Ultrafast pump-probe CXDI

Ian Robinson
Jesse Clark
Ross Harder
Gang Xiong
Xiaojing Huang
Johannes Ihli
Fiona Meldrum
Justin Wark
Alexander Korsunsky

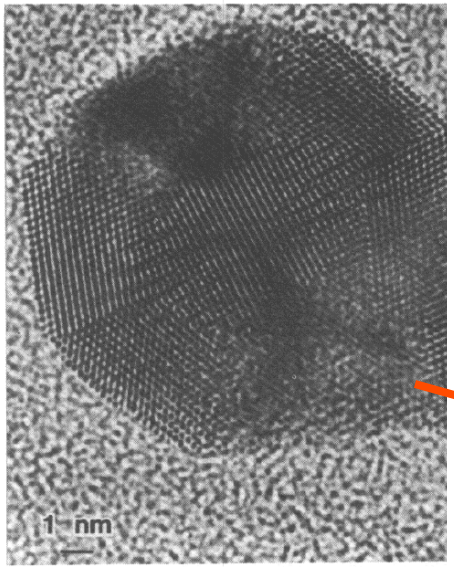
London Centre for Nanotechnology
Research Complex at Harwell

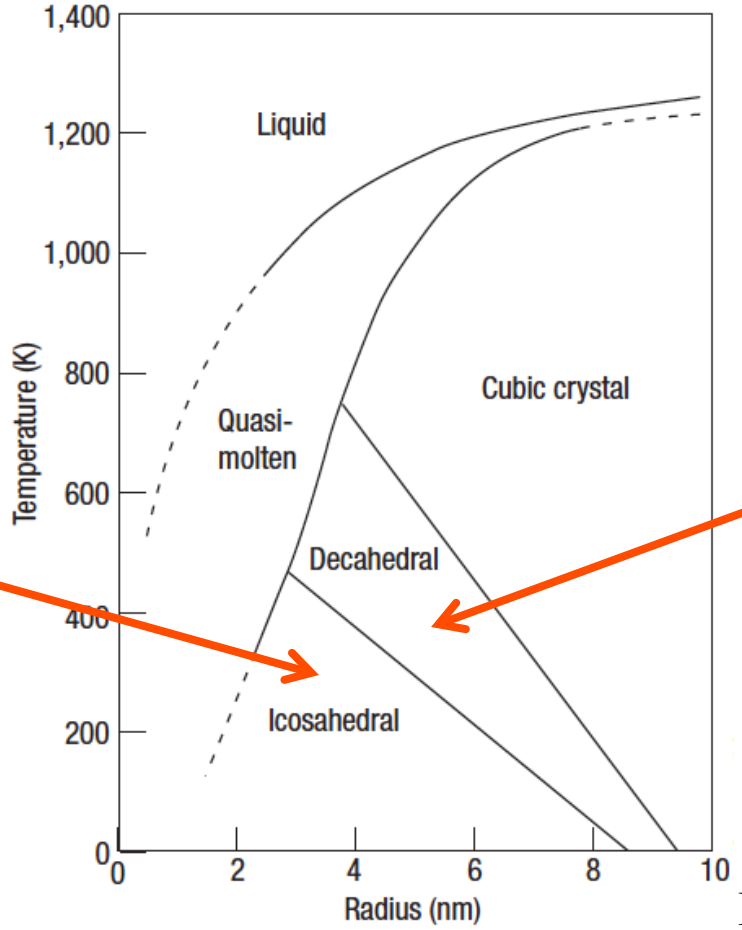
Early Science at MID
XFEL Users Meeting
January 2015

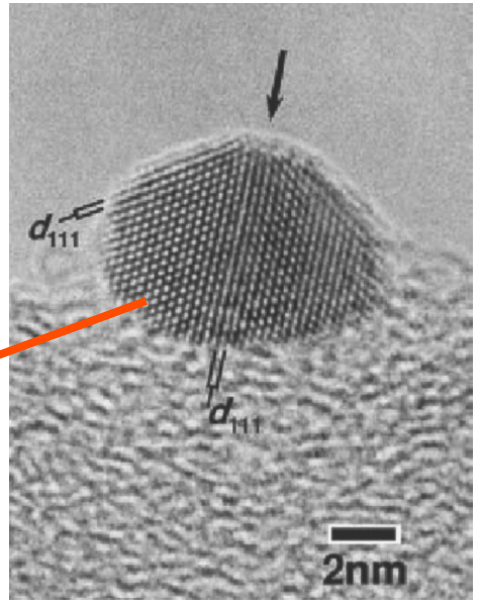
Outline

- Nanocrystal structures
- Coherent X-ray diffraction
- Crystal strain as complex density
- Dislocations during growth
- Ultrafast snapshots of moving matter
- Transient melting
- Plans for experiments at MID

Structure of Gold vs Size







L. D. Marks, RPP (1994)

Koga and Sugawara (2003)

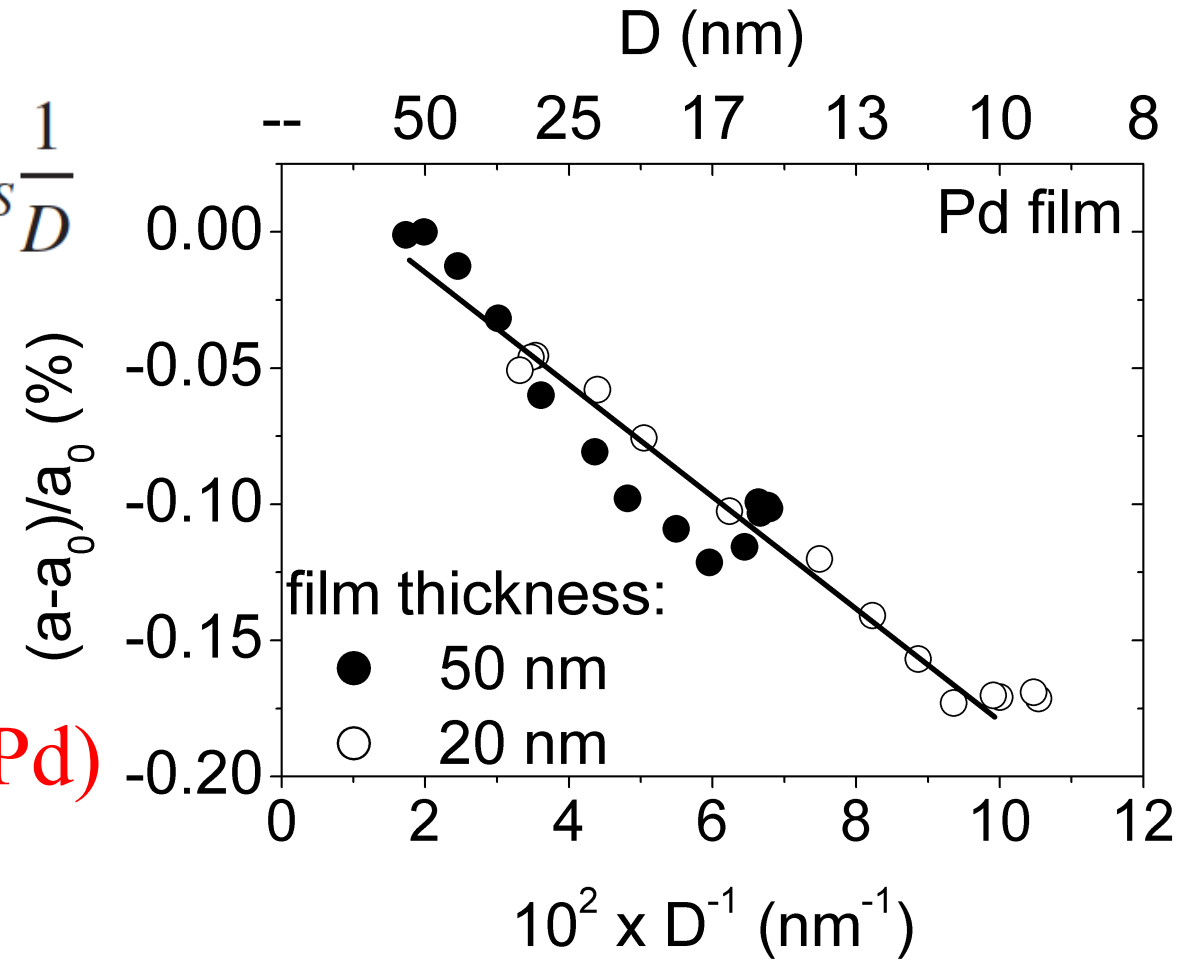
Contraction of Small Particles

Gibbs Thomson pressure + Bulk modulus

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

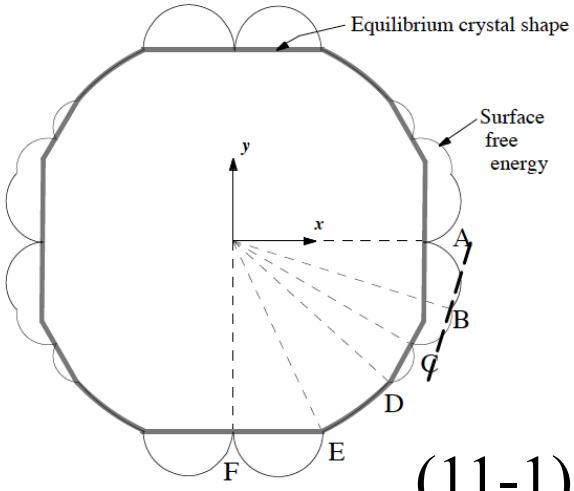
$$\frac{a - a_0}{a_0} = -\frac{4}{3K}\sigma_S\frac{1}{D}$$

