phase isosurface of residual strain

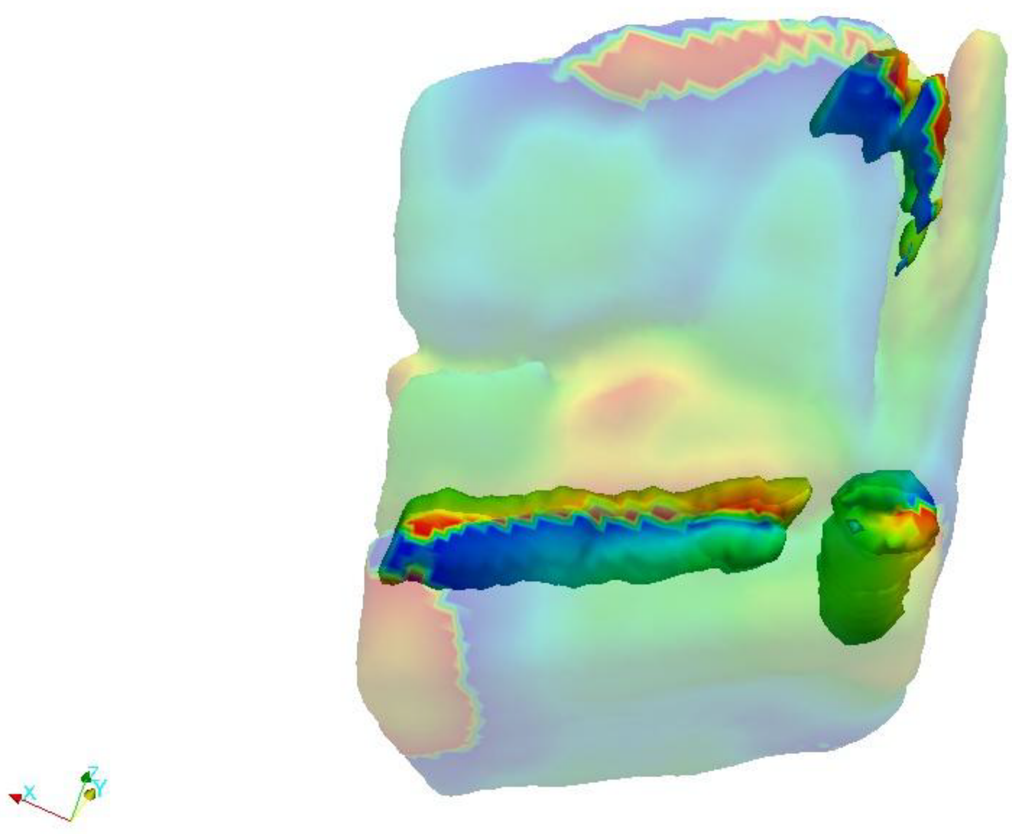
200nm Barium Titanate (BTO) crystals





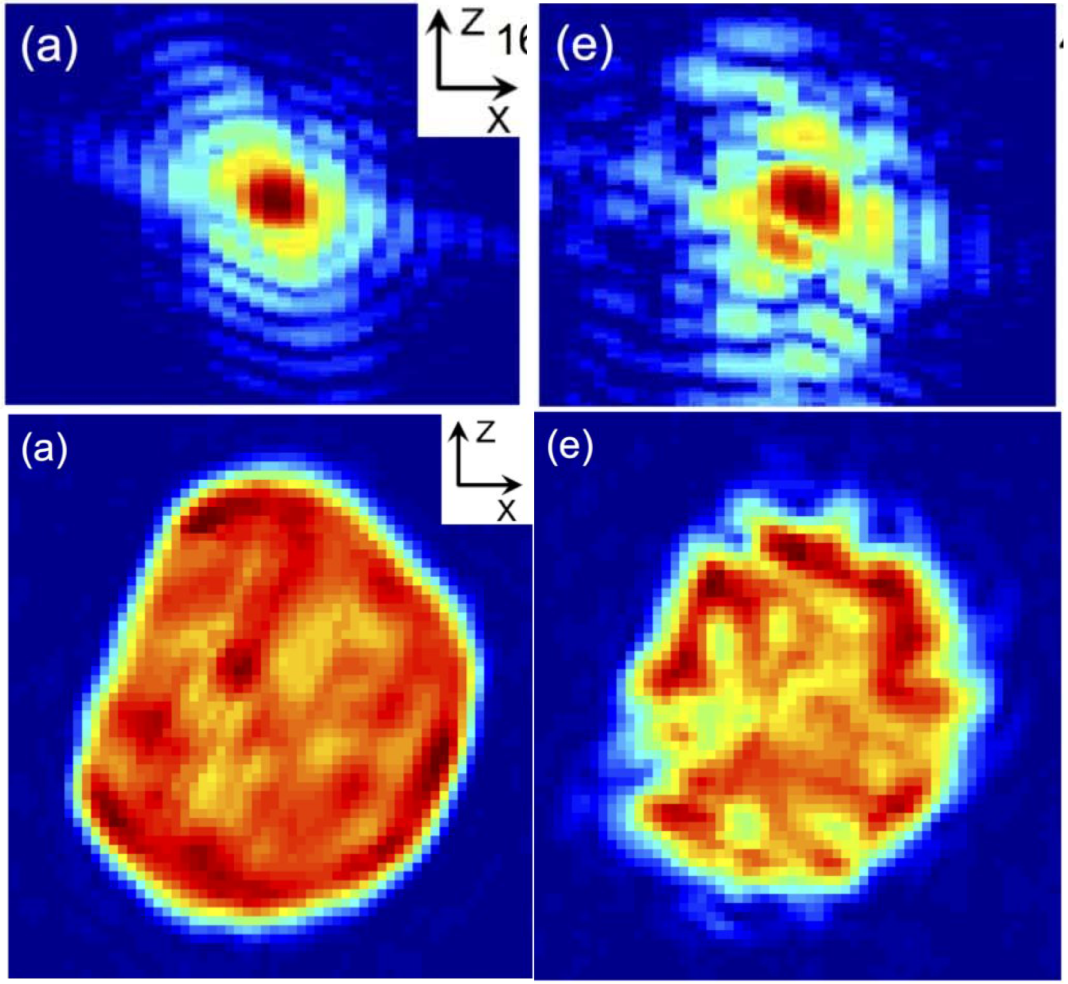
Screw dislocations in Calcite

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



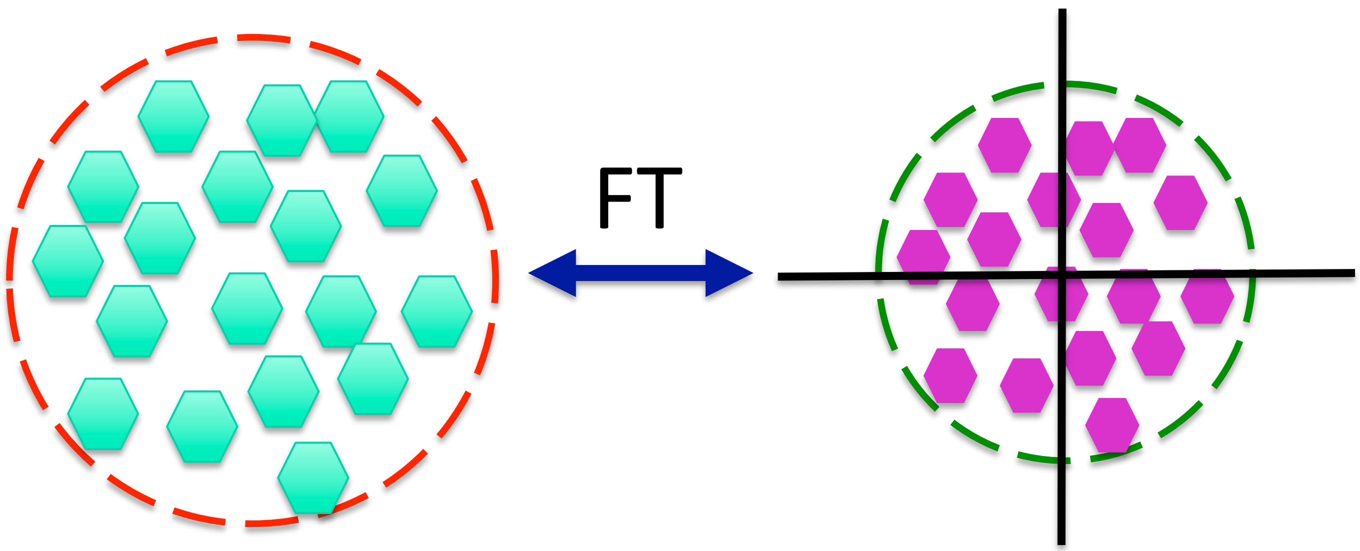
Copper Diffusion into Gold Nanocrystal

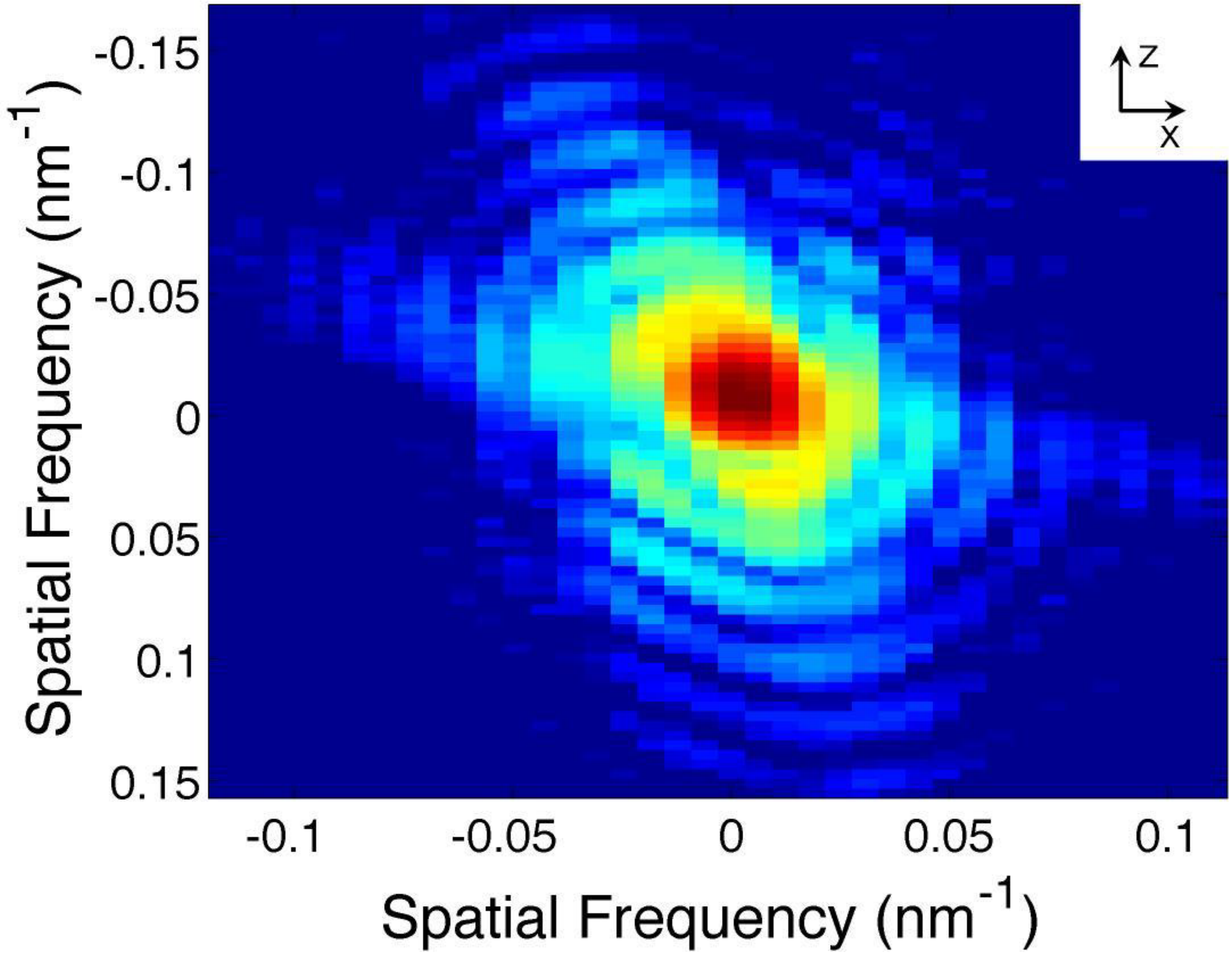
Gang Xiong, et al, Sci Rep 4 6765 (2013)



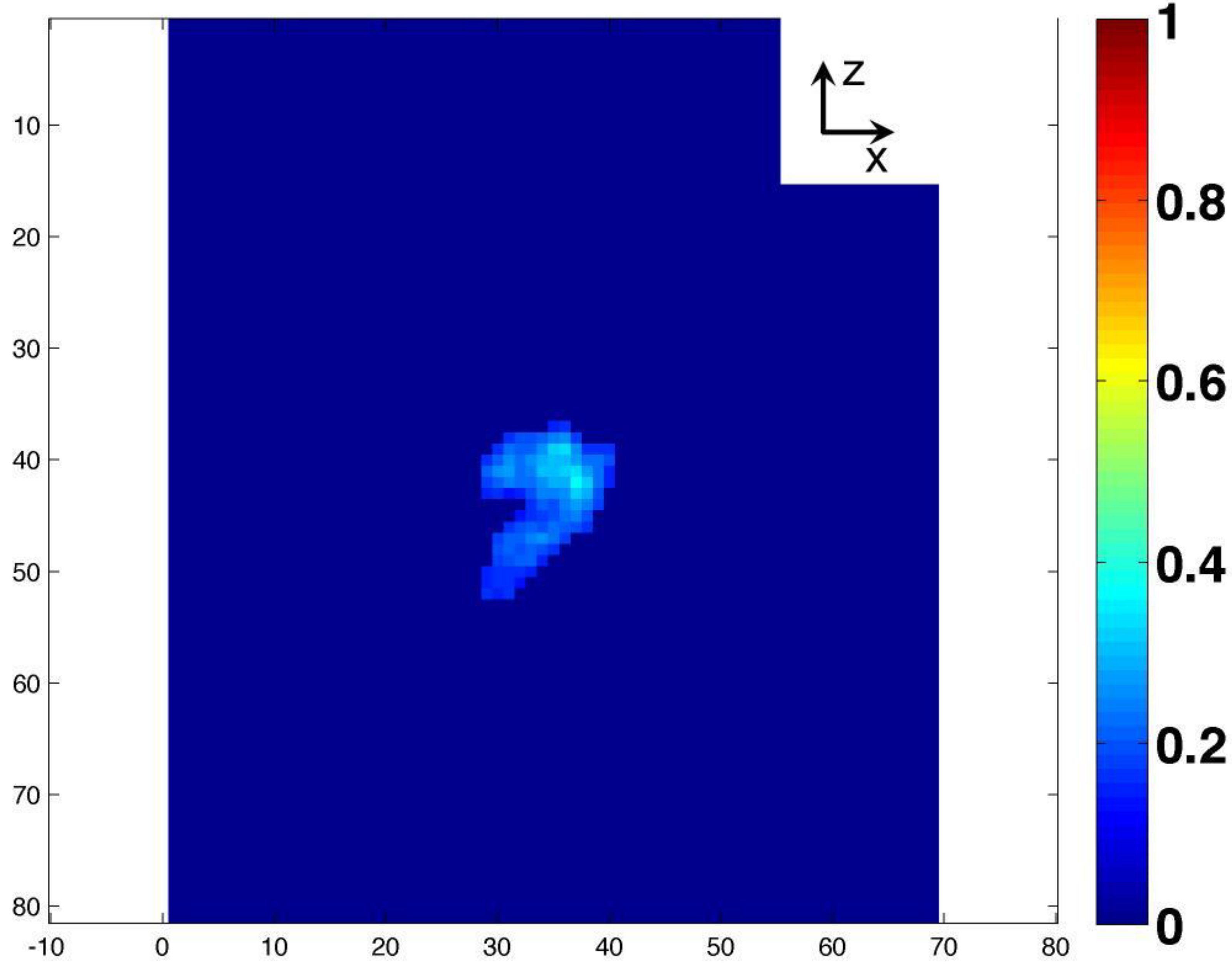
Domain structures give speckled diffraction