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



Equilibrium crystal shape

Wulff construction + Gibbs Thomson (Young-Laplace) pressure



γ = 2N/m

P = 2γ/R = 70MPa

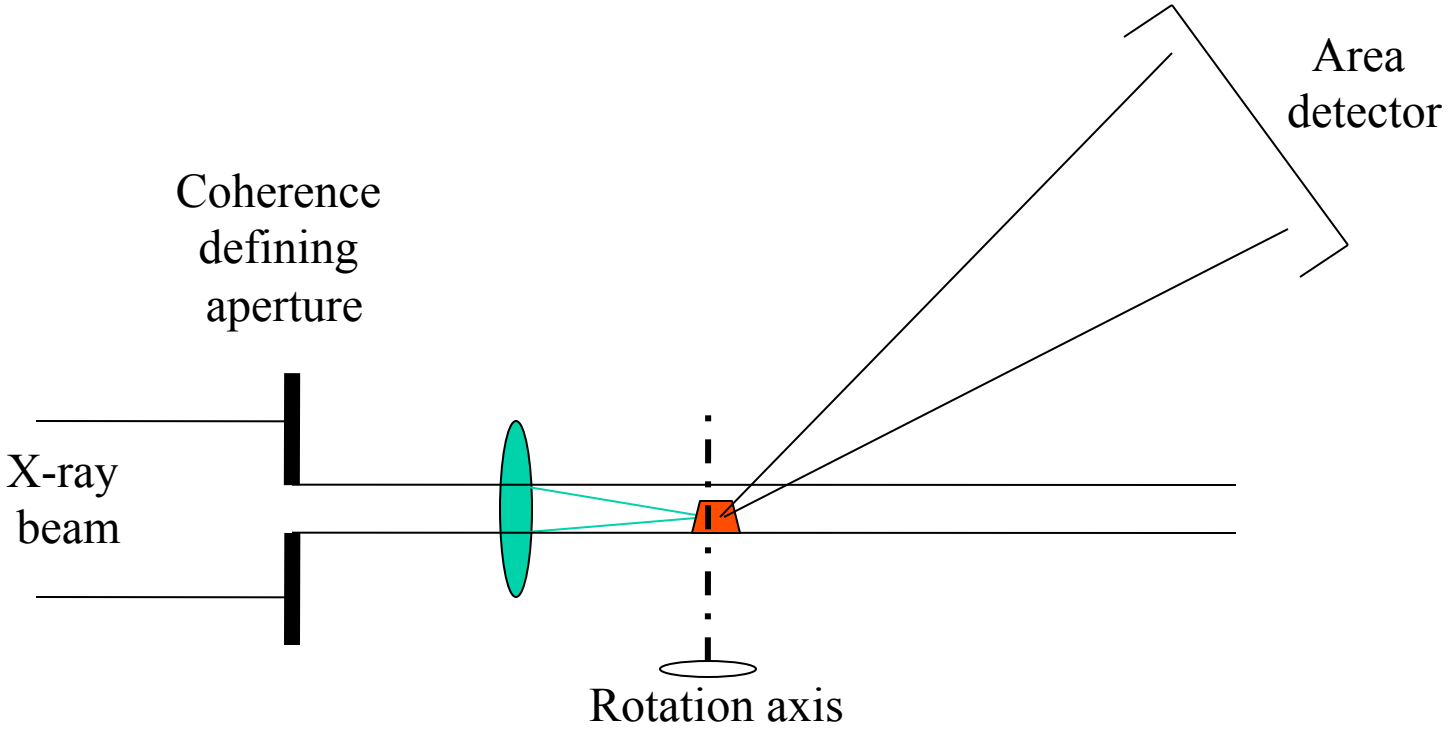
ε = 0.1%, Φ = 0.6 rad

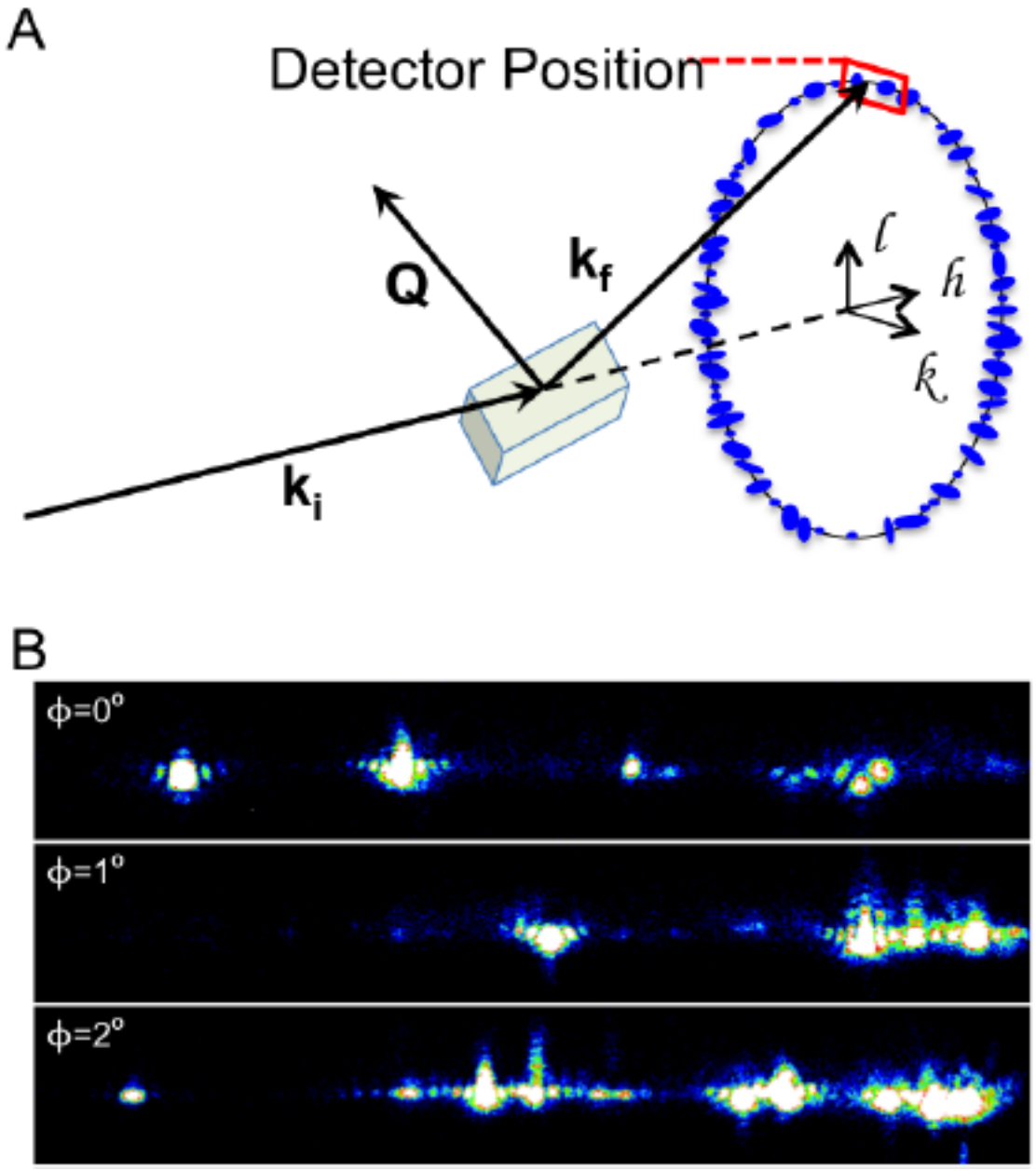
(111)

R = 30nm

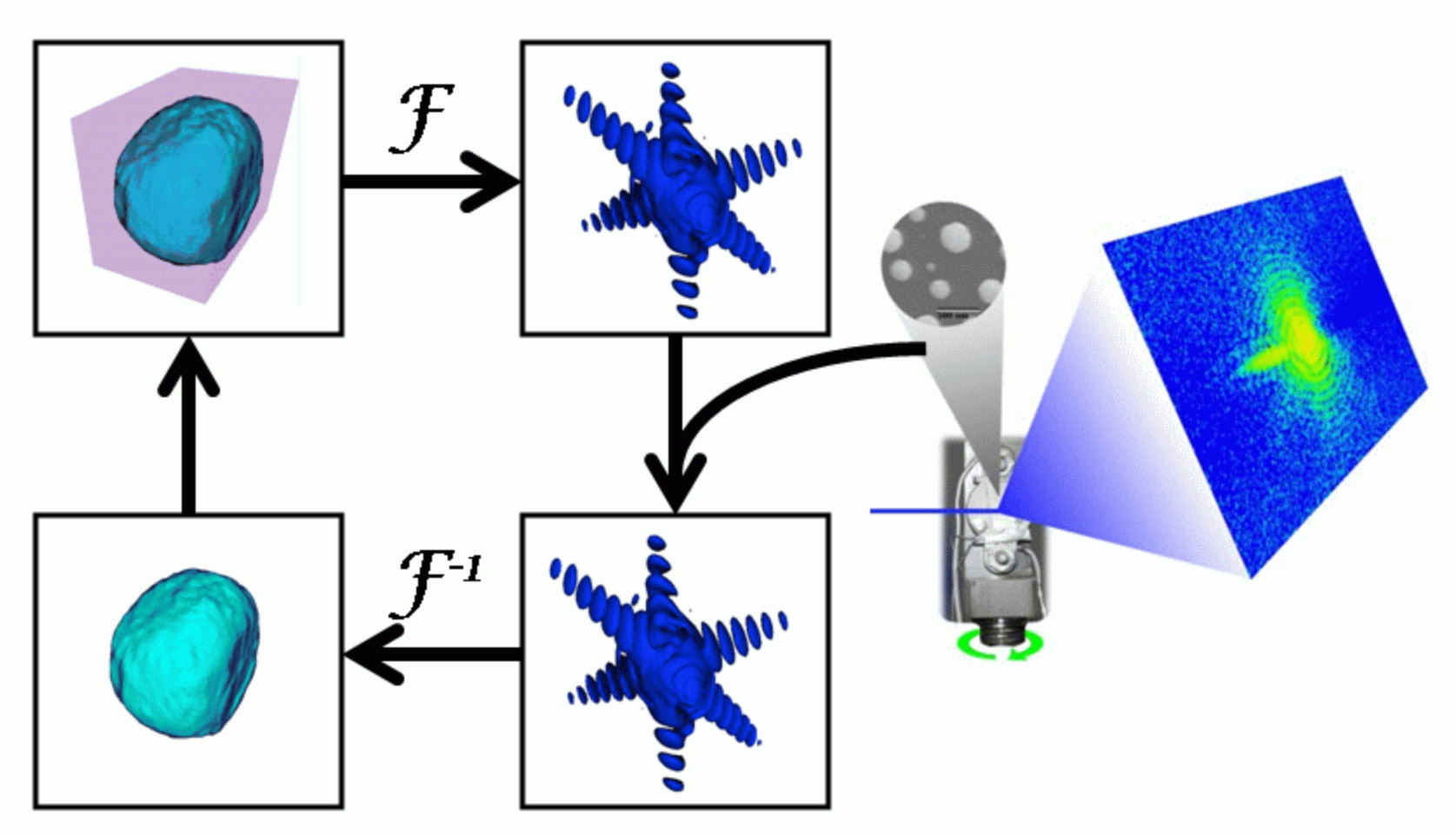
(11-1)