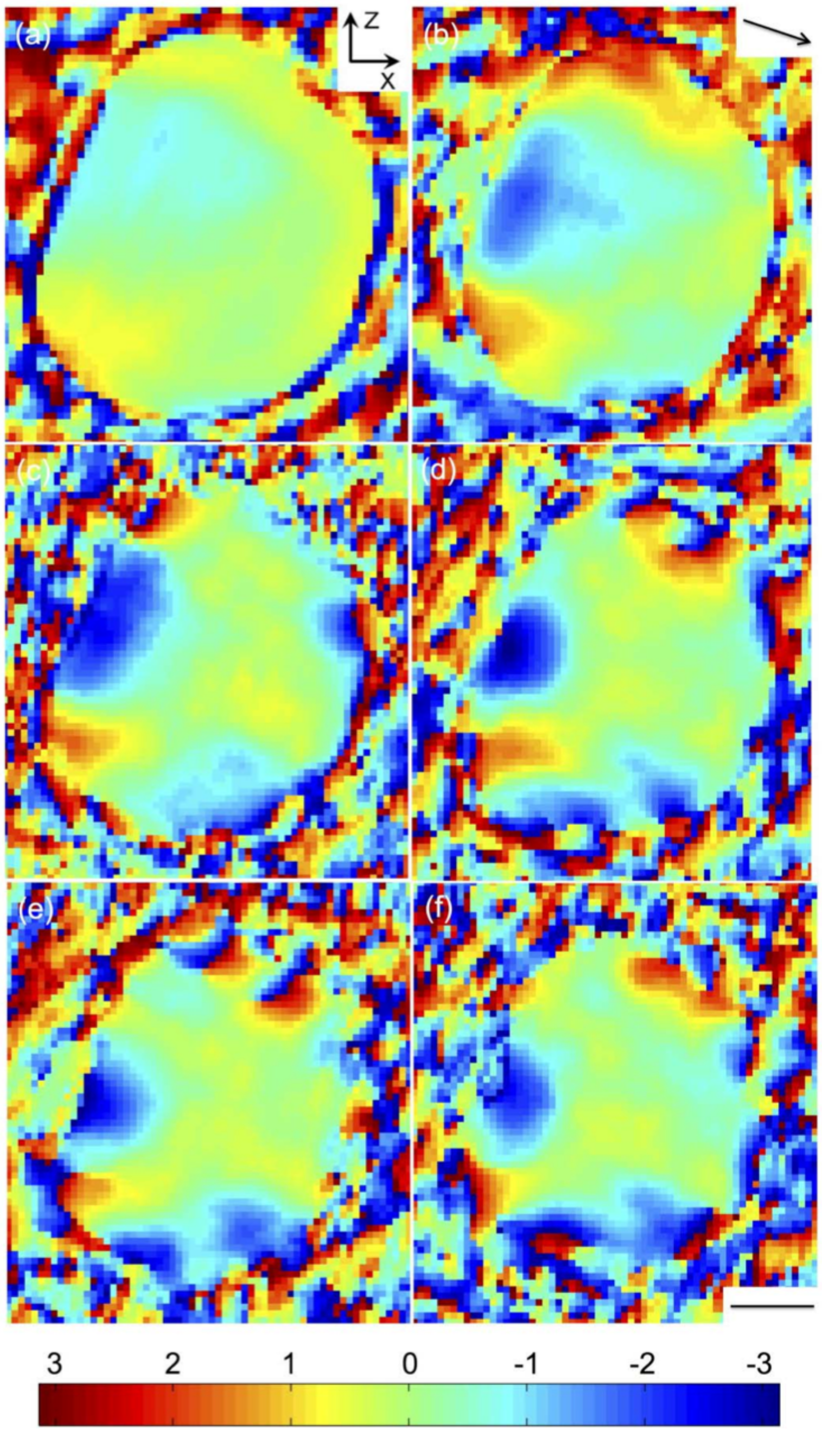
Real Space Reciprocal Space

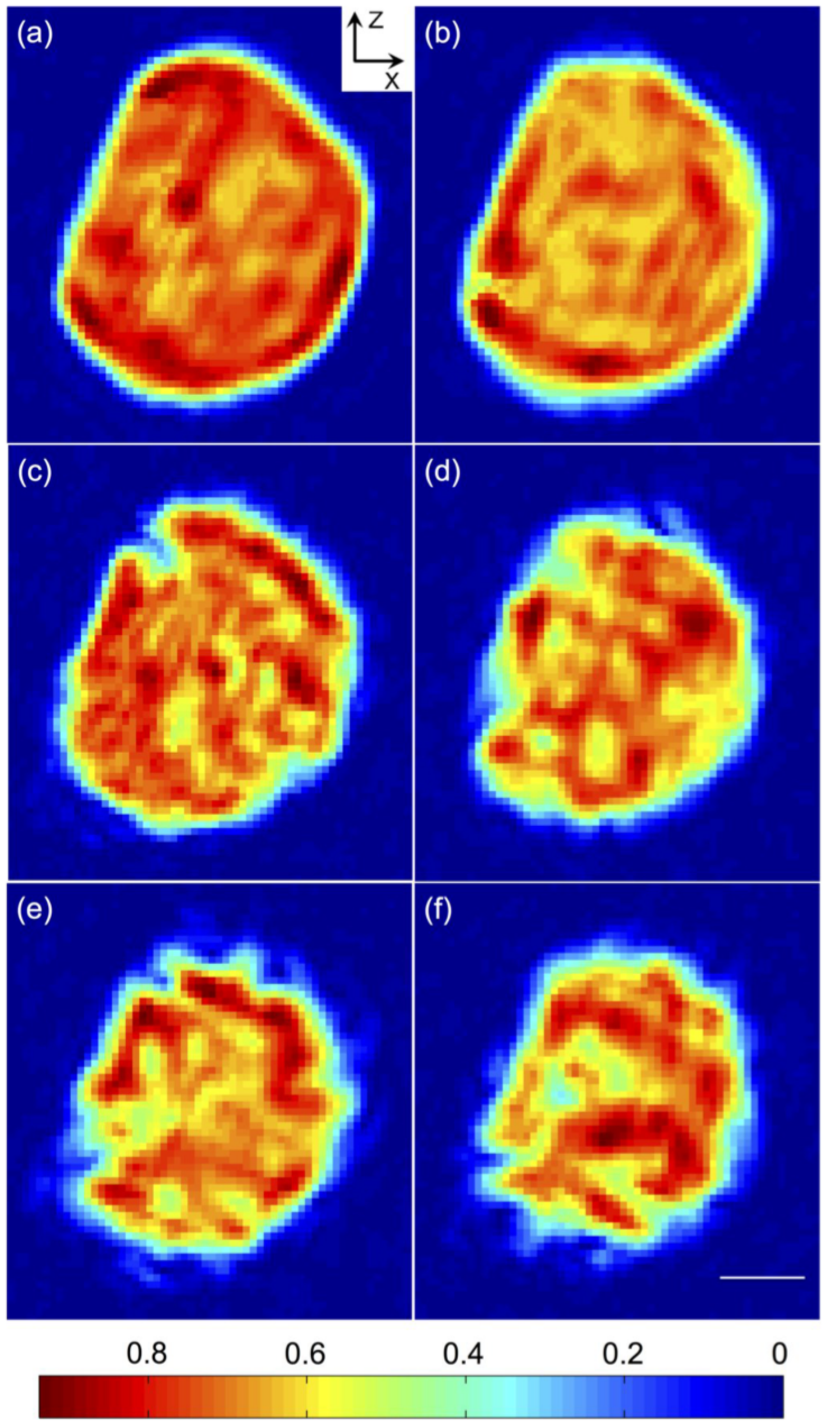




z
x
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
Spatial Frequency (nm^{-1})
-0.1
-0.05
0
0.05
0.1
Spatial Frequency (nm^{-1})

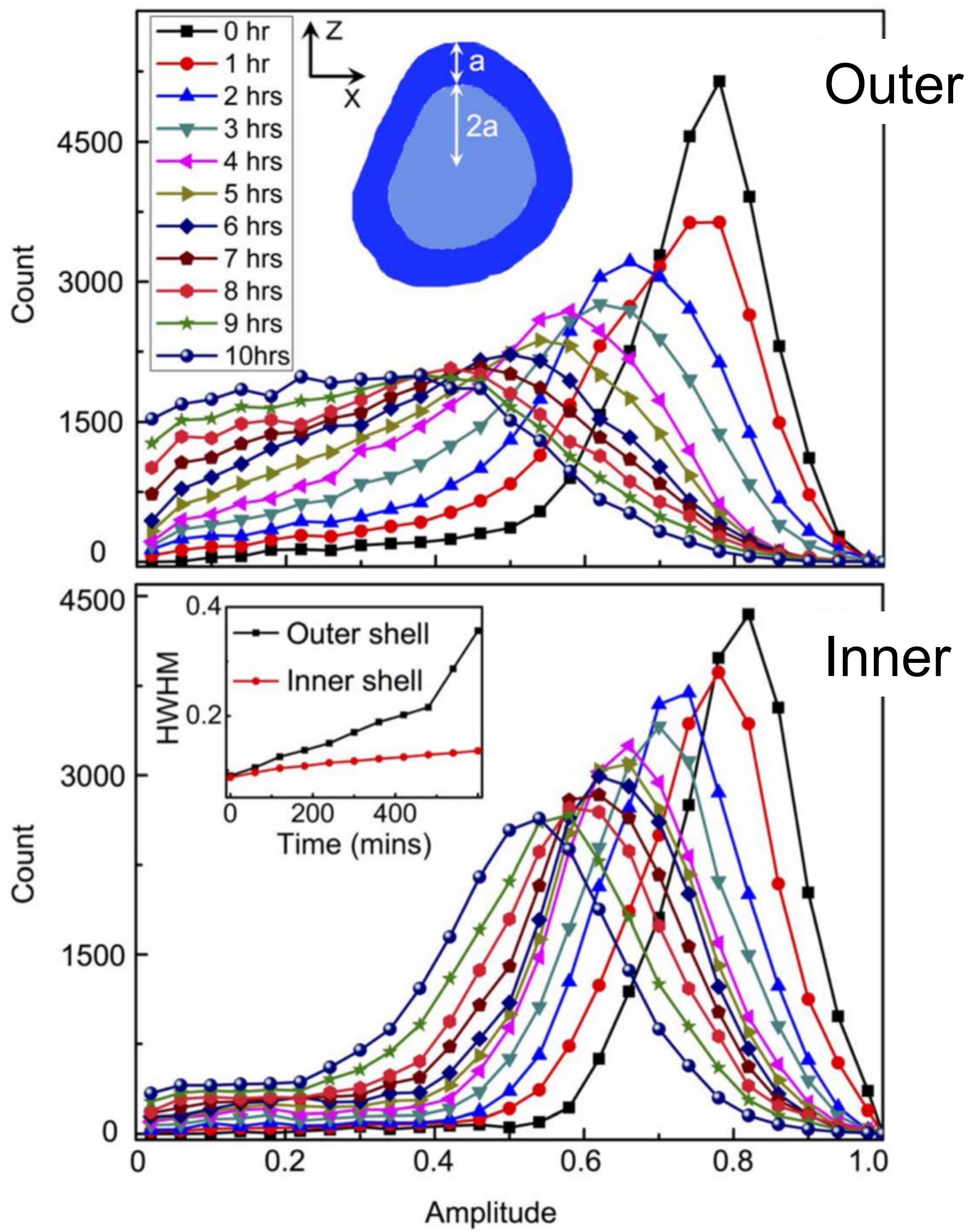

z
x
10
20
30
40
50
60
70
80
-10
0
10
20
30
40
50
60
70
80
1
0.8
0.6
0.4
0.2
0


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


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

Atomic Diffusion within Individual Gold Nanocrystal

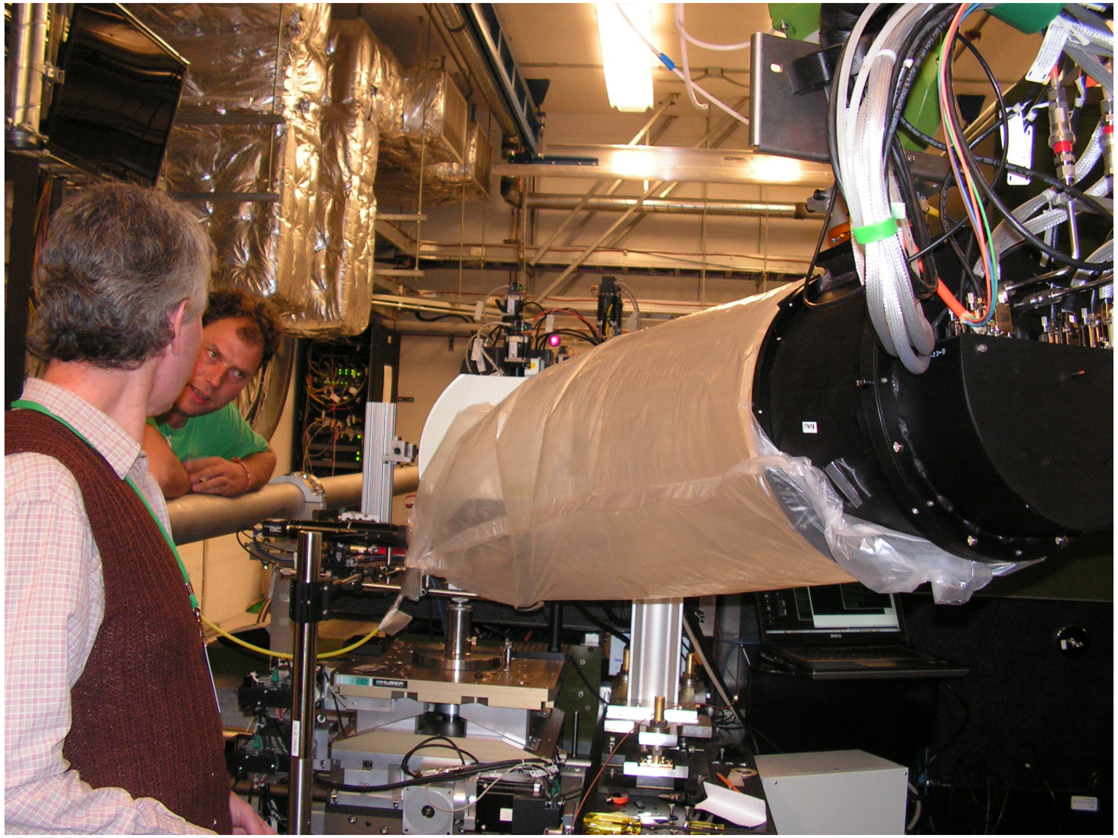
Gang Xiong,
J. N. Clark,
C. Nicklin,
J. Rawle &
I. K. Robinson
Sci Rep **4** 6765
(2013)