Lensless X-ray Microscope, 2003




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

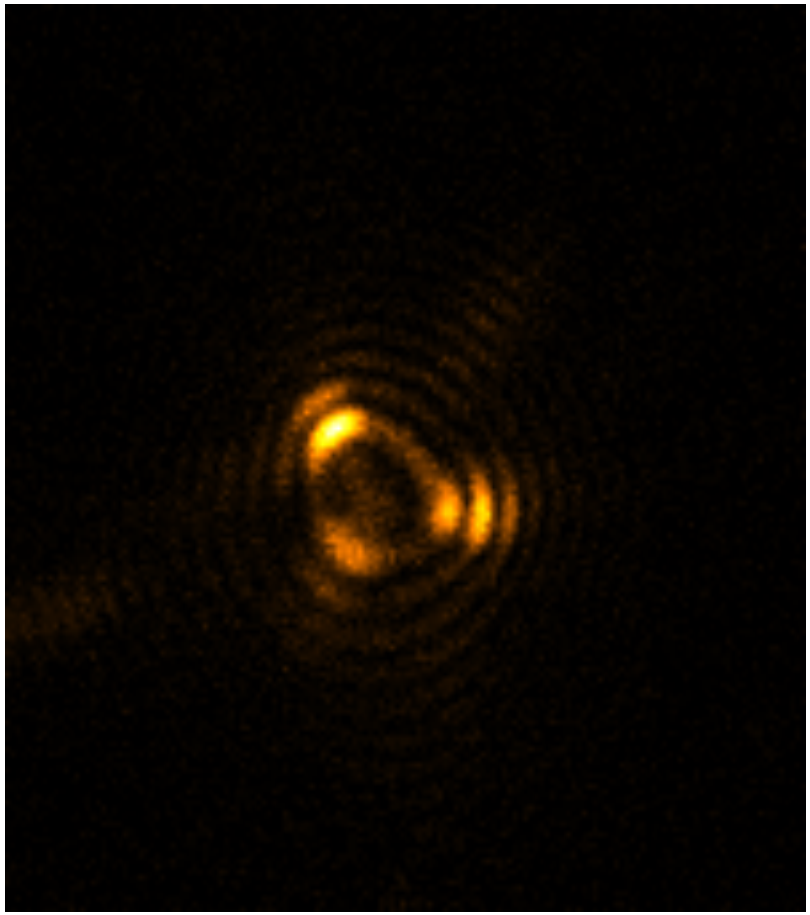
Generic "Error Reduction" method

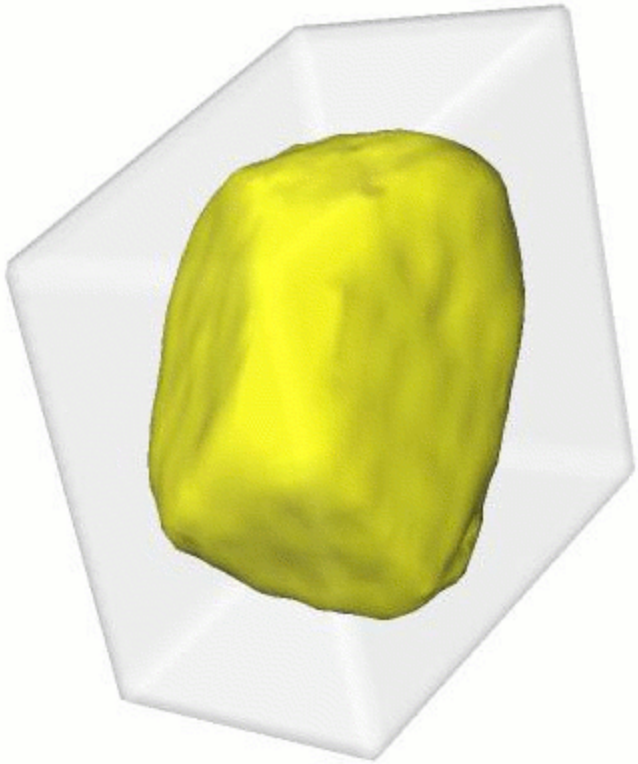


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

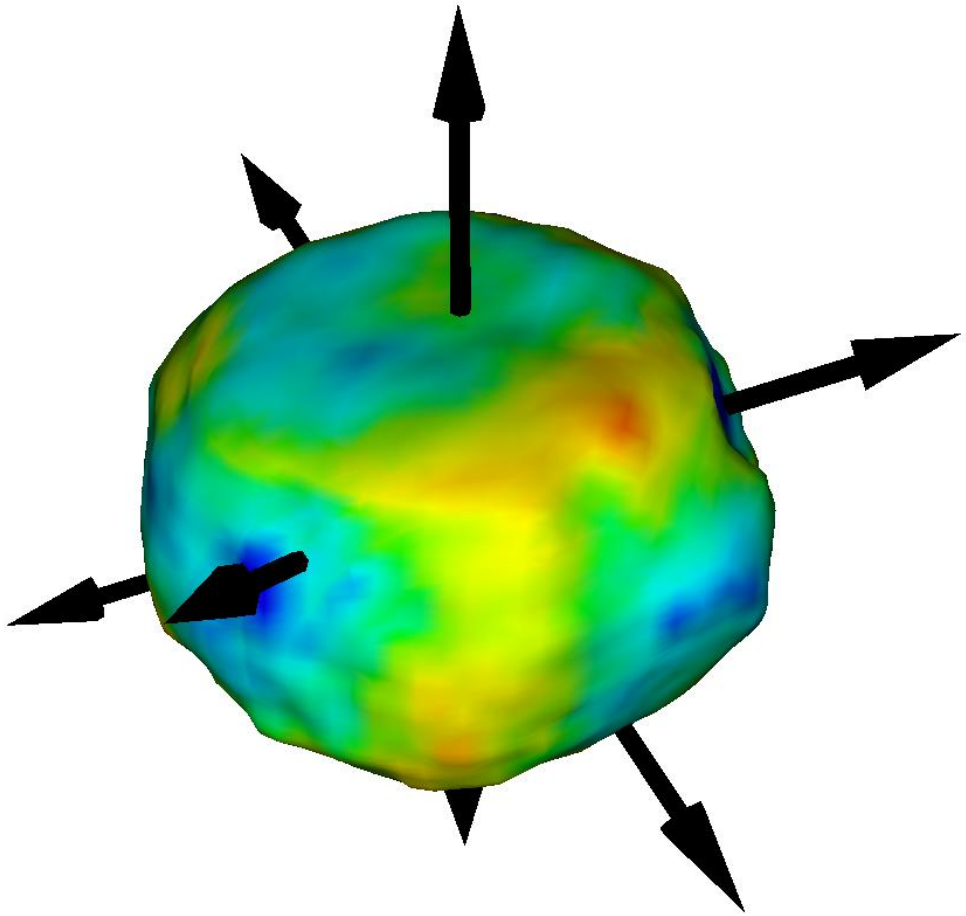
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



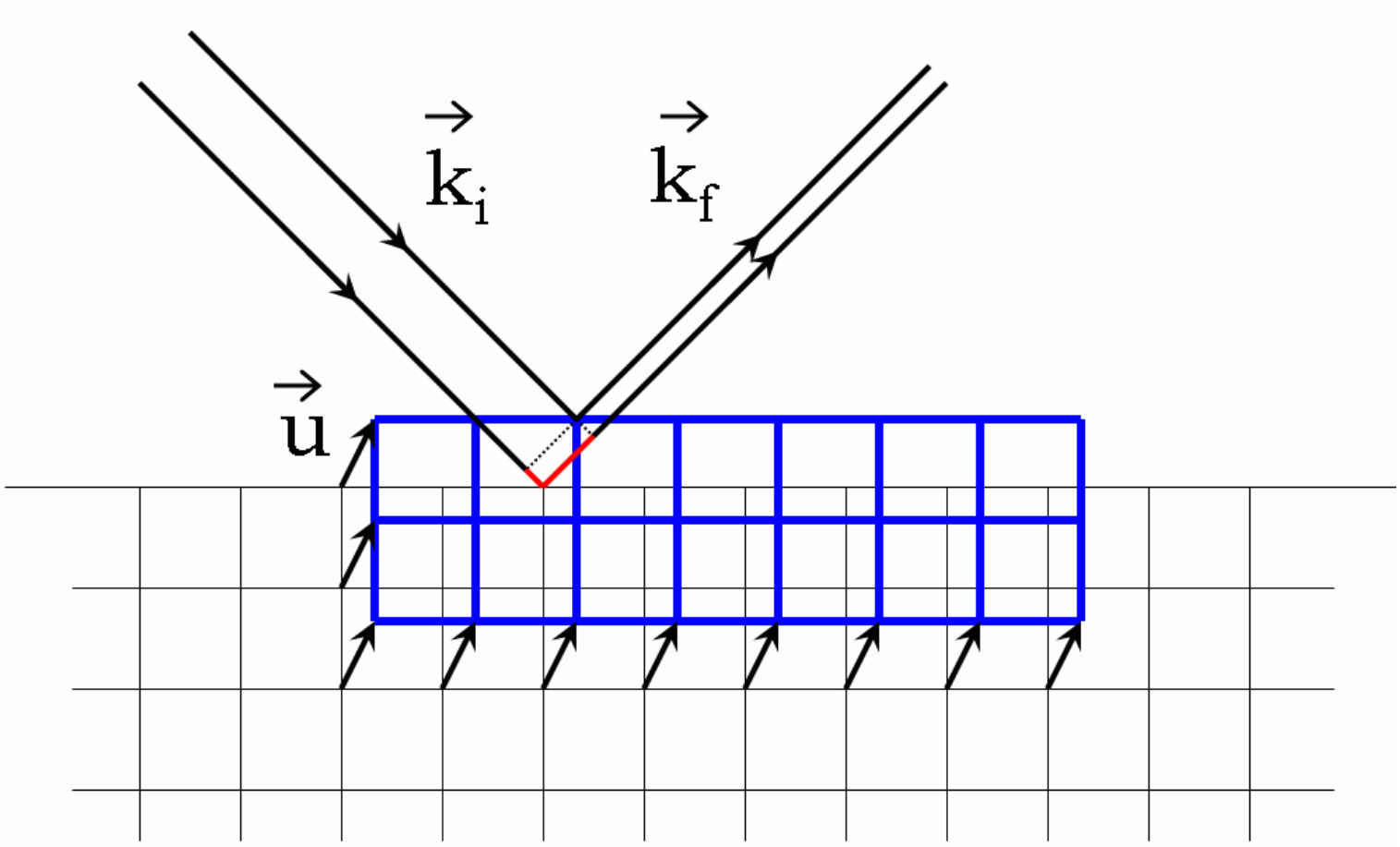


Phase isosurface of residual strain



Sensitivity to strain

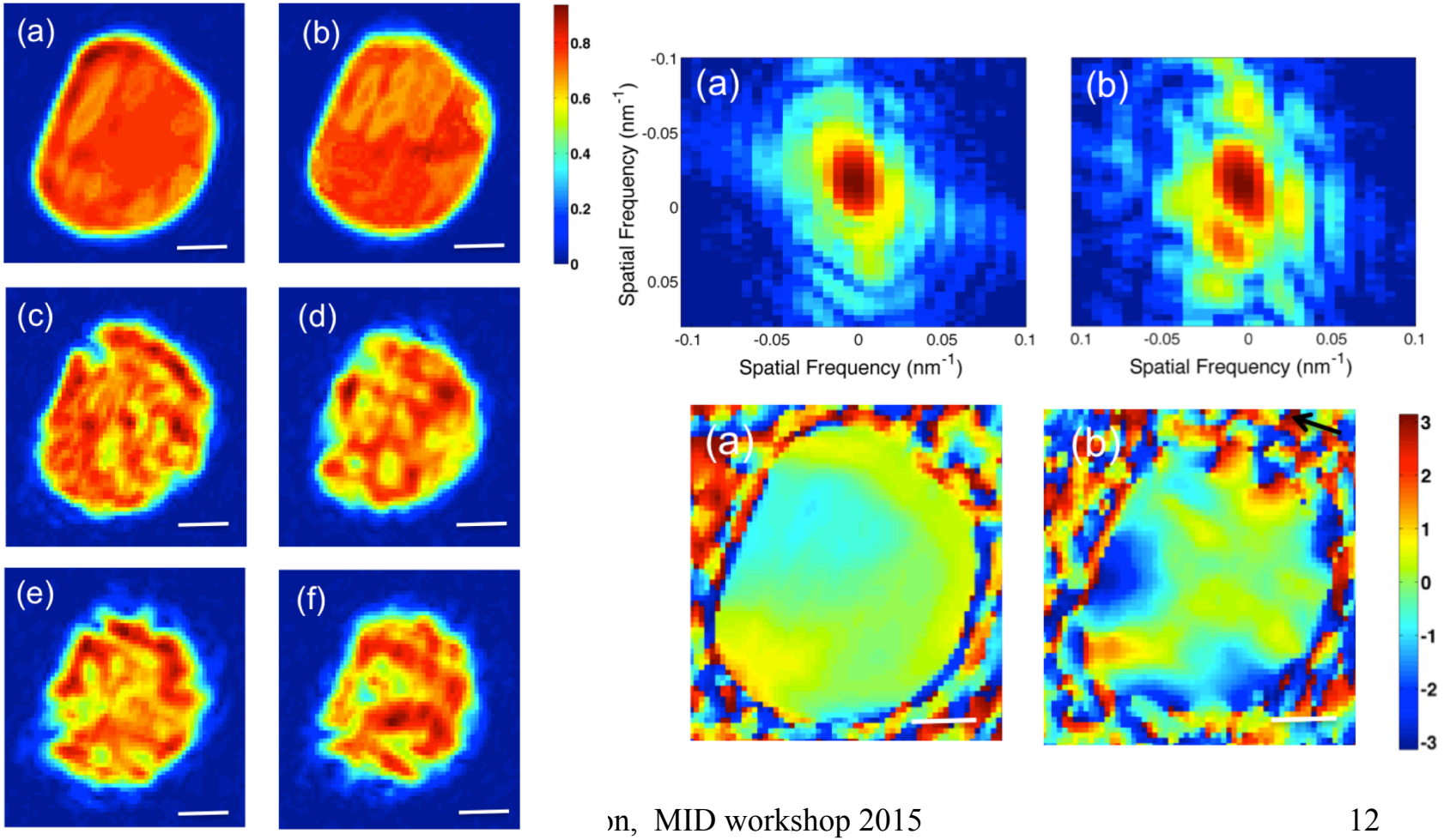
$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$



BCDI on a traditional SXRD beamline

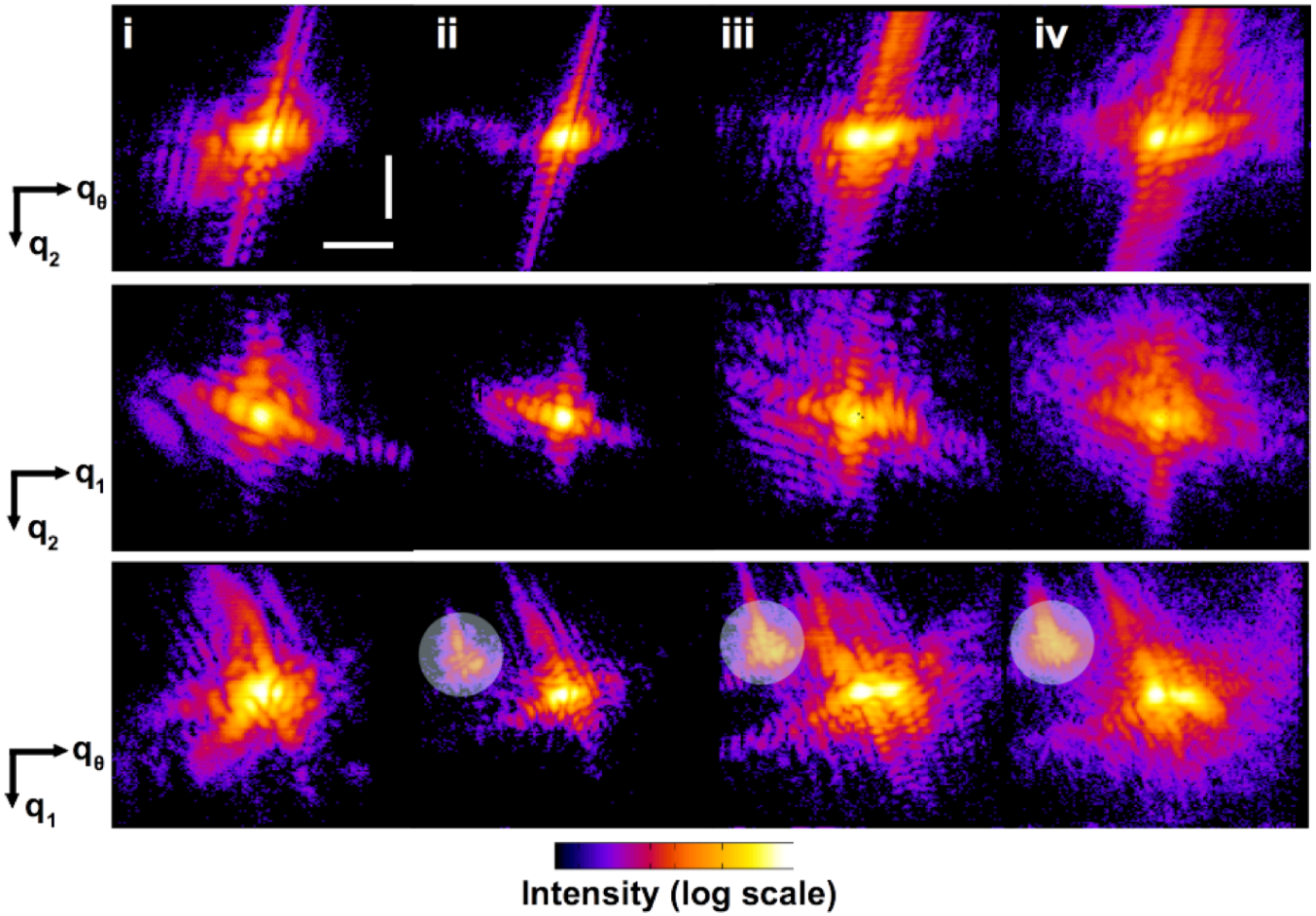
Gang Xiong, Chris Nicklin, I-07 Diamond

in-situ Cu deposition on 250nm Au crystal at 600C



Dissolution and Growth

J. Clark, J. Ihli, A. Schenk, Y. Kim, A. Kulak, J. Campbell, G. Nisbet, F. Meldrum, I. Robinson, unpublished



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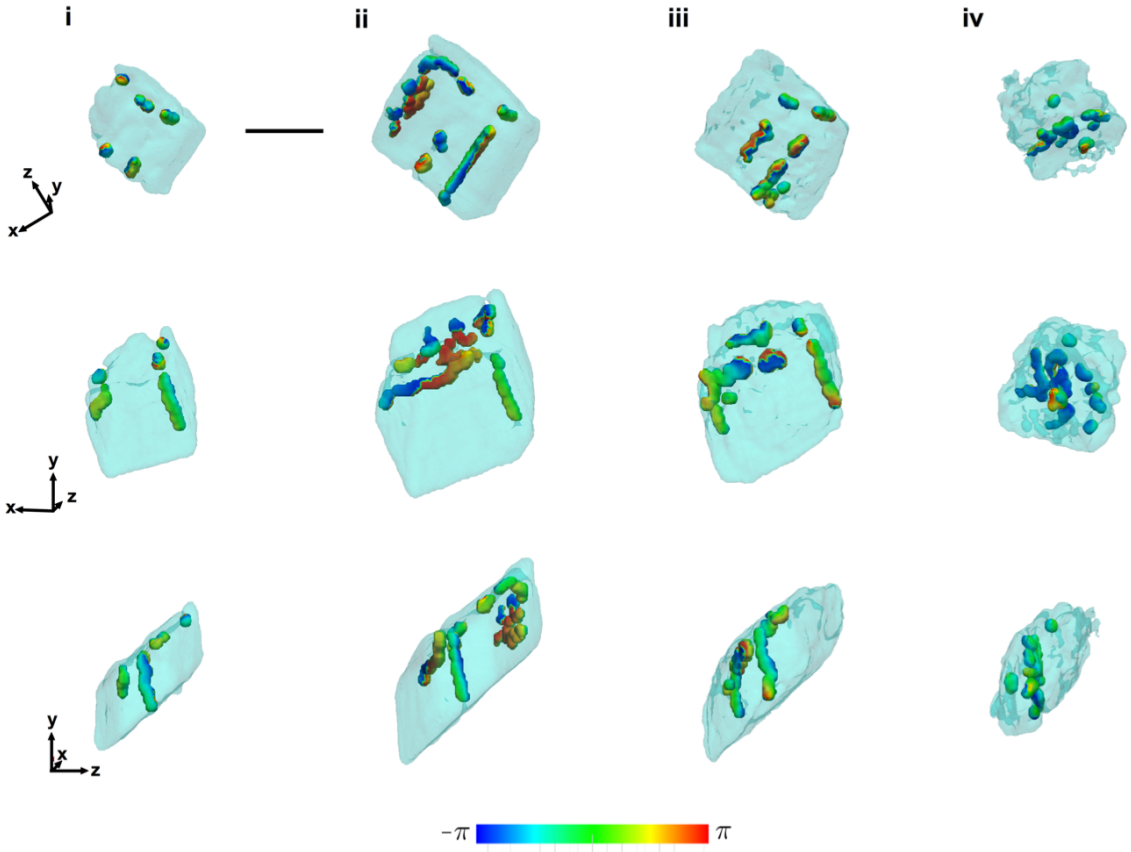
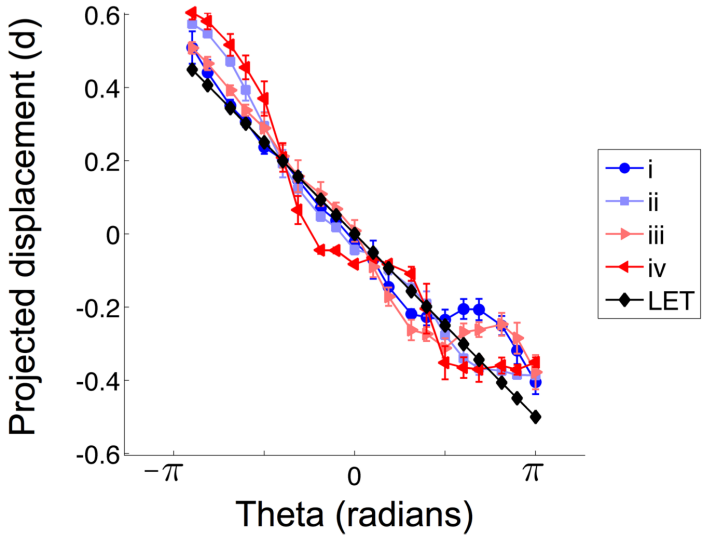
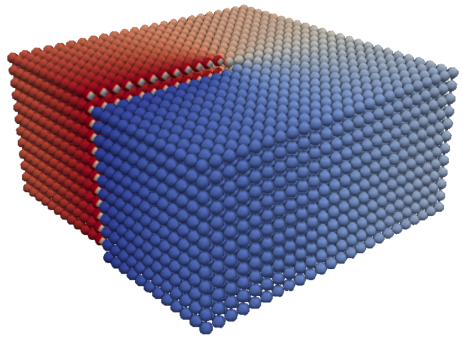
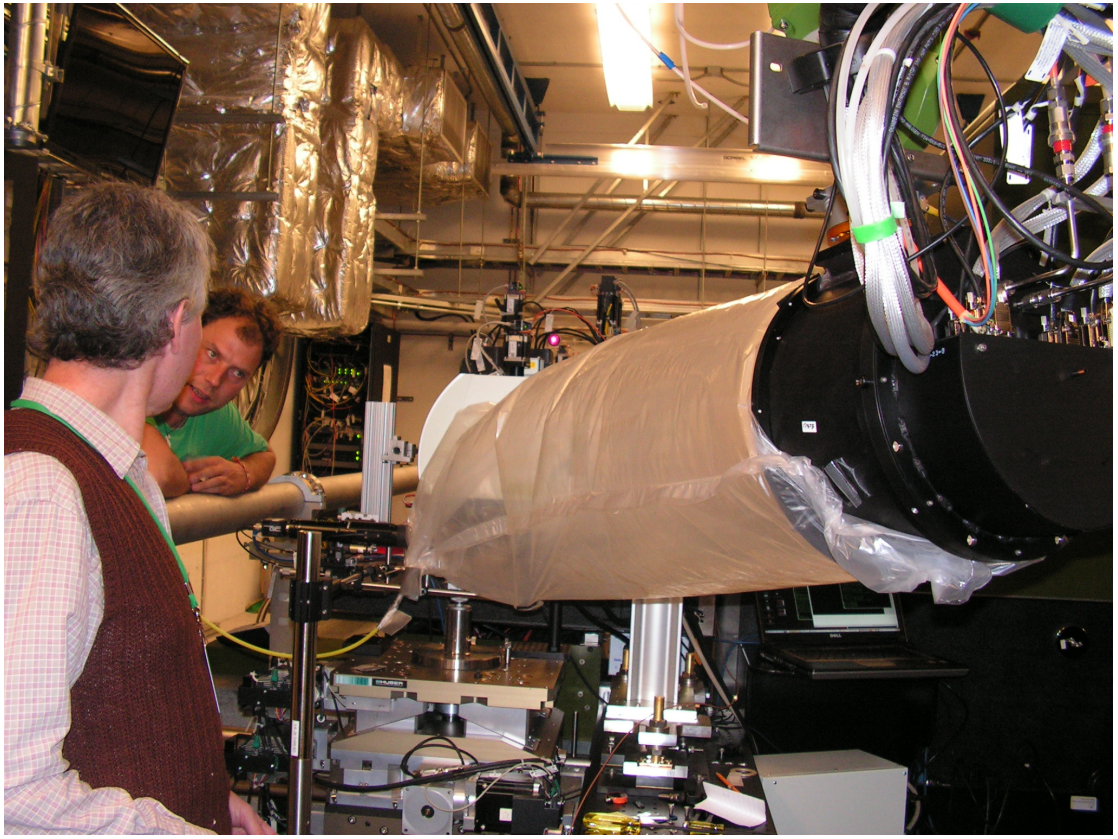