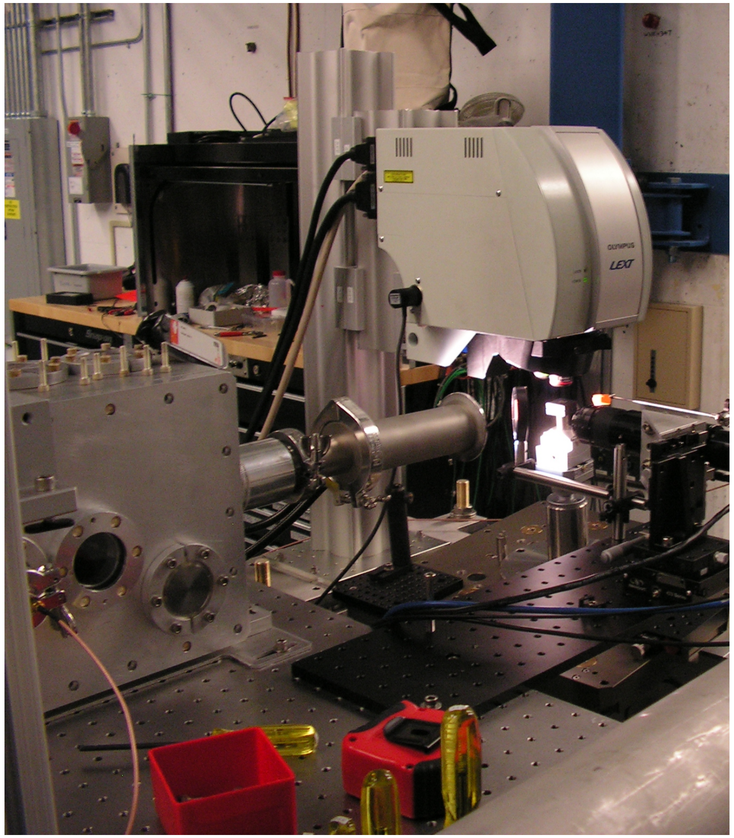


I

Pump-probe at LCLS (XPP)

Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz ,
Sebastien Boutet, Jesse Clark, Garth Williams, Brian Abbey, Andy Higginbotham,
Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt

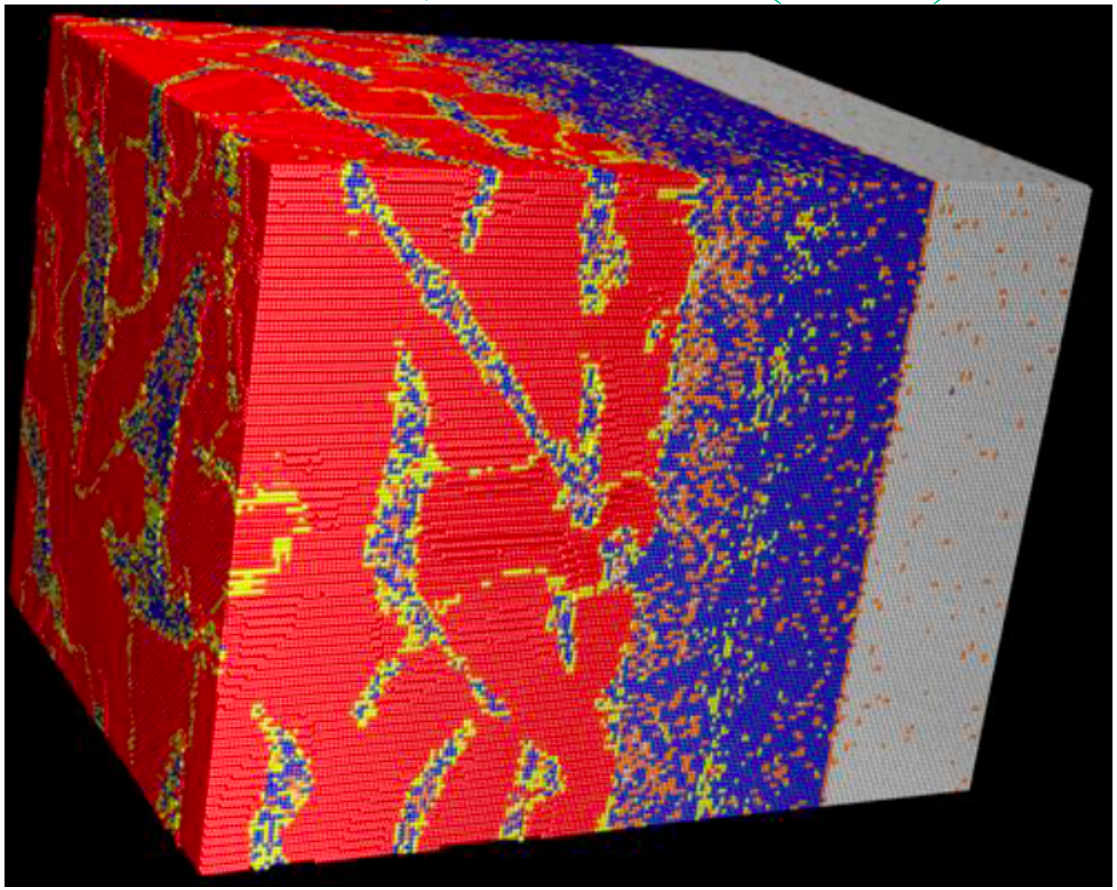




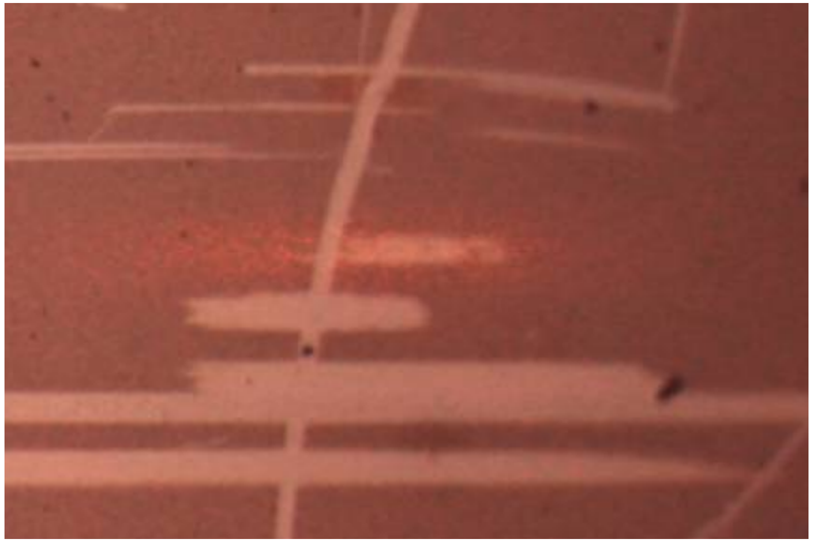
MD simulation of Shock Wave

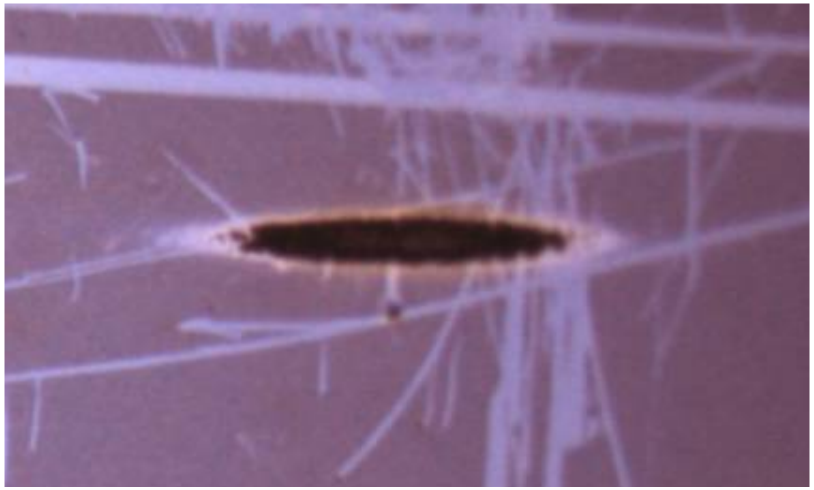
Damage in Fe along (001) direction

K Kadau, TC Germann, PS Lomdahl, and BL Holian. Science, 296 1681 (2002)



Visible and Confocal microscopy





Pump-probe at LCLS (XPP)

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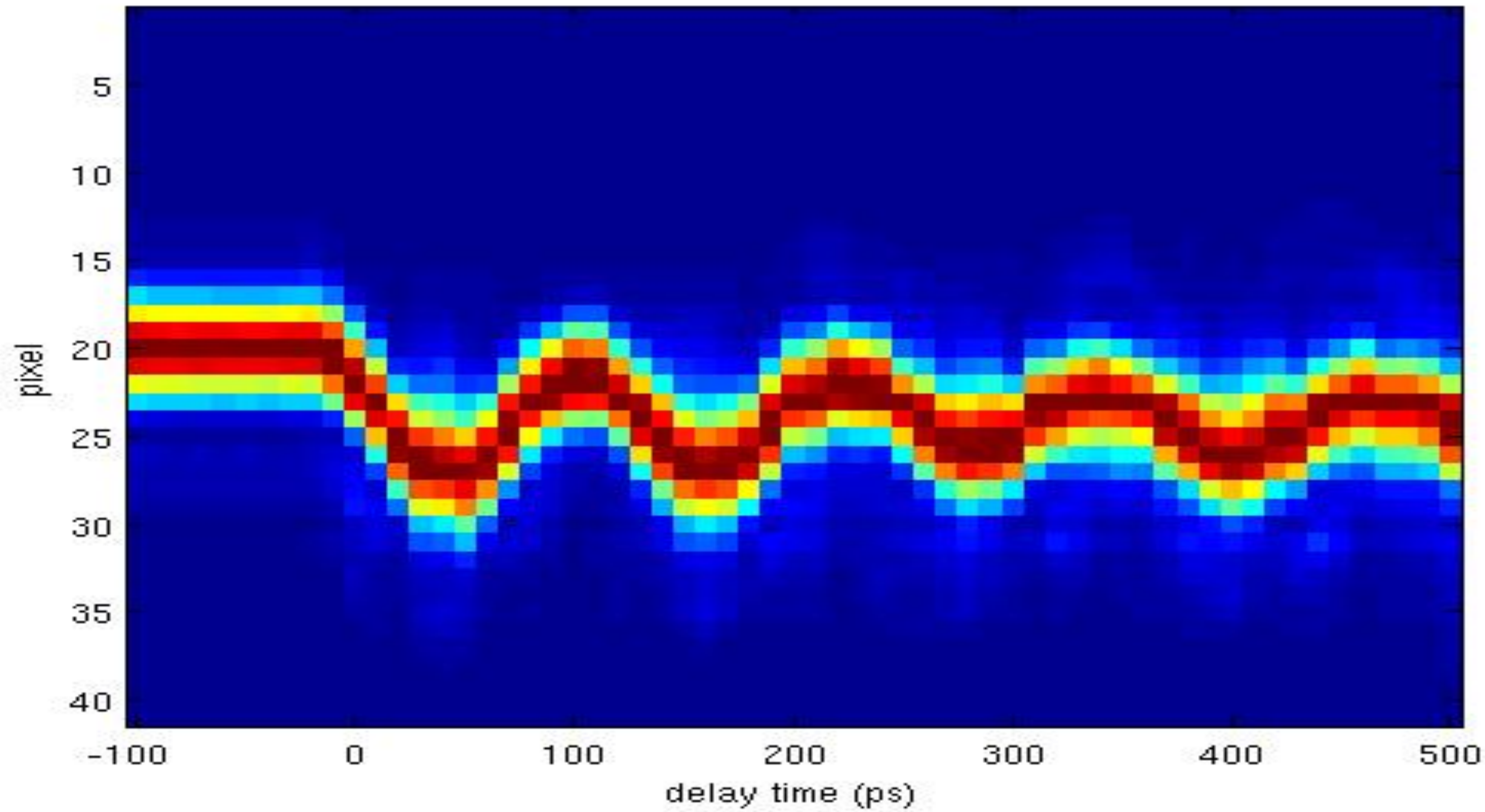
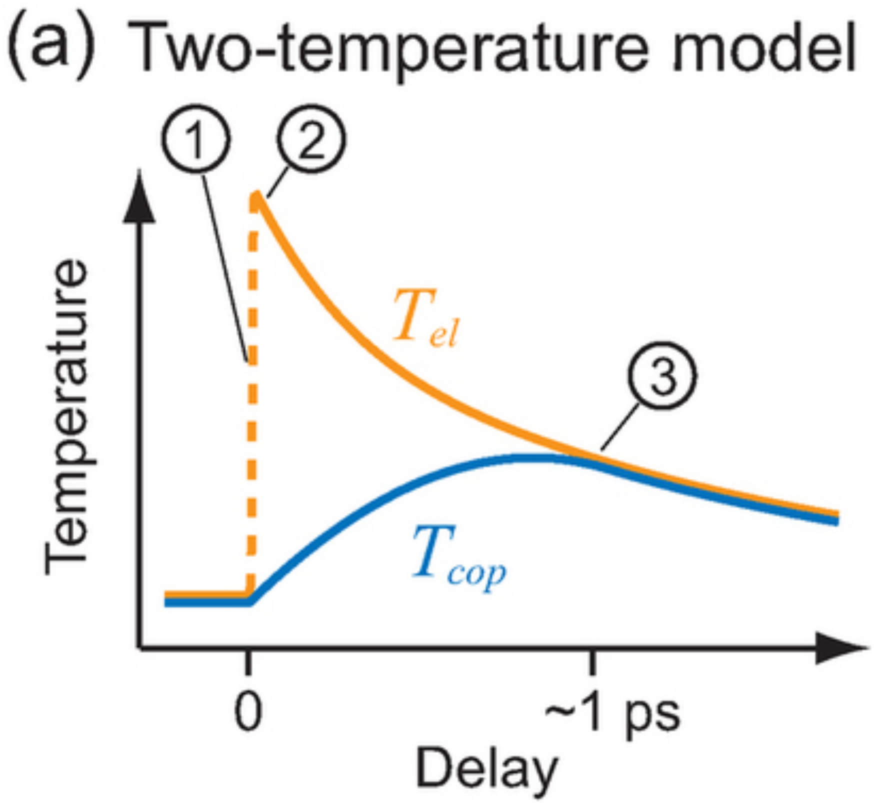
Sebastien Boutet, Jesse Clark, Garth Williams, Brian Abbey, Andy Higginbotham,
Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt