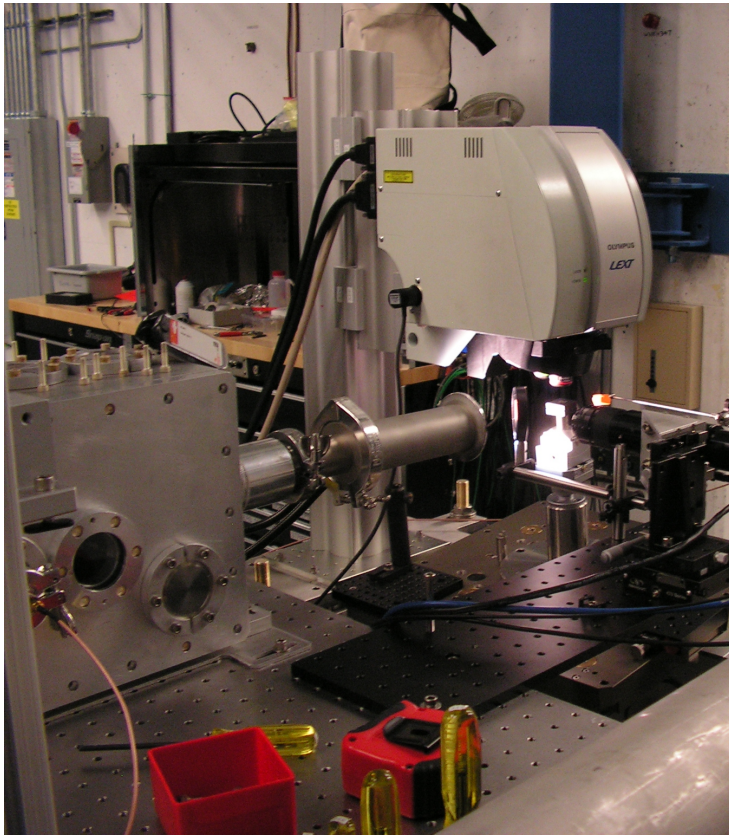




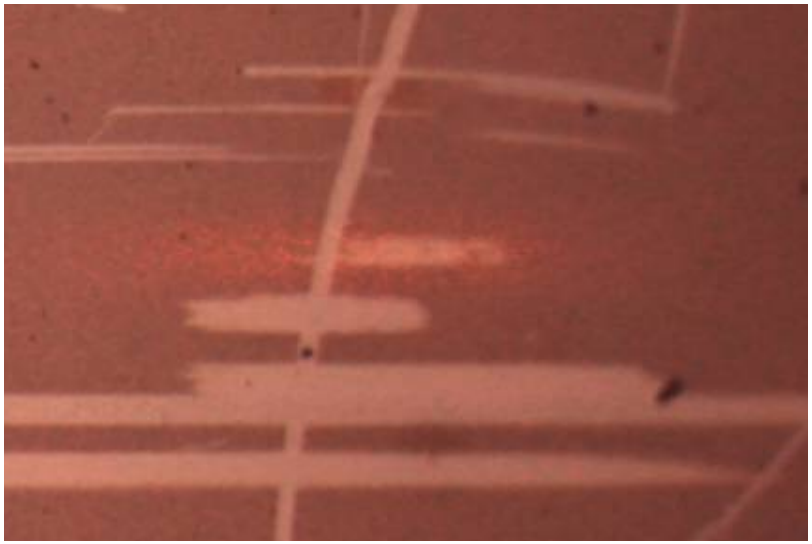
Pump-probe at LCLS (XPP)

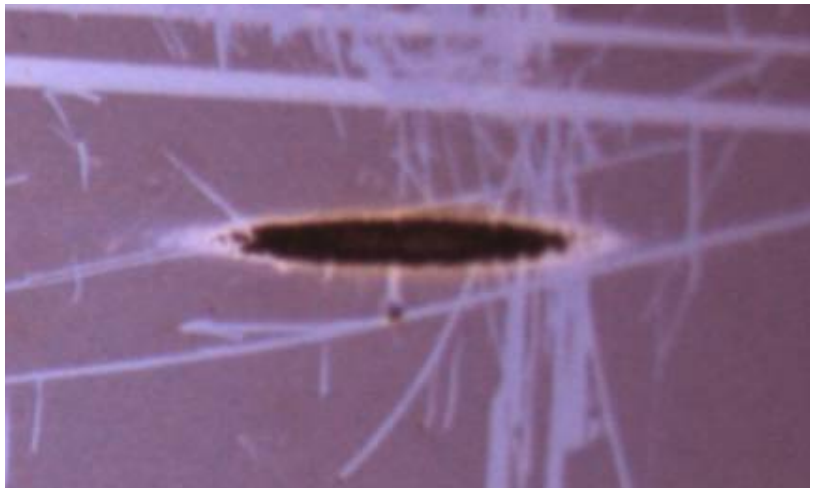
Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz ,
Sebastien Boutet, Jesse Clark, Garth Williams, Brian Abbey, Andy Higginbotham,
Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt

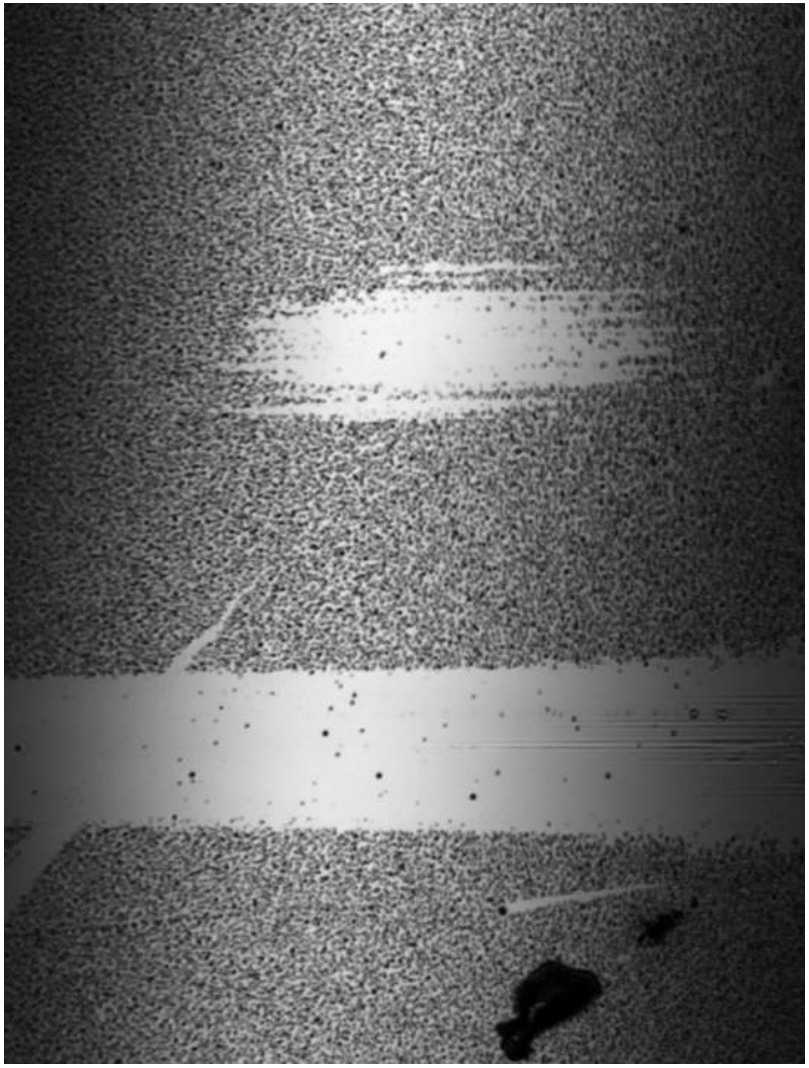




Visible and Confocal microscopy







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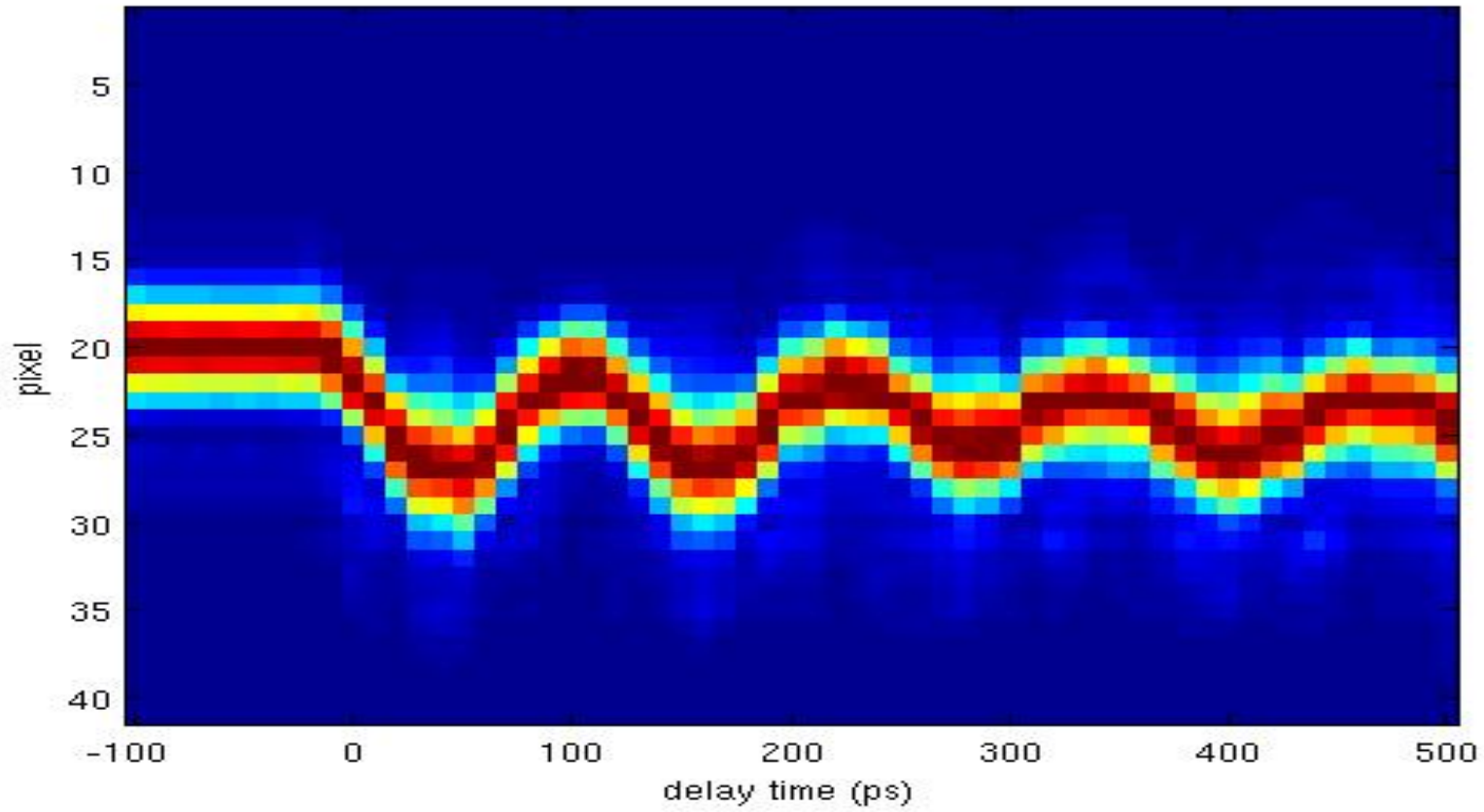
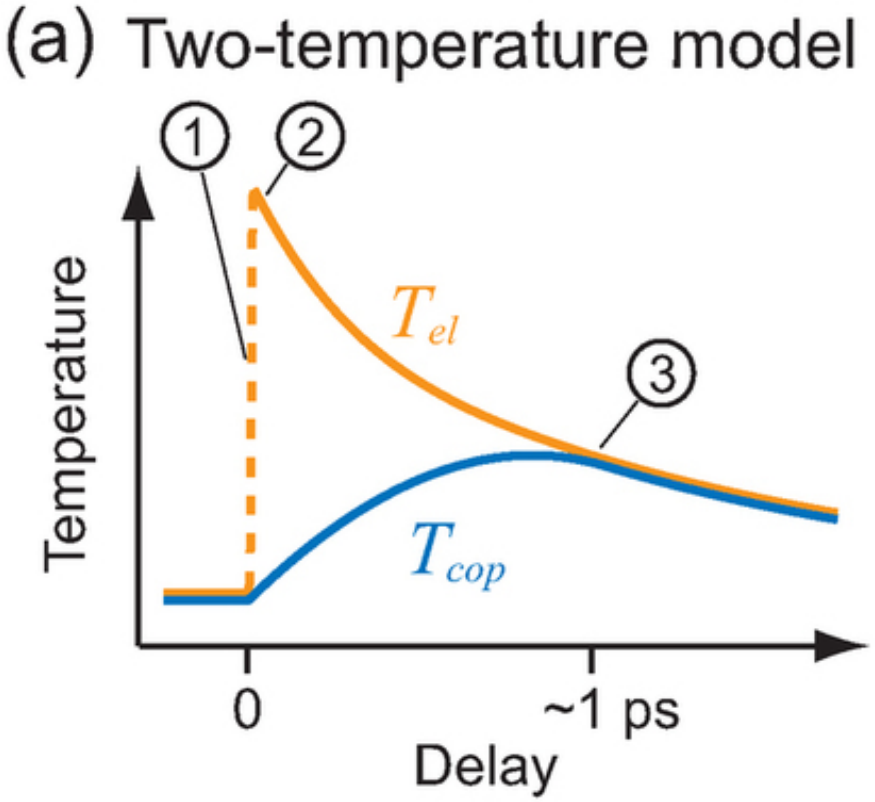
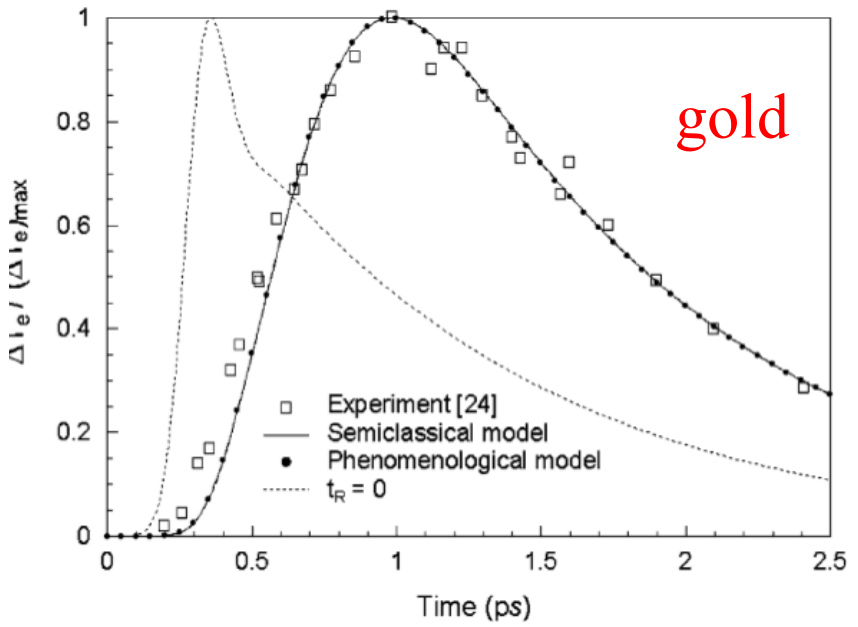


"Two-temperature" model

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

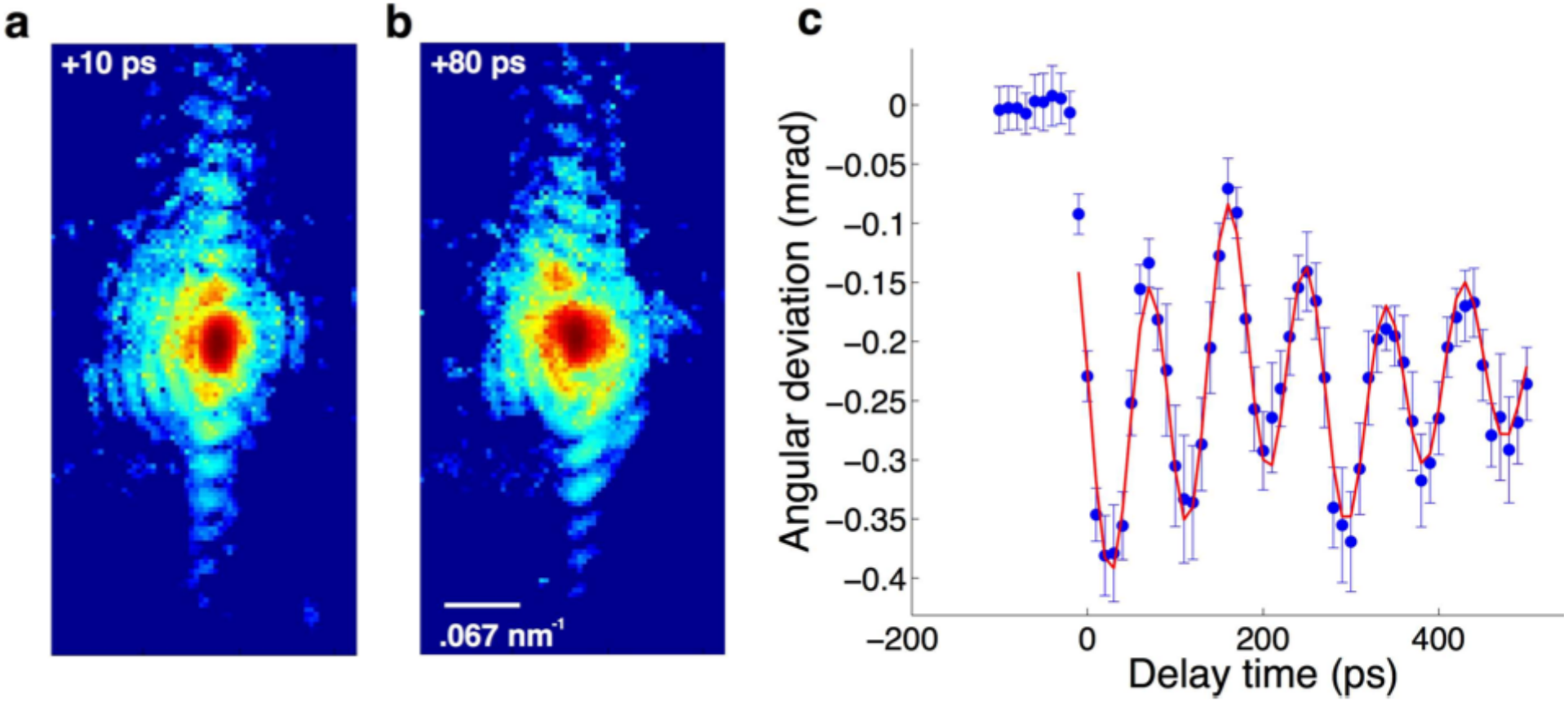
J.K. Chen et al, Int J. Heat Transfer 49 307 (2006)





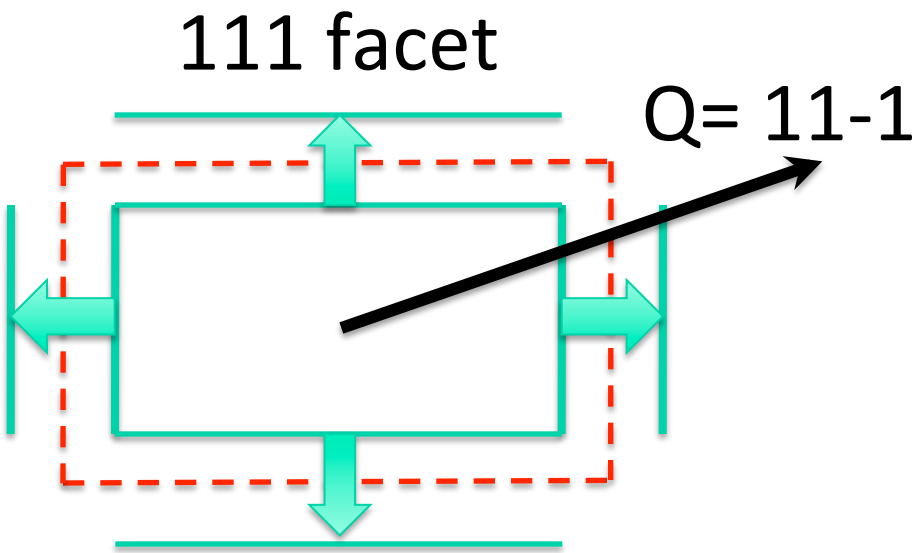
ig. 2. Comparison of the change in electron temperature at ıe front surface of an 80-nm gold film irradiated by a 2.8 mJ/ n^2, 800 nm, 150-fs laser pulse.