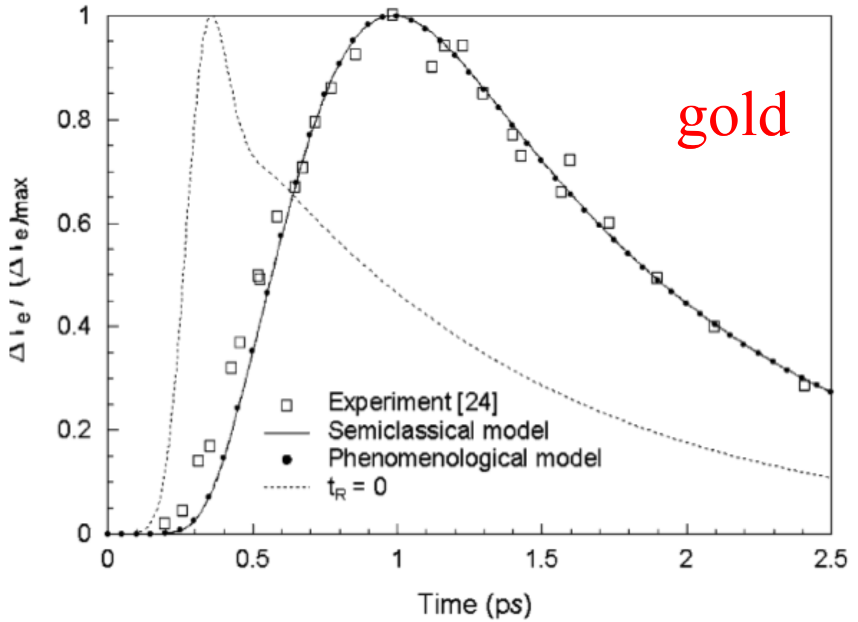


“Two-temperature” model

Y. Ishida et al, Nature Scientific Reports 1 64 (2011)

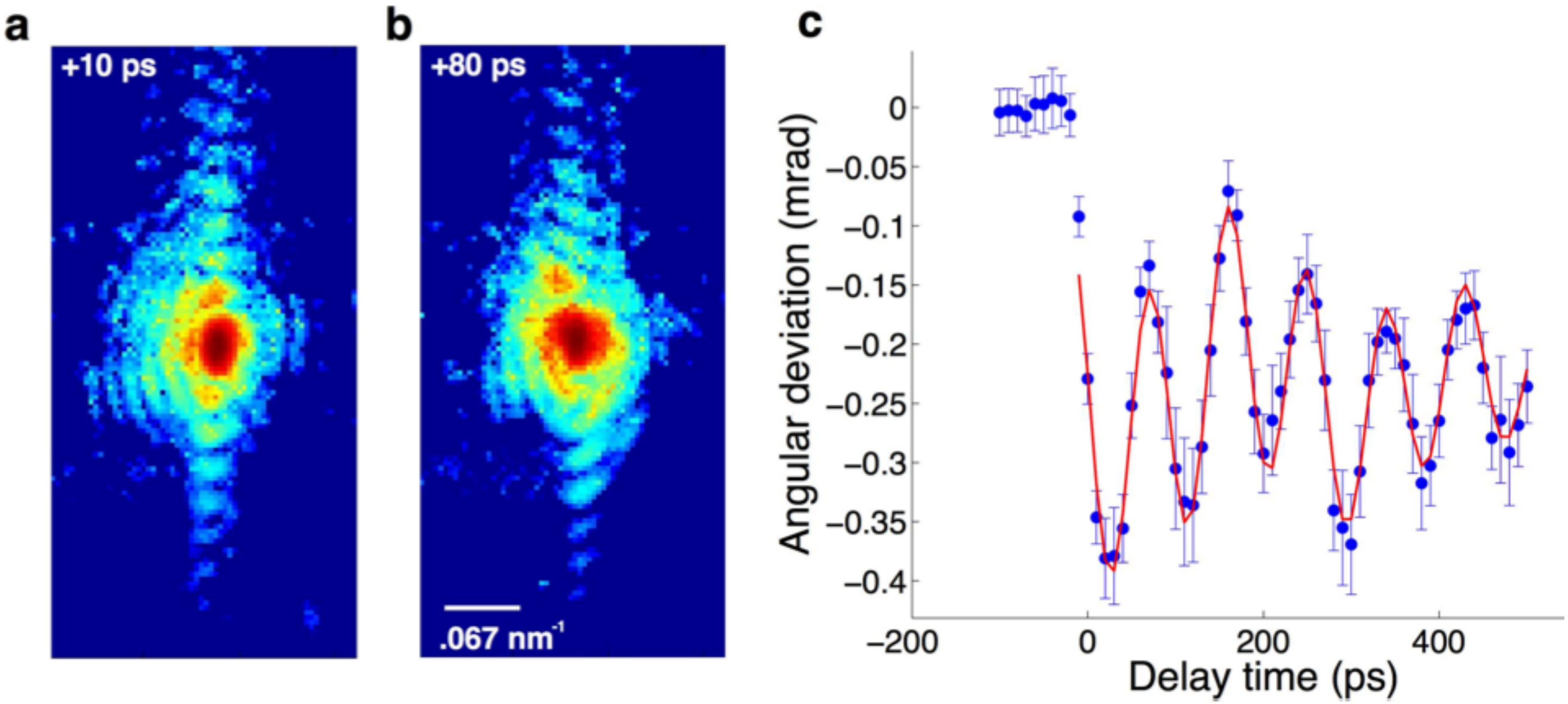
J.K. Chen et al, Int J. Heat Transfer 49 307 (2006)





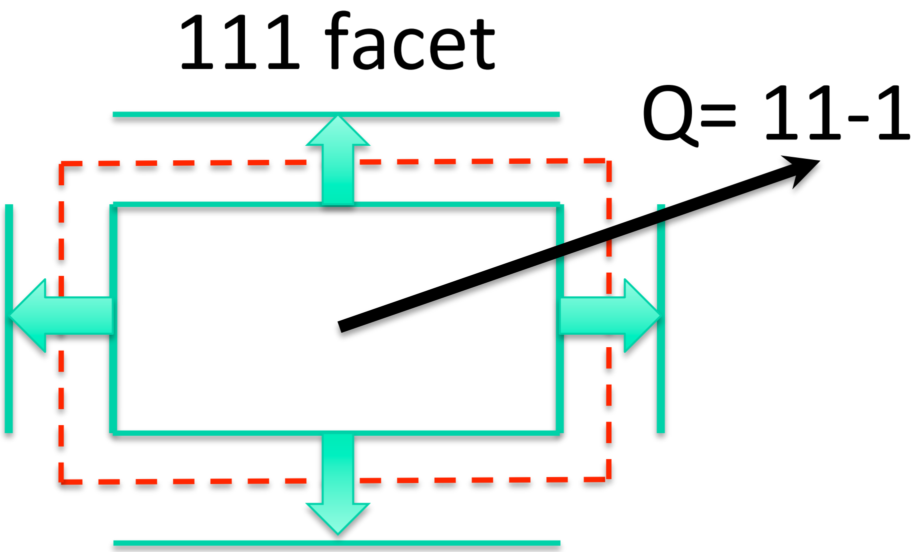
ig. 2. Comparison of the change in electron temperature at ie front surface of an 80-nm gold film irradiated by a 2.8 mJ/ n^2, 800 nm, 150-fs laser pulse.

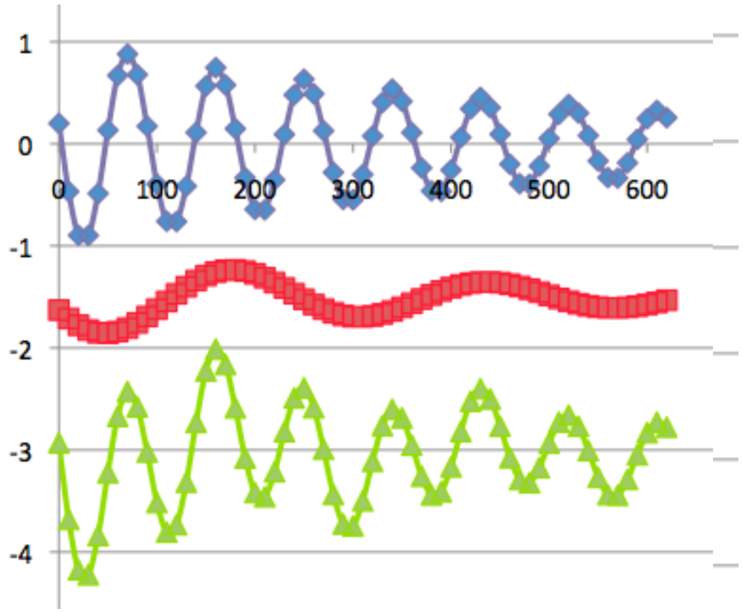
Time resolved Bragg peak position



Two Normal Modes of Vibration

$$S(\tau) = \sum_{n=1}^{N} A_n \exp\left[-\left(\tau/\tau_{d,n}\right)^2\right] \cos\left(\omega_n \tau + \varphi_{0,n}\right)$$



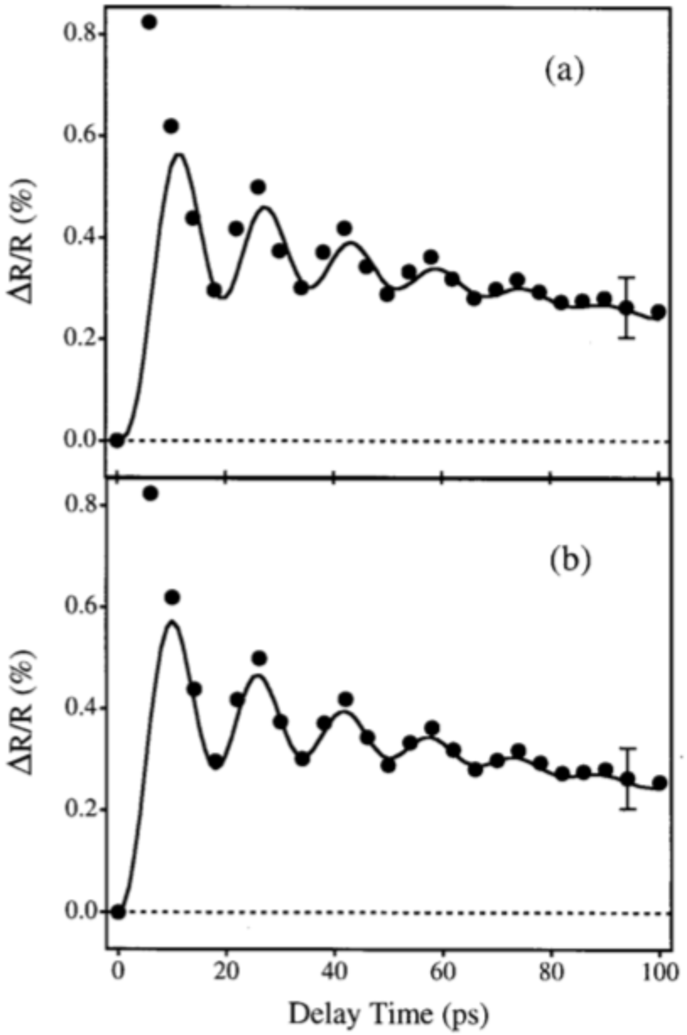


T_1 = 90ps h_1 = 145nm c_S = 3240 m/s

T_2 = 259ps h_2 = 420nm

Ultrafast Absorption Spectroscopy

24nm Au nanoparticles in H_2O, converted to radius
G. V. Hartland, J. Chem. Phys. 116, 8048 (2002)

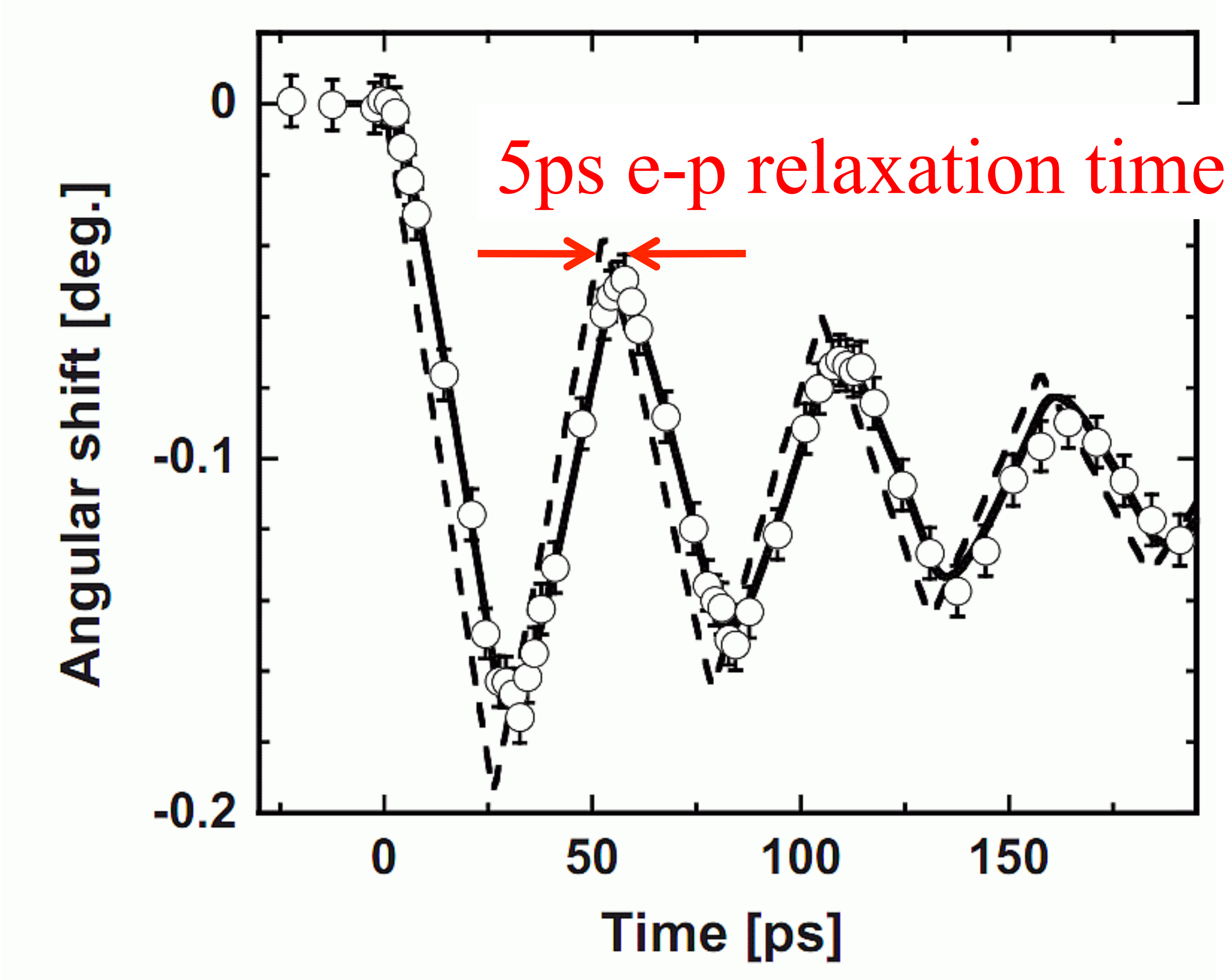


(a) Simple normal mode analysis with impulse heating.

(b) Corrected by adding 2T model and electronic contribution to thermal expansion coefficient.

Plasma Source on 90nm Au film

M. Nicoul et al, APL 98 191902 (2011)

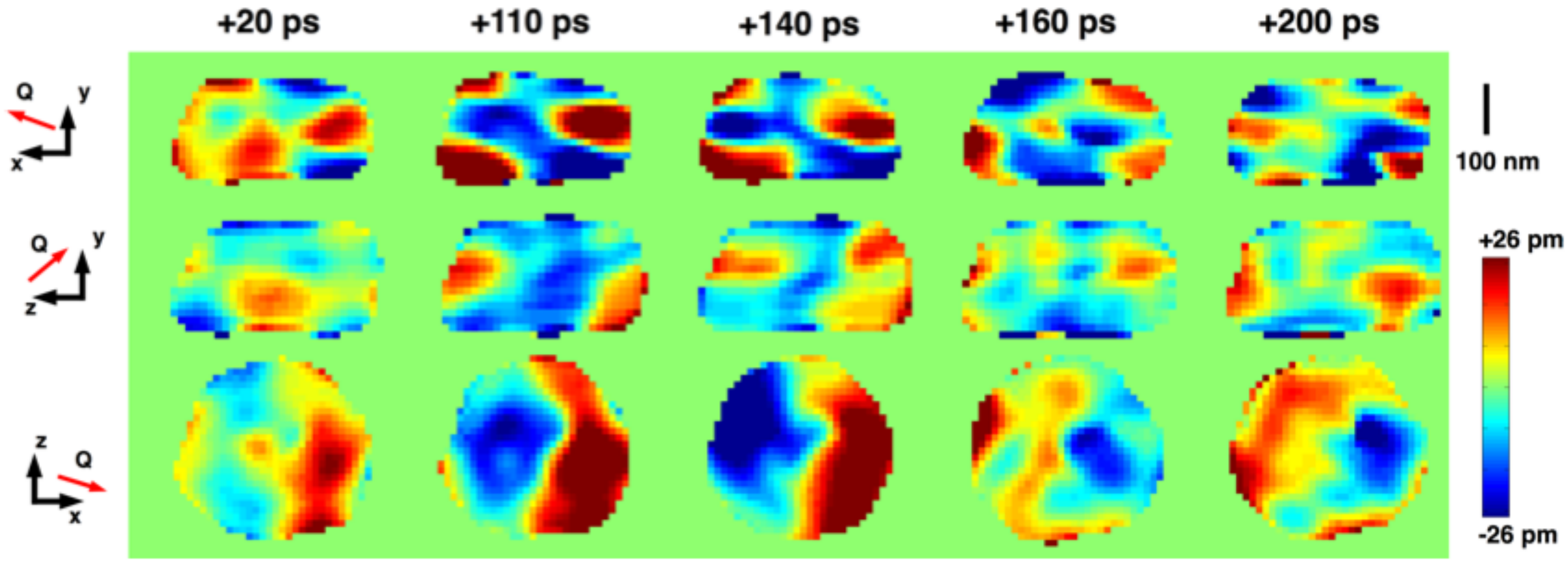


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

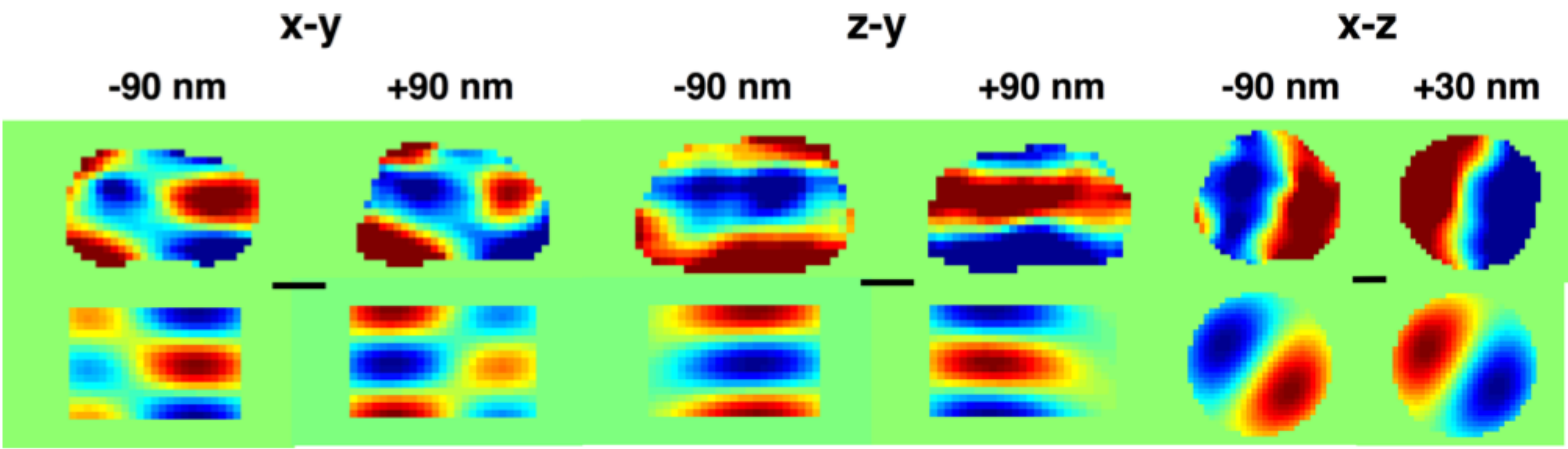
1000 frames averaged at each point of rocking curve

Jesse Clark et al, Science 341 56 (2013)



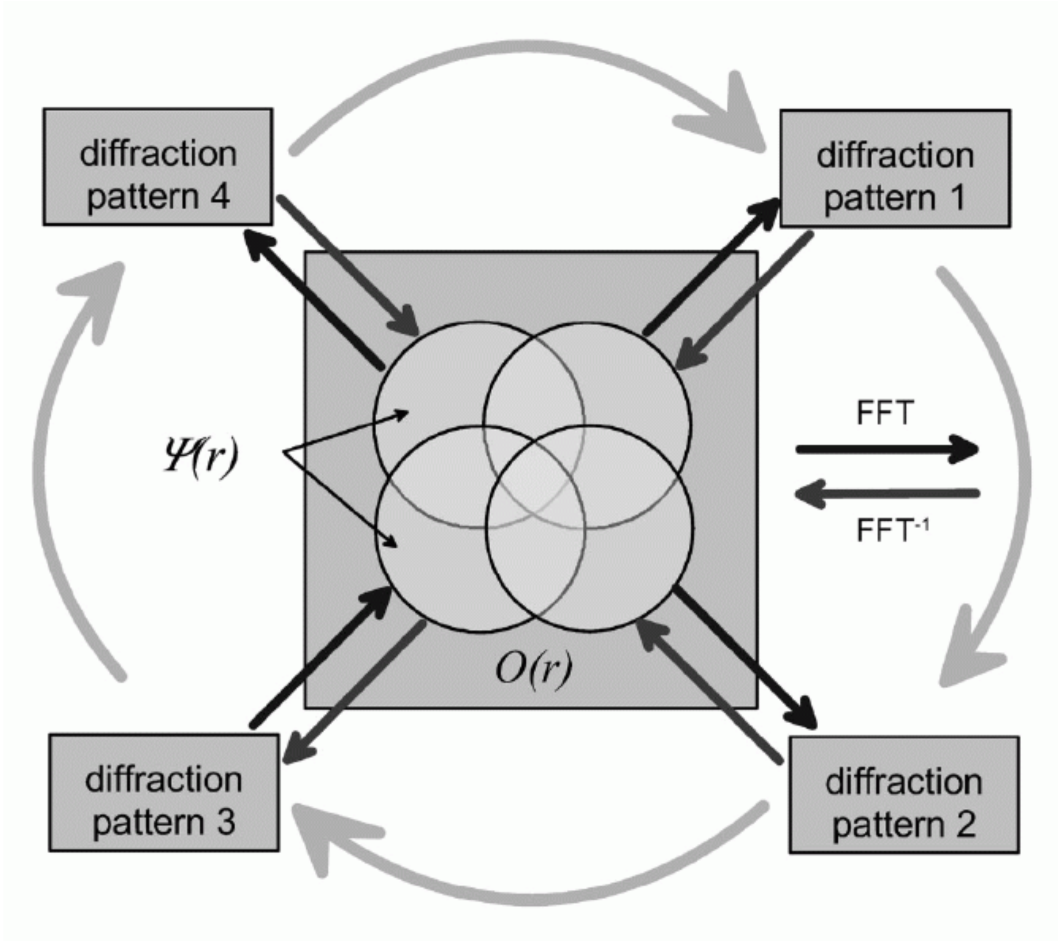
Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns
Comparison with (1,1) normal mode of cylinder
Jesse Clark et al, Science 341 56 (2013)



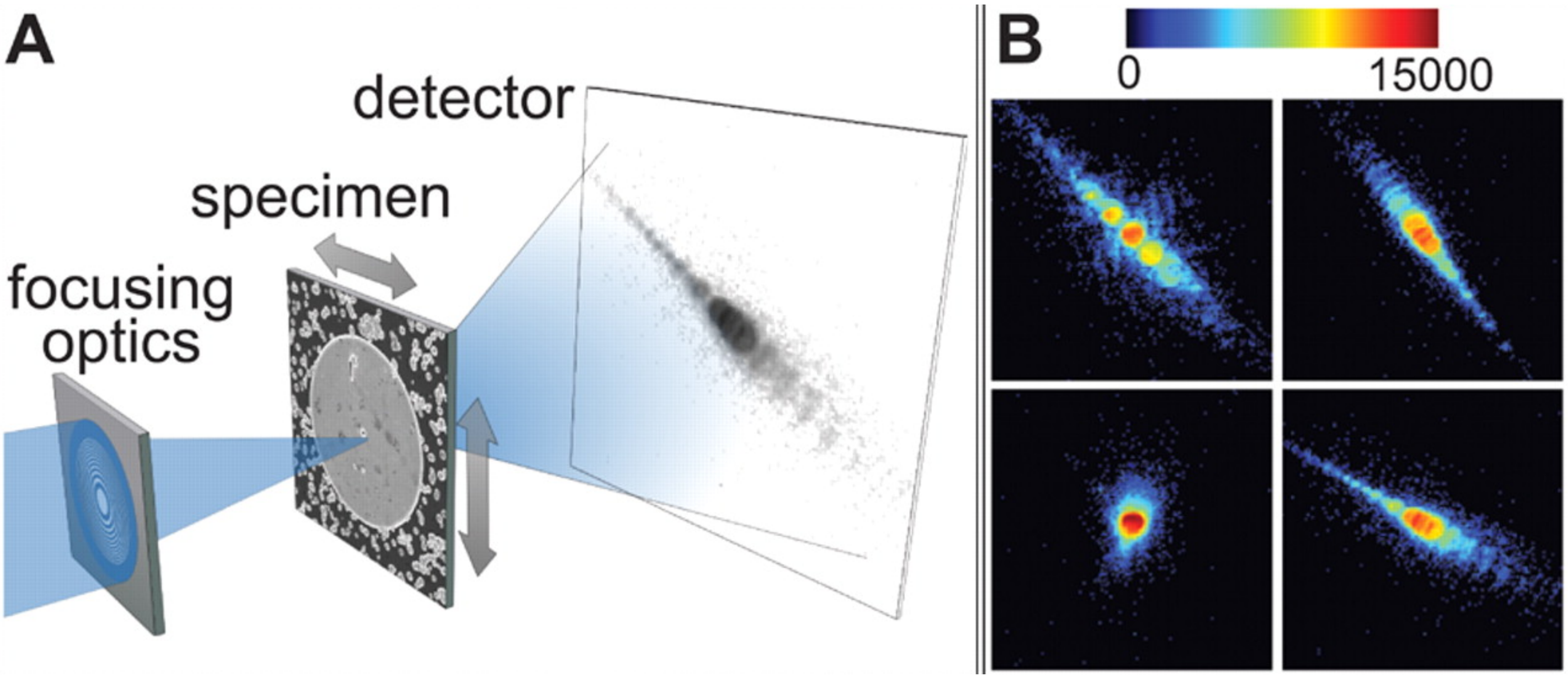
X-ray Ptychography

J. Rodenburg et al, PRL 98, 034801 (2007)



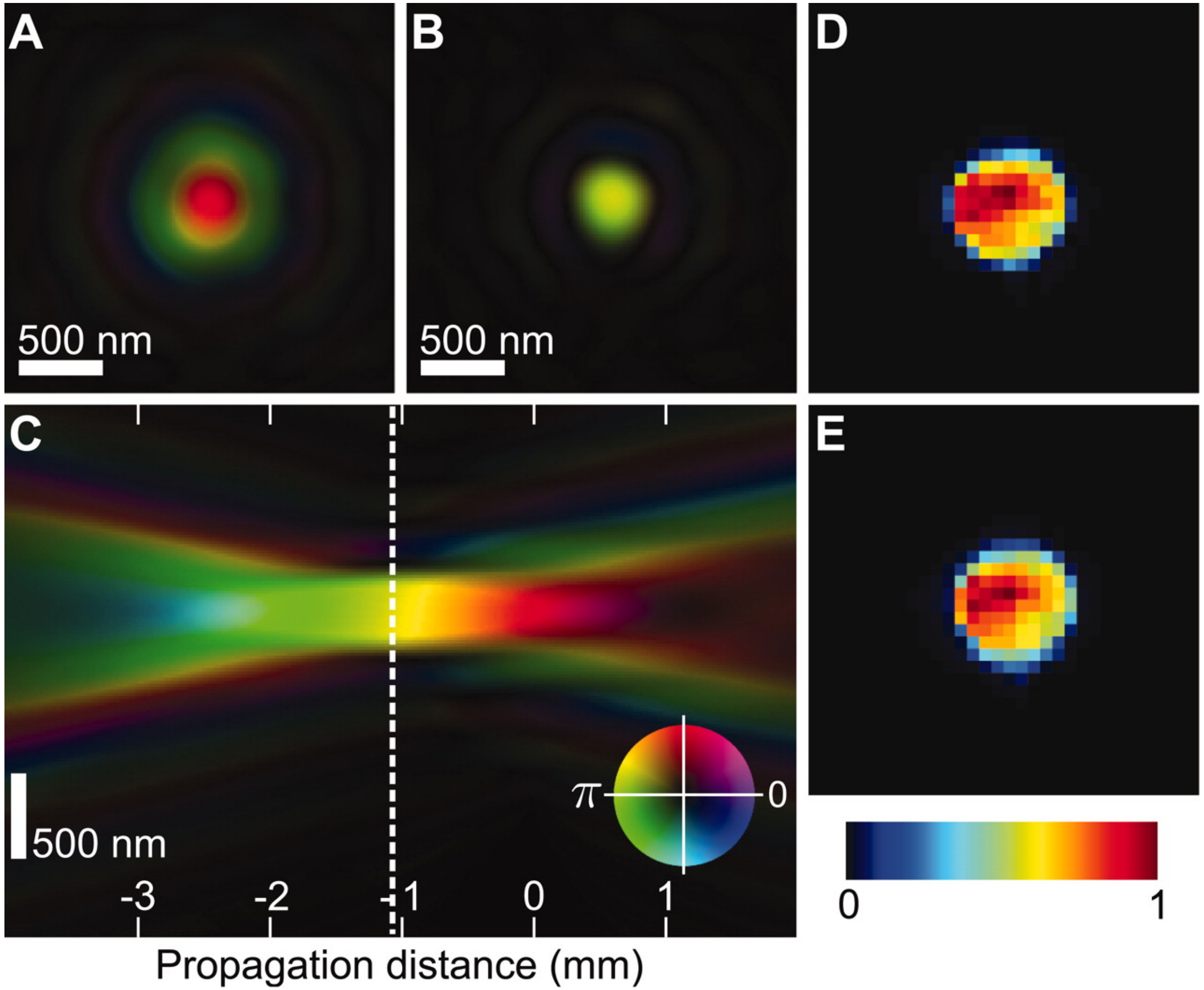
X-ray Ptychography

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



Reconstruction of Probe

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



Solution of the Phase Problem in the Theory of Structure Determination of Crystals from X-Ray Diffraction Experiments

Emil Wolf*
Department of Physics and Astronomy and the Institute of Optics, University of Rochester, Rochester, New York 14627, USA
(Received 6 May 2009; published 10 August 2009)

We present a solution to a long-standing basic problem encountered in the theory of structure determination of crystalline media from x-ray diffraction experiments; namely, the problem of determining phases of the diffracted beams.