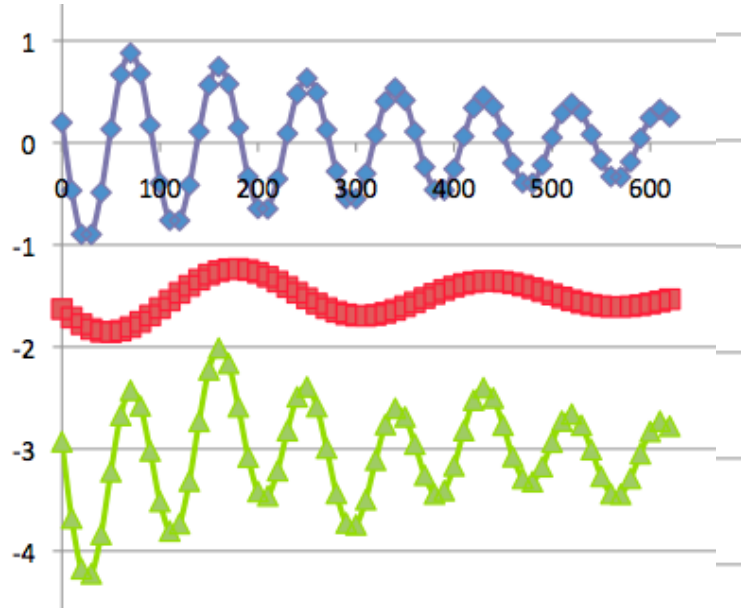
Time resolved Bragg peak position



Two Normal Modes of Vibration

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





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

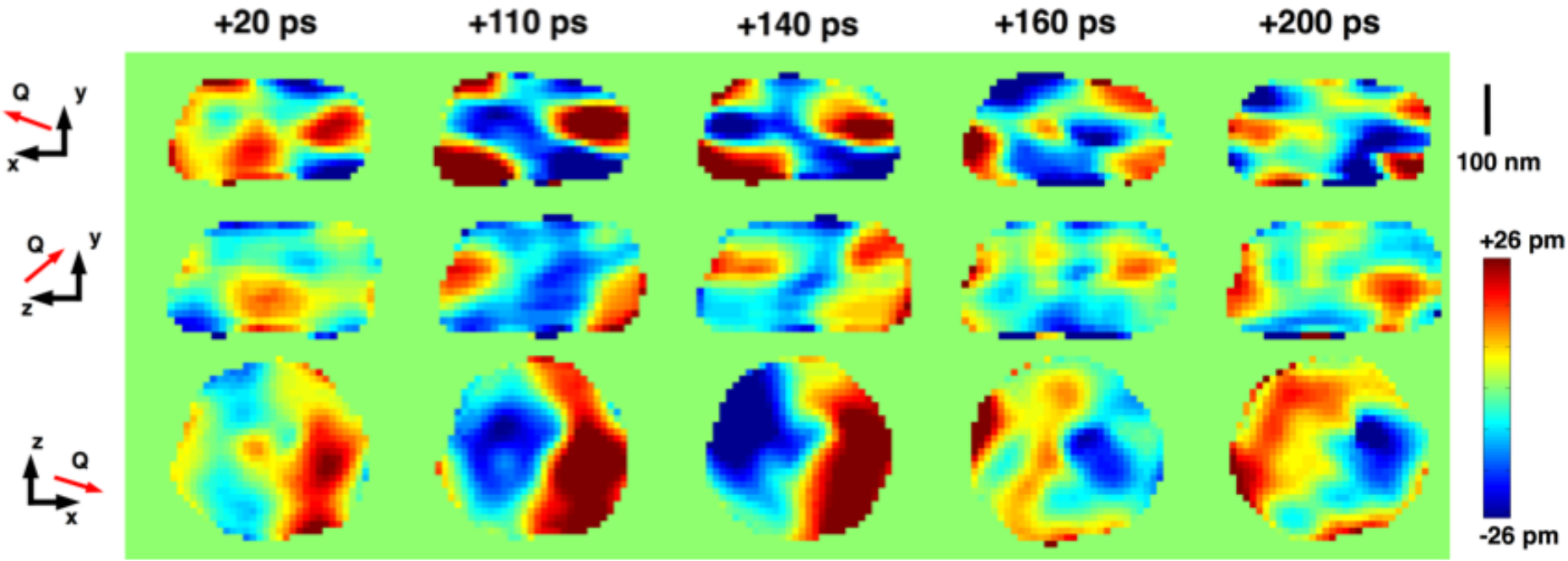
T_2 = 259ps h_2 = 420nm

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)

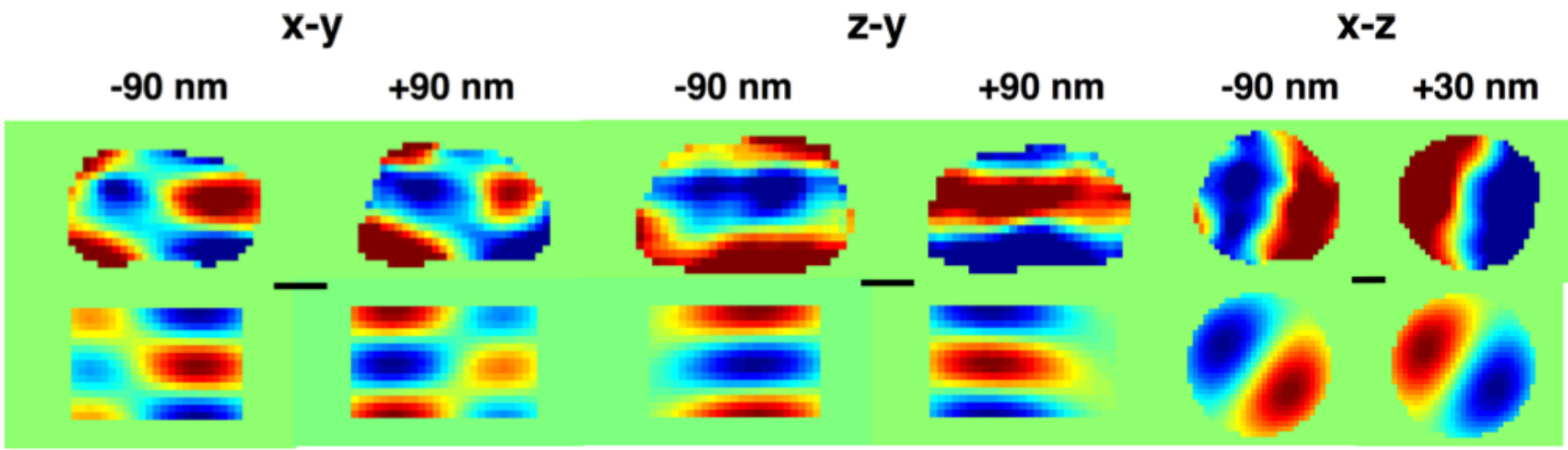


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

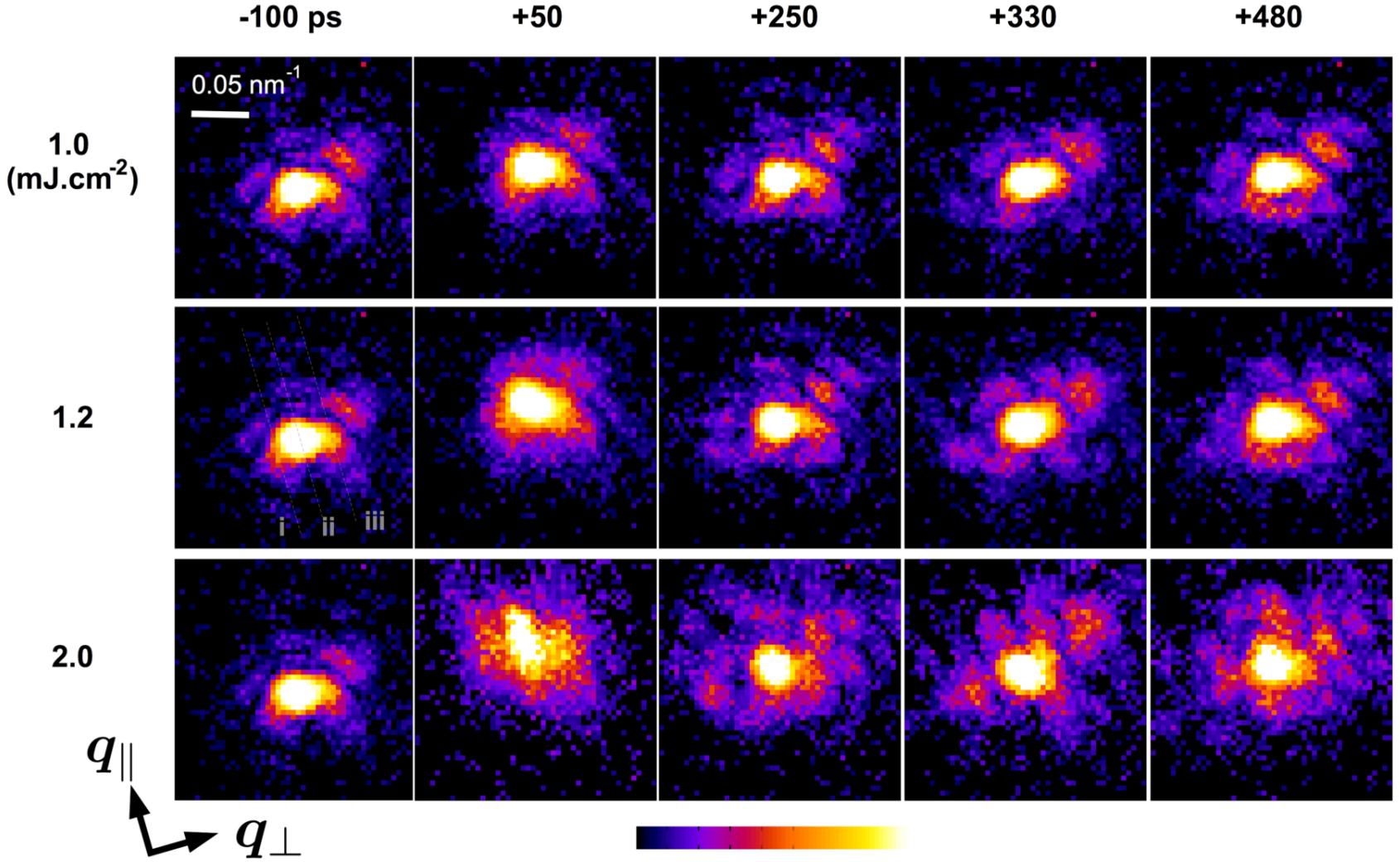
Comparison with (1,1) normal mode of cylinder