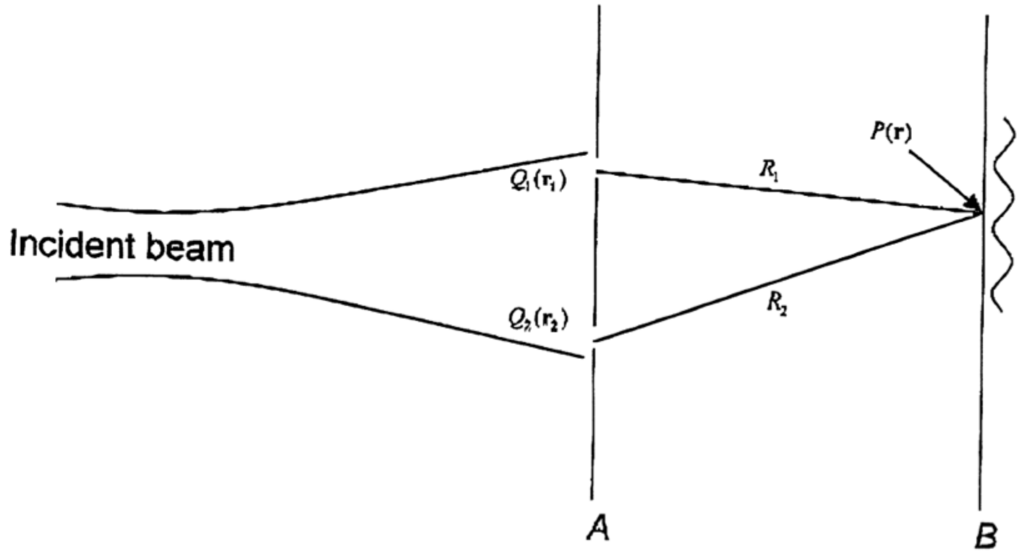
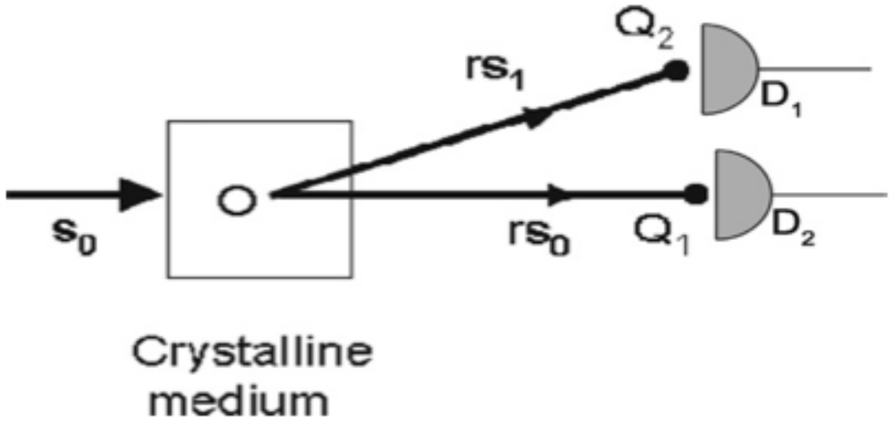


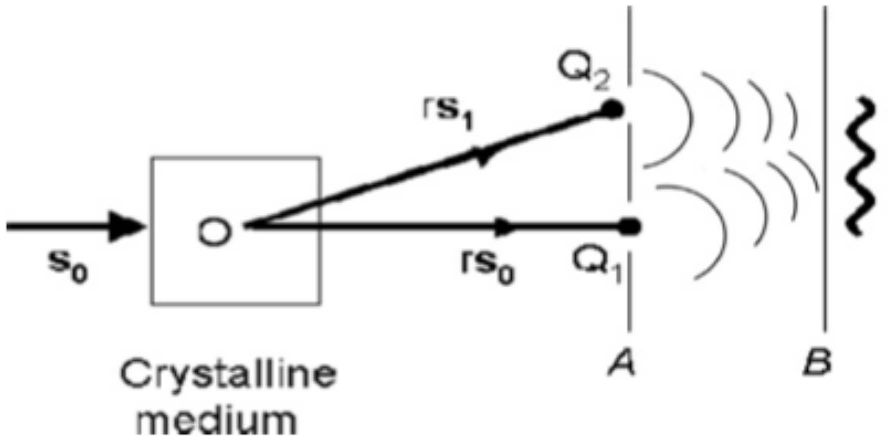
FIG. 1. Illustrating notation relating to Young's interference experiment.

Emil Wolf's Phasing Scheme

Physics Letters A 374 491 (2010)



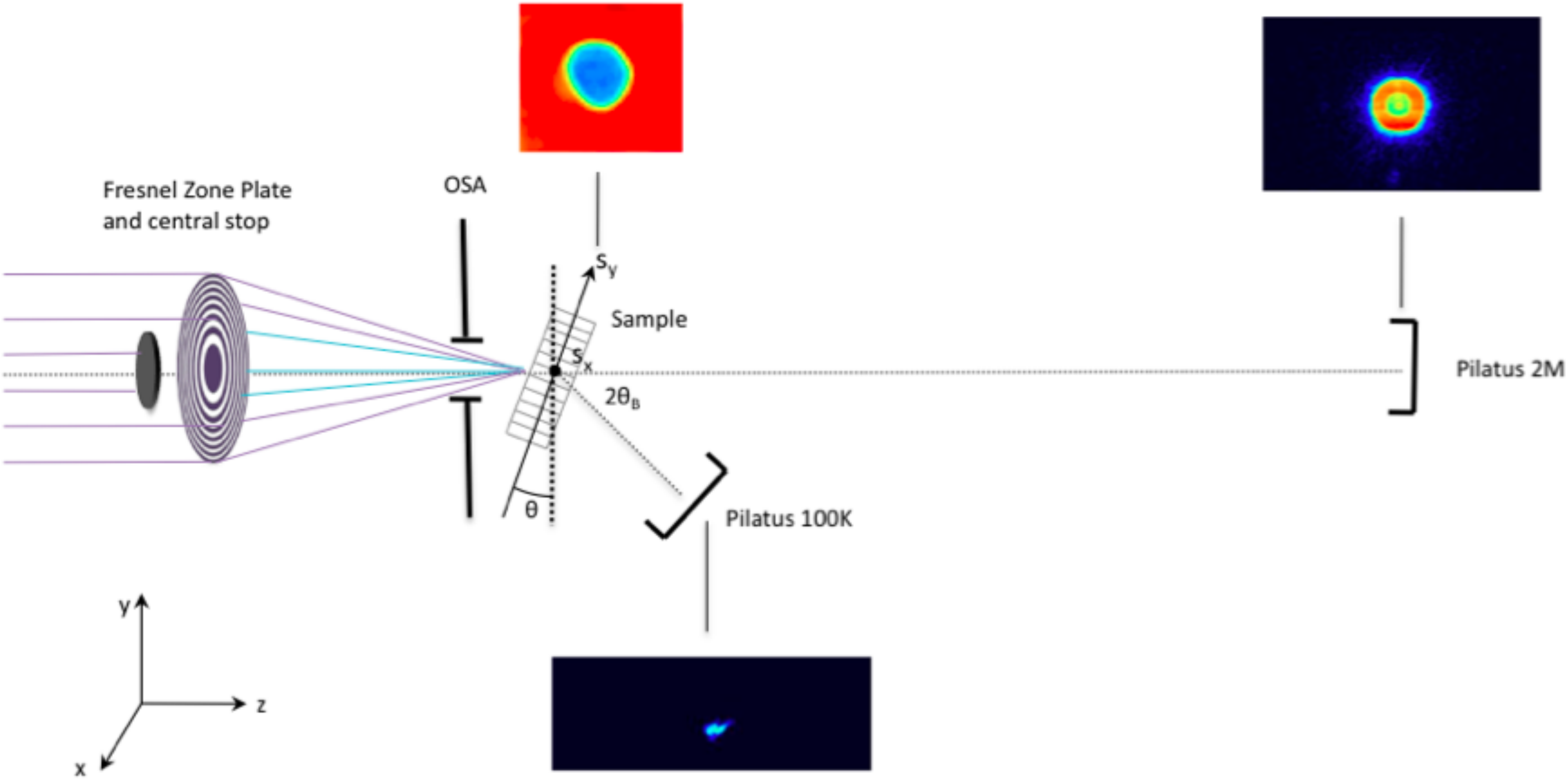
(a) In the usual technique one tries to measure *the phase difference between monochromatic beams at a pair of points* $Q_1(r\mathbf{s}_0)$ and $Q_2(r\mathbf{s}_1)$ in the far zone using detectors D_1 and D_2.



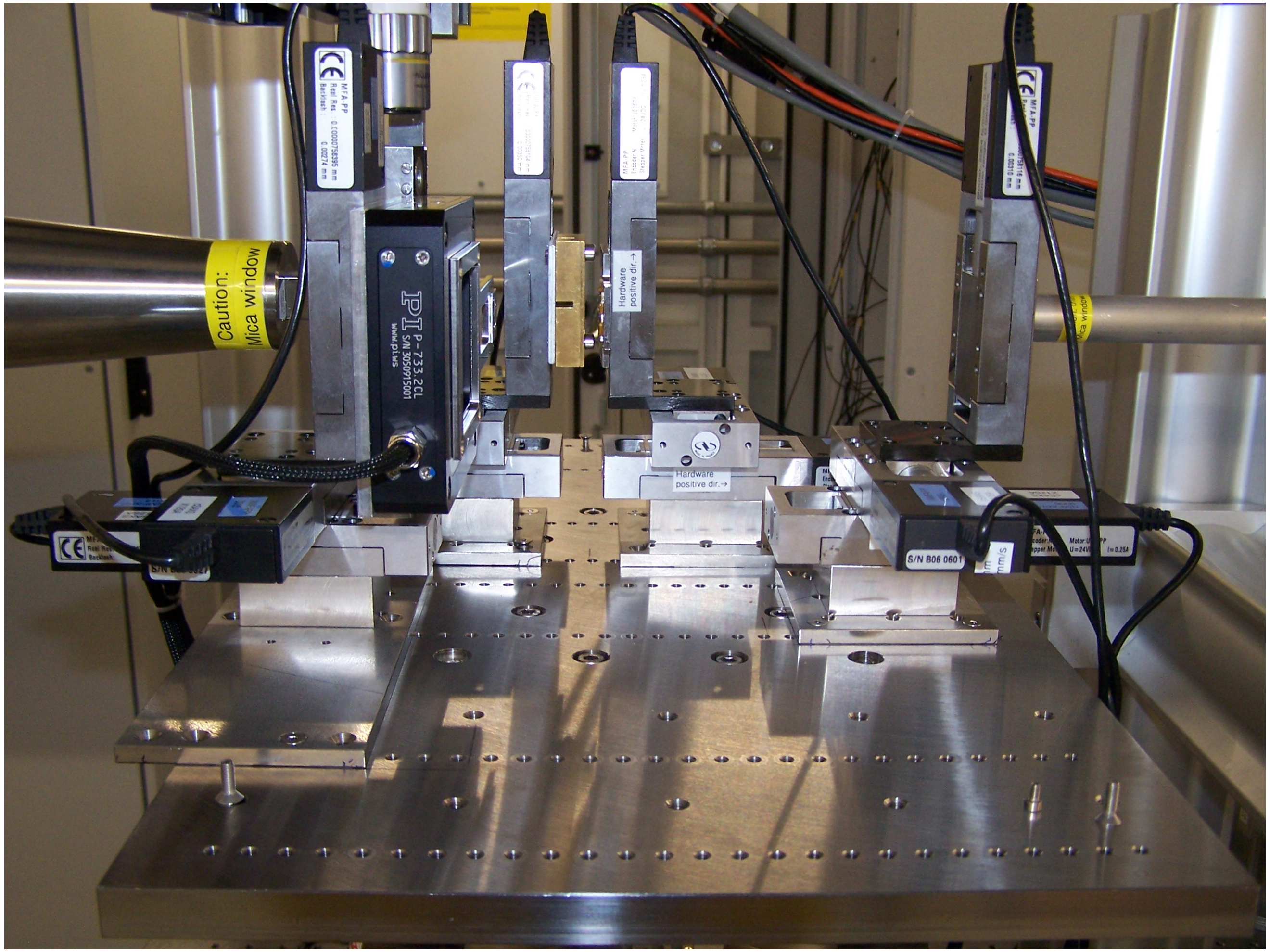
(b) In the technique described in the present Letter one would determine *the phase of the spectral degree of coherence* $\mu_{s0}(r\mathbf{s}_0, r\mathbf{s}_1; \bar{\omega})$ at a pair of points $Q_1(r\mathbf{s}_0)$ and $Q_2(r\mathbf{s}_1)$ in the far zone from an interference experiment.

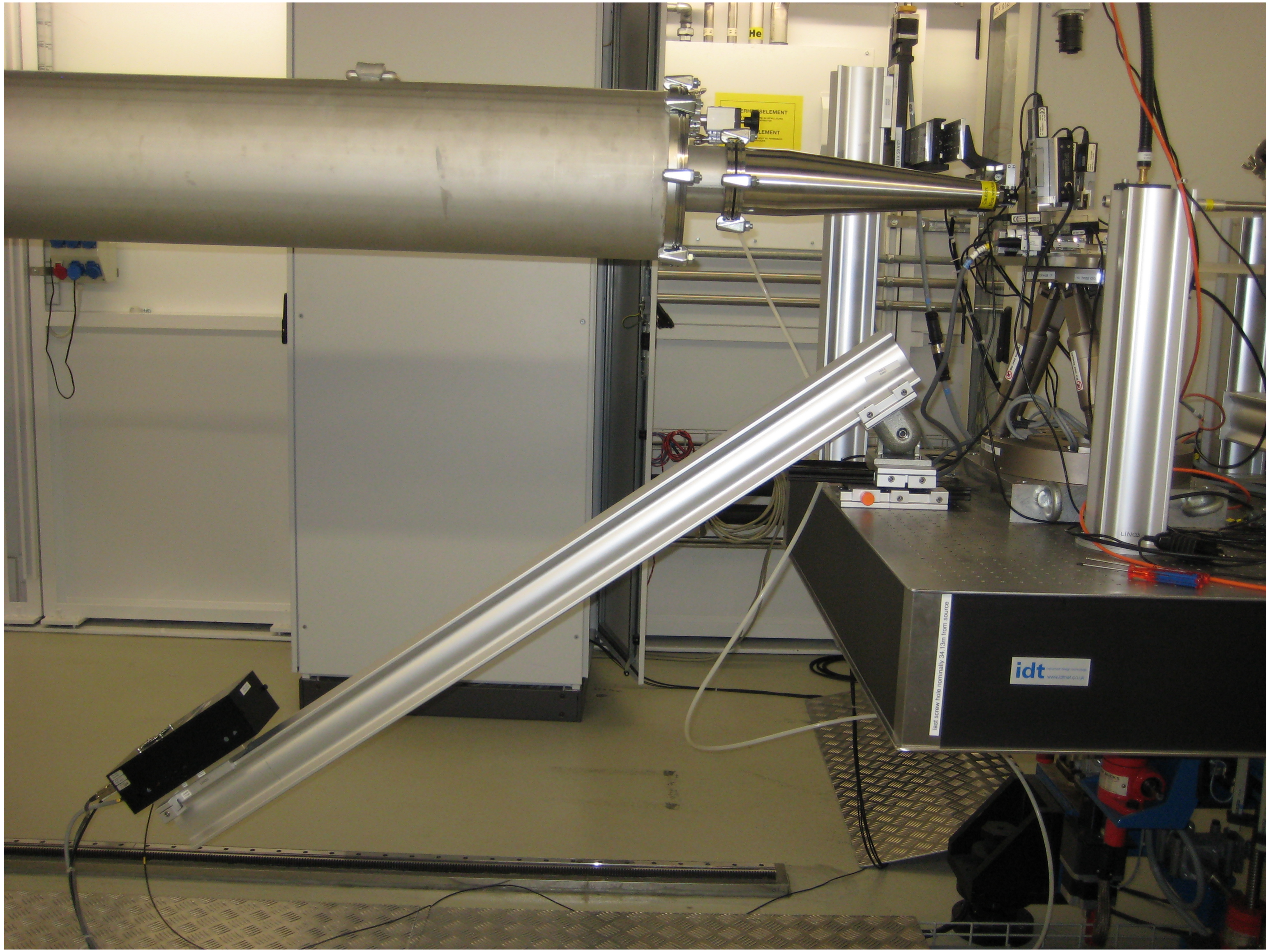
Ptychography of Gold Nanocrystals

Maria Civita, UCL, Ana Diaz, Swiss Light Source



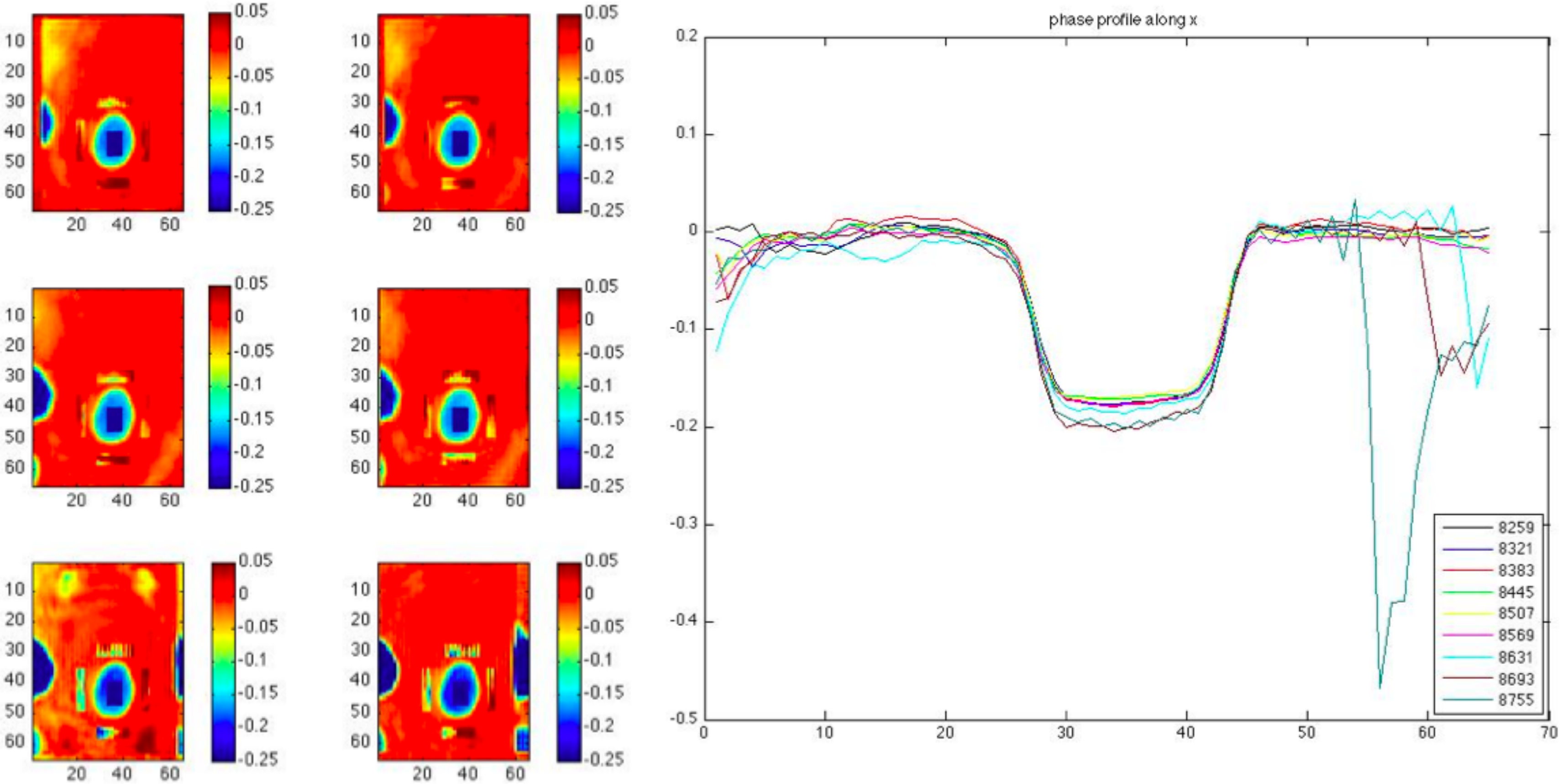
Swiss Light Source cSAXS beamline




He
idt

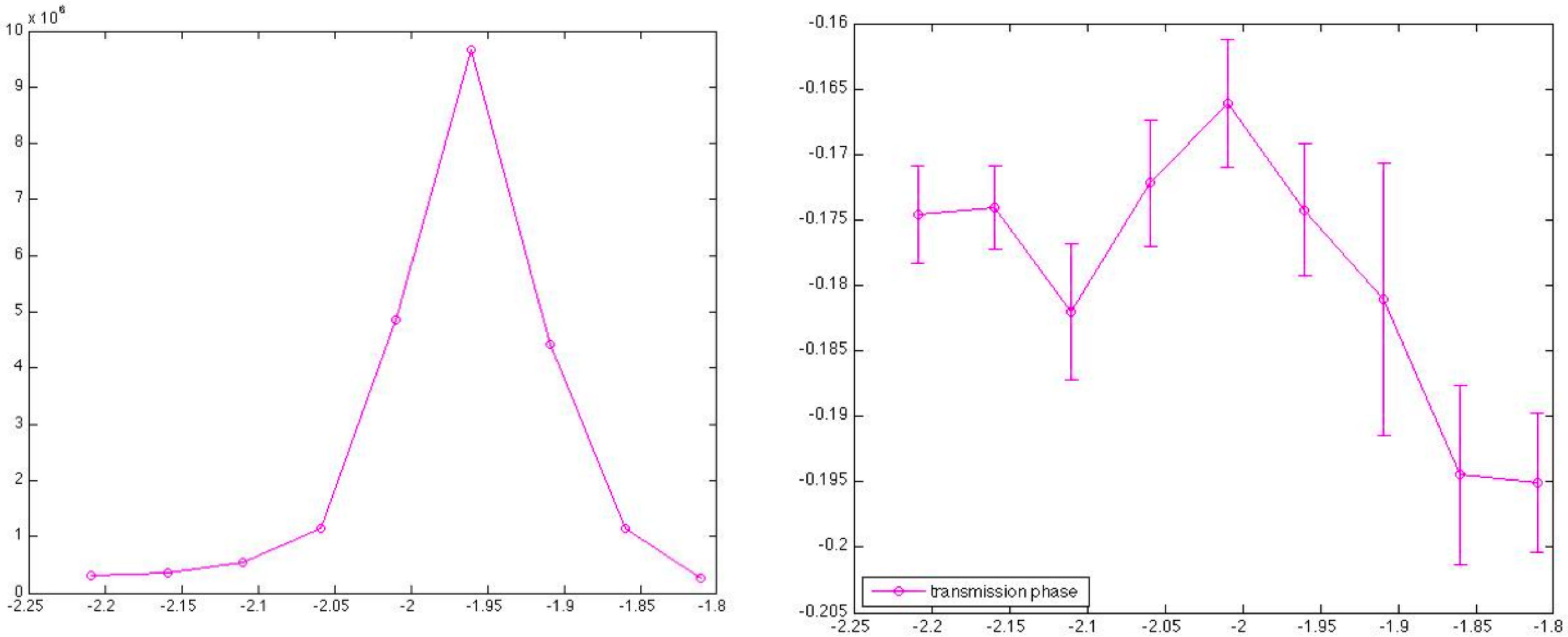
Ptychography of Gold Nanocrystals

Maria Civita, UCL, Ana Diaz, Swiss Light Source



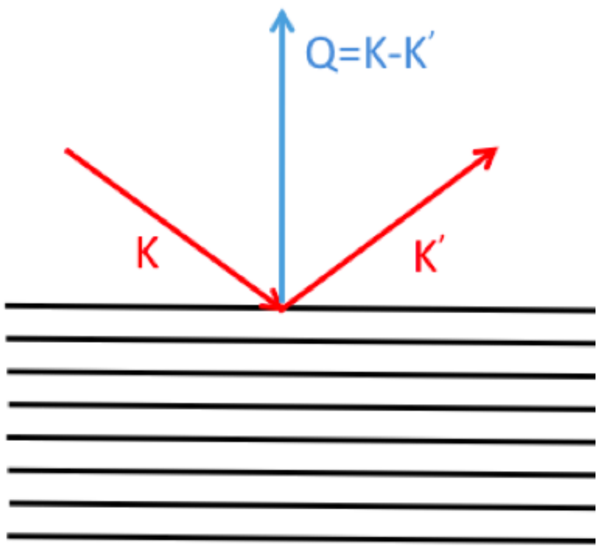
Transmitted Phase of Gold Nanocrystals

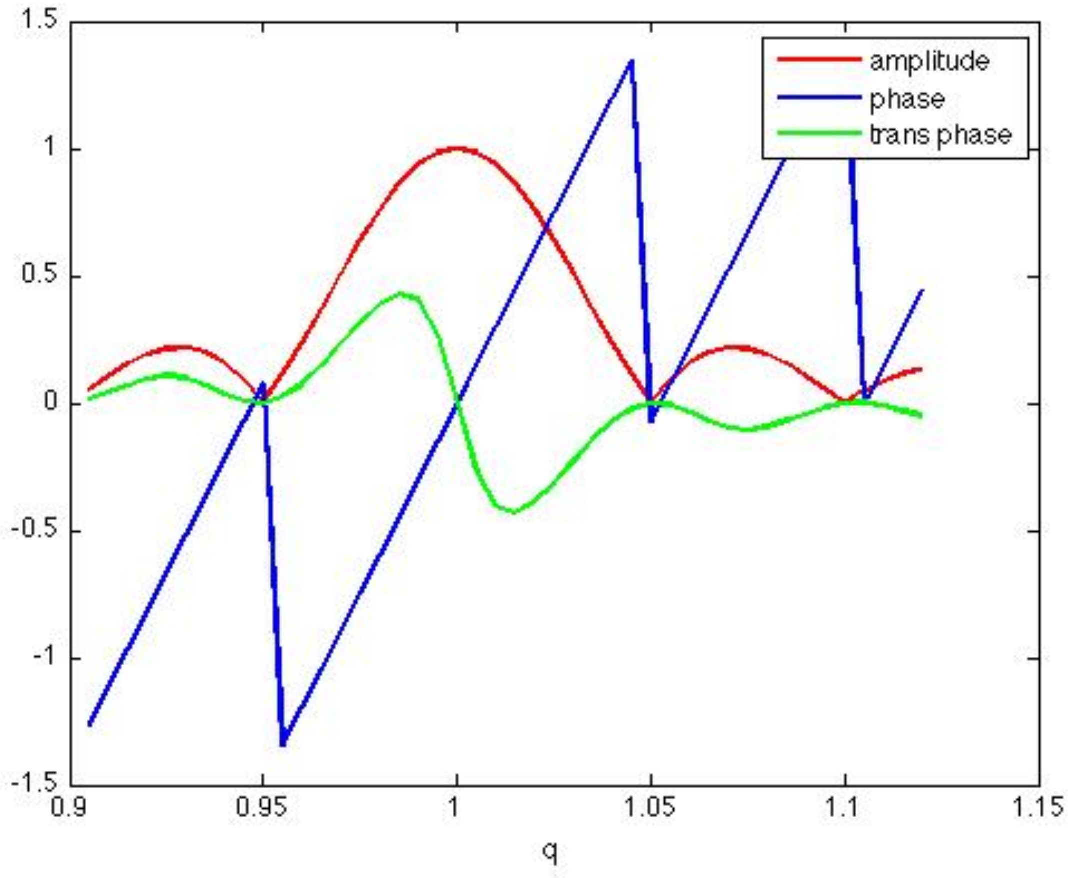
Maria Civita, UCL, Ana Diaz, Swiss Light Source



Diffraction from a Finite Slab

Als-Nielsen and McMorrow, "Modern X-ray Physics"





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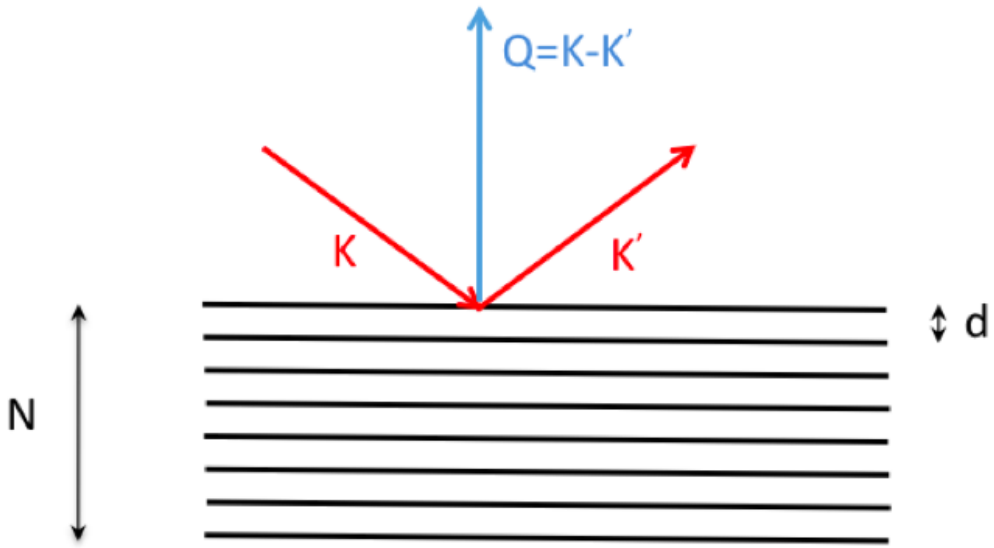
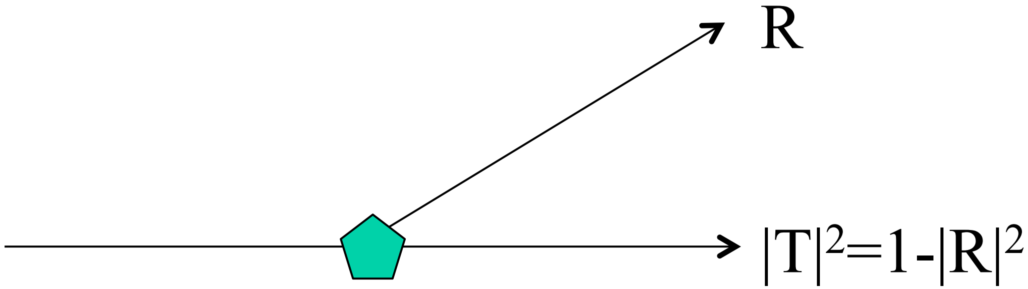
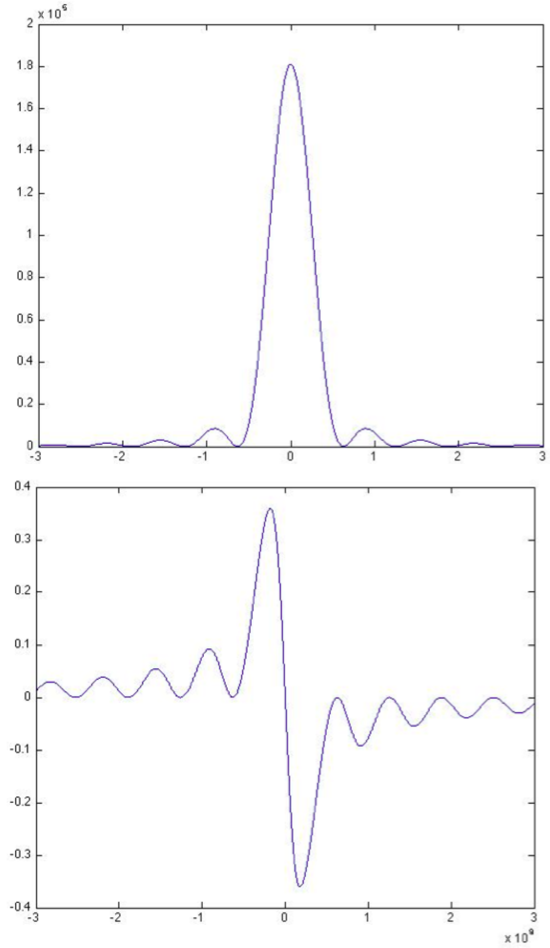
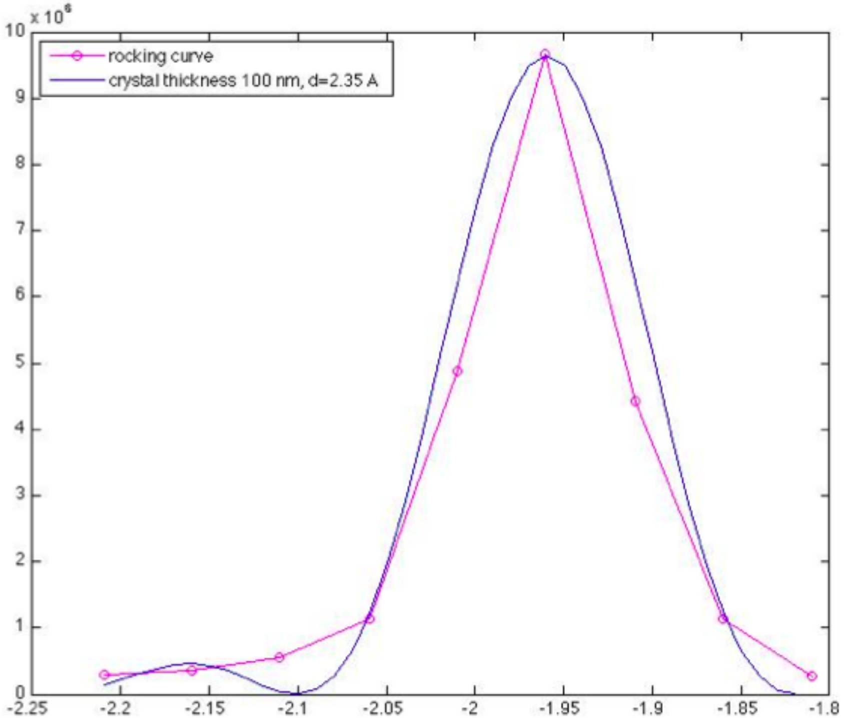


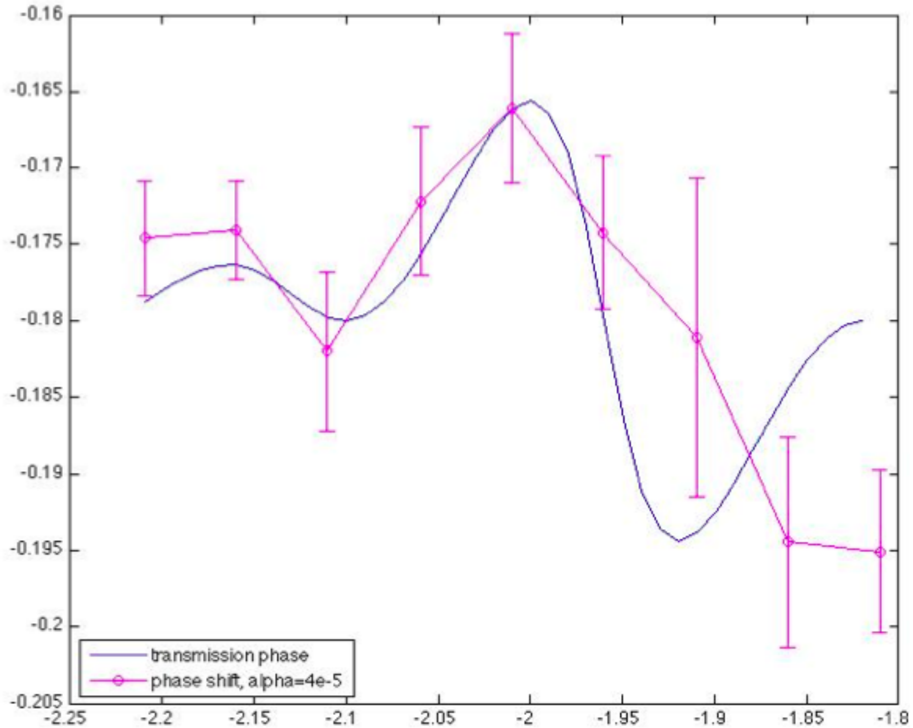




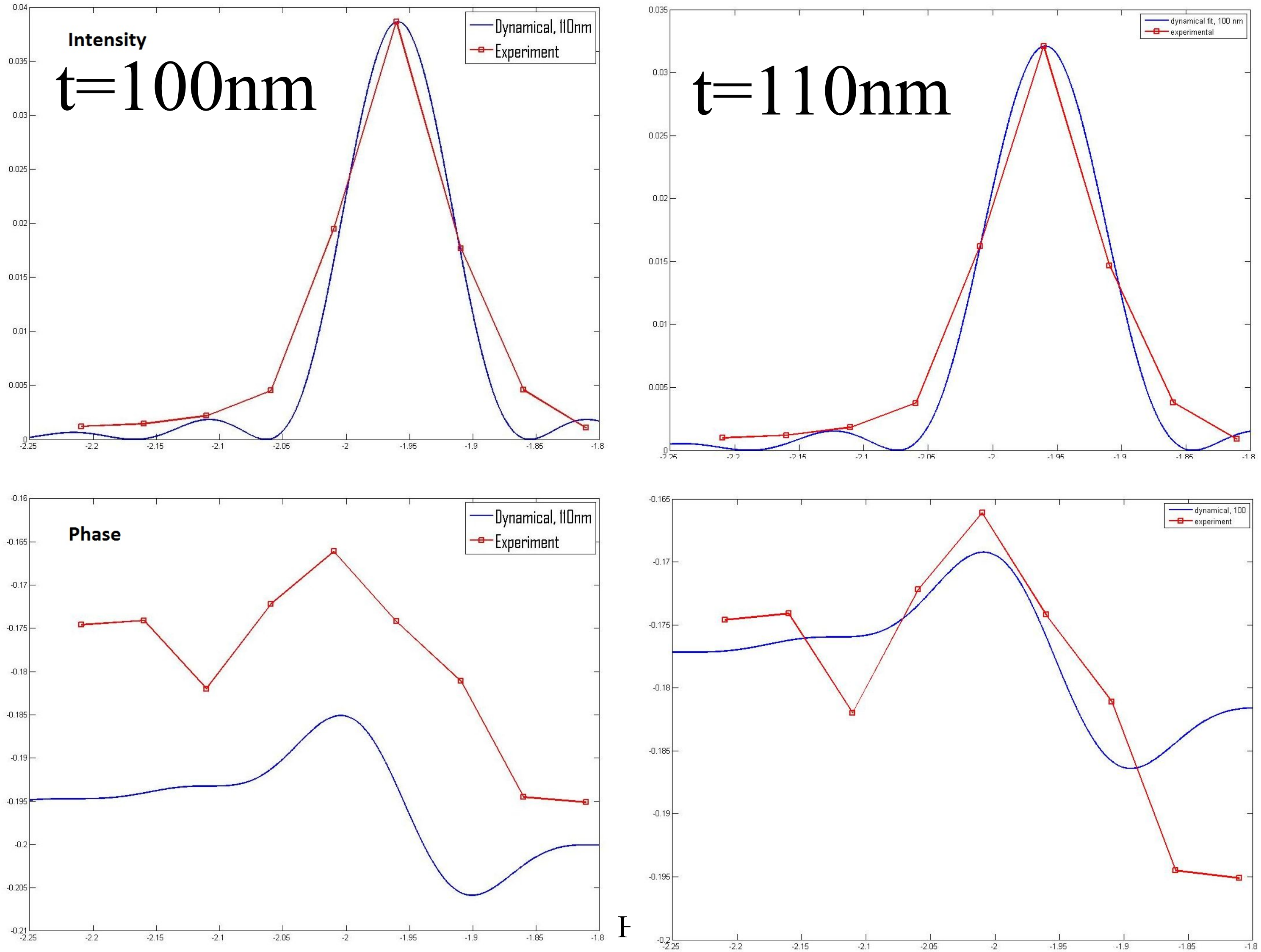
Ptychography of Gold Nanocrystals

Maria Civita, UCL, Ana Diaz, Swiss Light Source



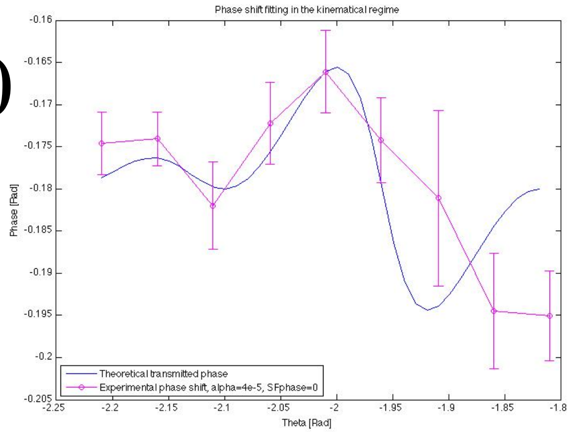


Dynamical Theory (Ivan Vartaniants)

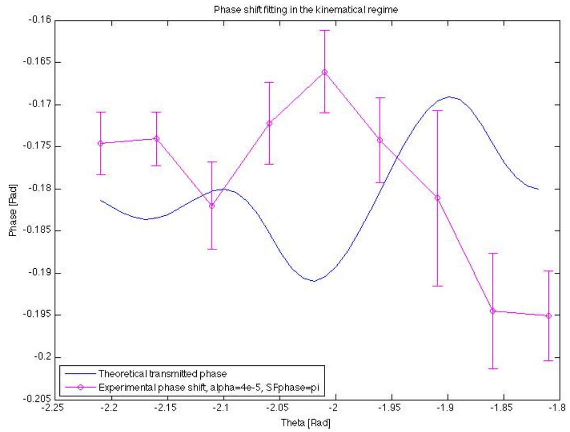


Sensitive to Crystallographic Phase

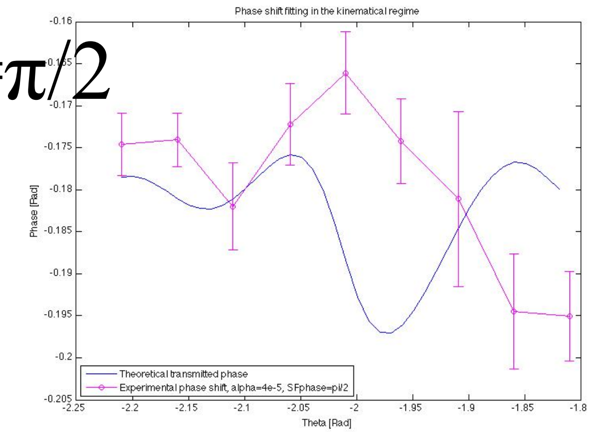
$\phi_{SF}=0$



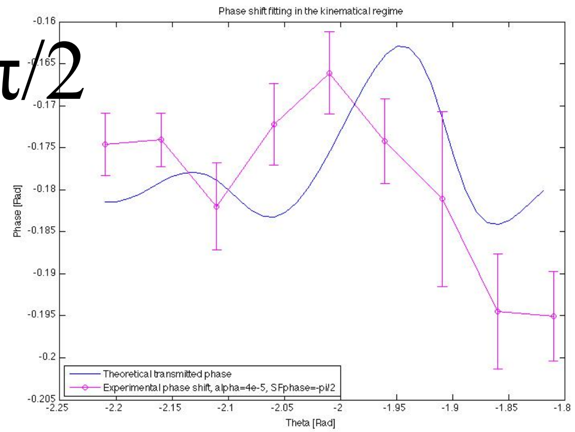
$\phi_{SF}=\pi$



$\phi_{SF}=\pi/2$



$\phi_{SF}=-\pi/2$



Coherent x-ray diffraction (CXD)

- Complex density can image strain
- Strain associated with nano-shape
- Diffusion of Cu in Au nanoparticle
- Ultrafast snapshots of vibrations
- Transient melting of nanoparticles
- Crystallographic phase determination