Jesse Clark et al, Science 341 56 (2013)



Dependence on Laser Fluence

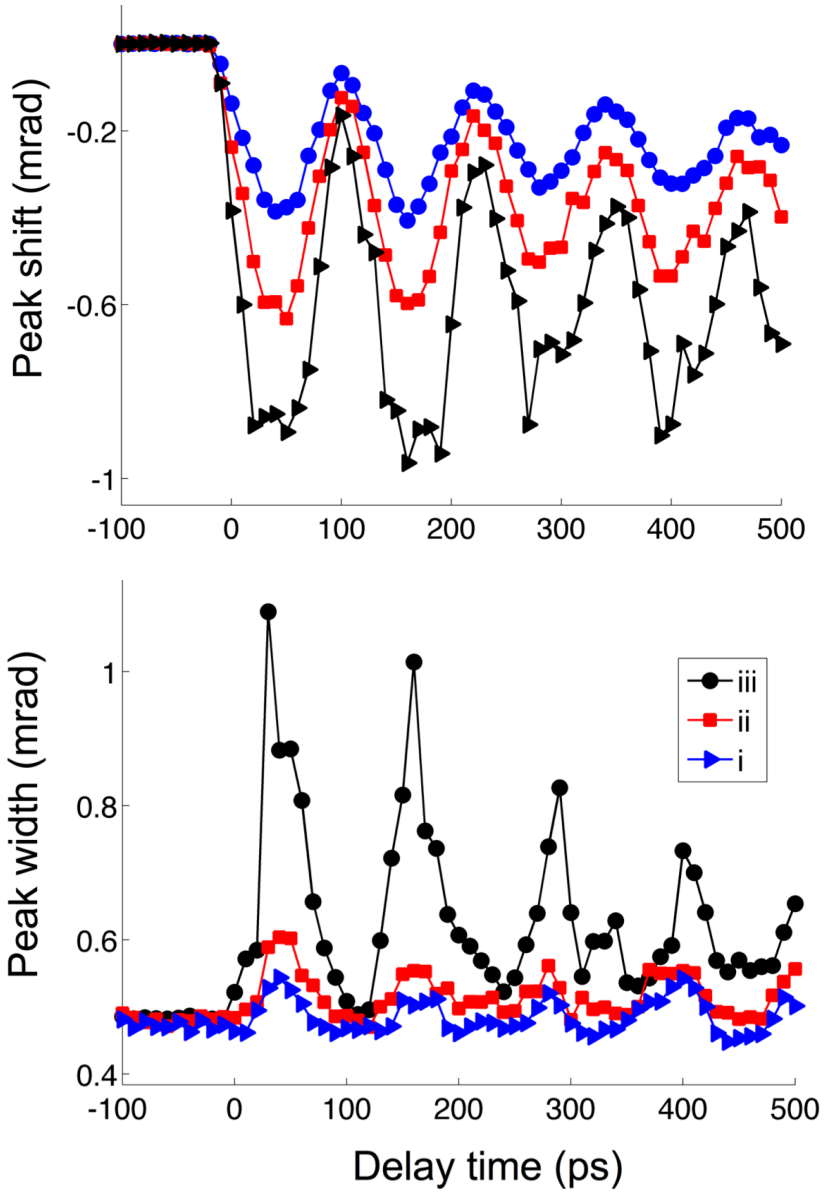
Jesse Clark et al, to be published



Dependence on Laser Fluence

Jesse Clark et al, to be published

1.0 mJ cm^{-2}
1.2 mJ cm^{-2}
2.0 mJ cm^{-2}



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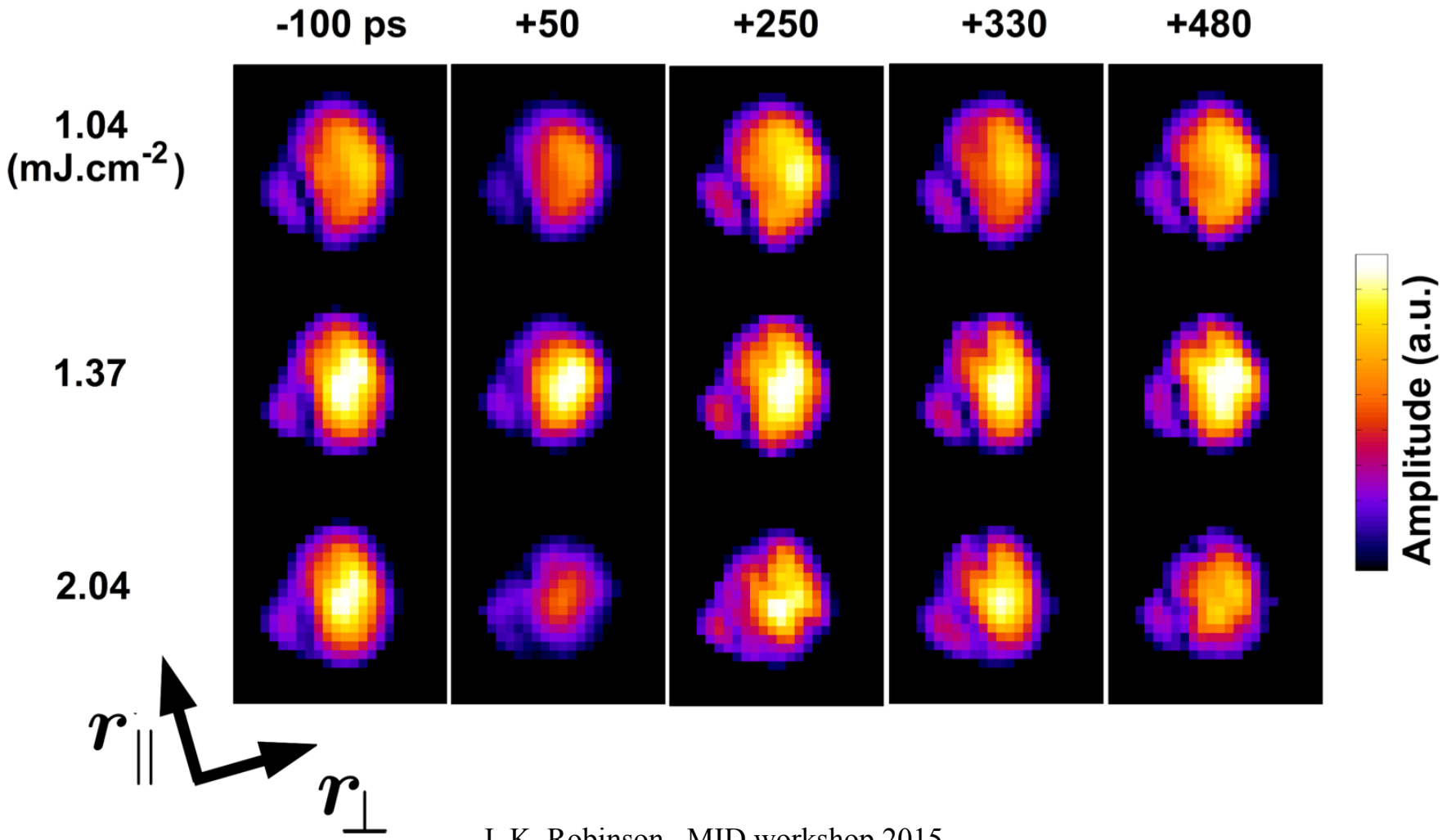
Jesse Clark et al, to be published

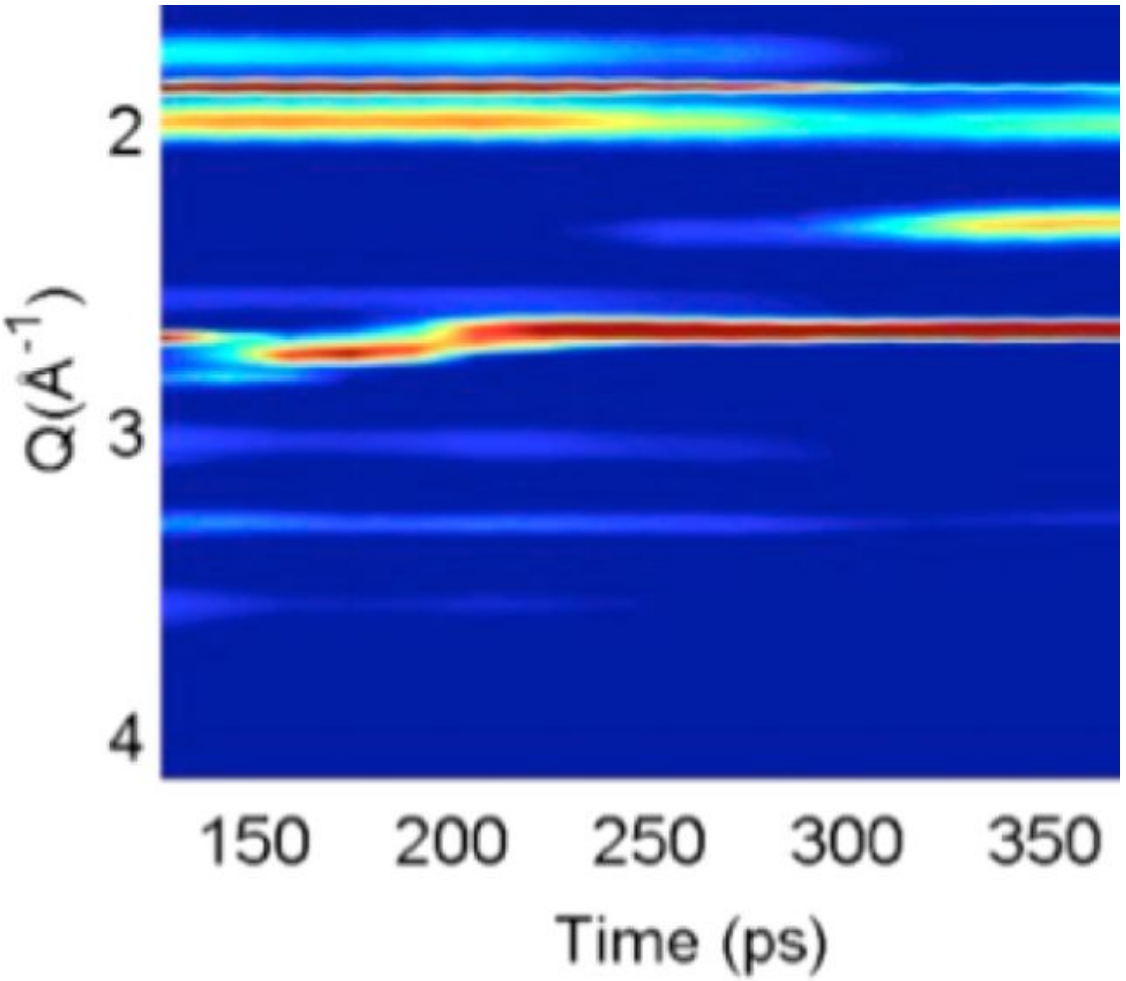


Materials Science using XFELs

- Synthesize samples in nanoparticle format
- Nanoparticle array scanned through beam
- Pump-Probe has two state variables
  - Optical fluence = sample temperature
  - Delay time after ‘instantaneous’ heating
- Laser “pump” pulse to create new states
- Explore transient phase diagrams

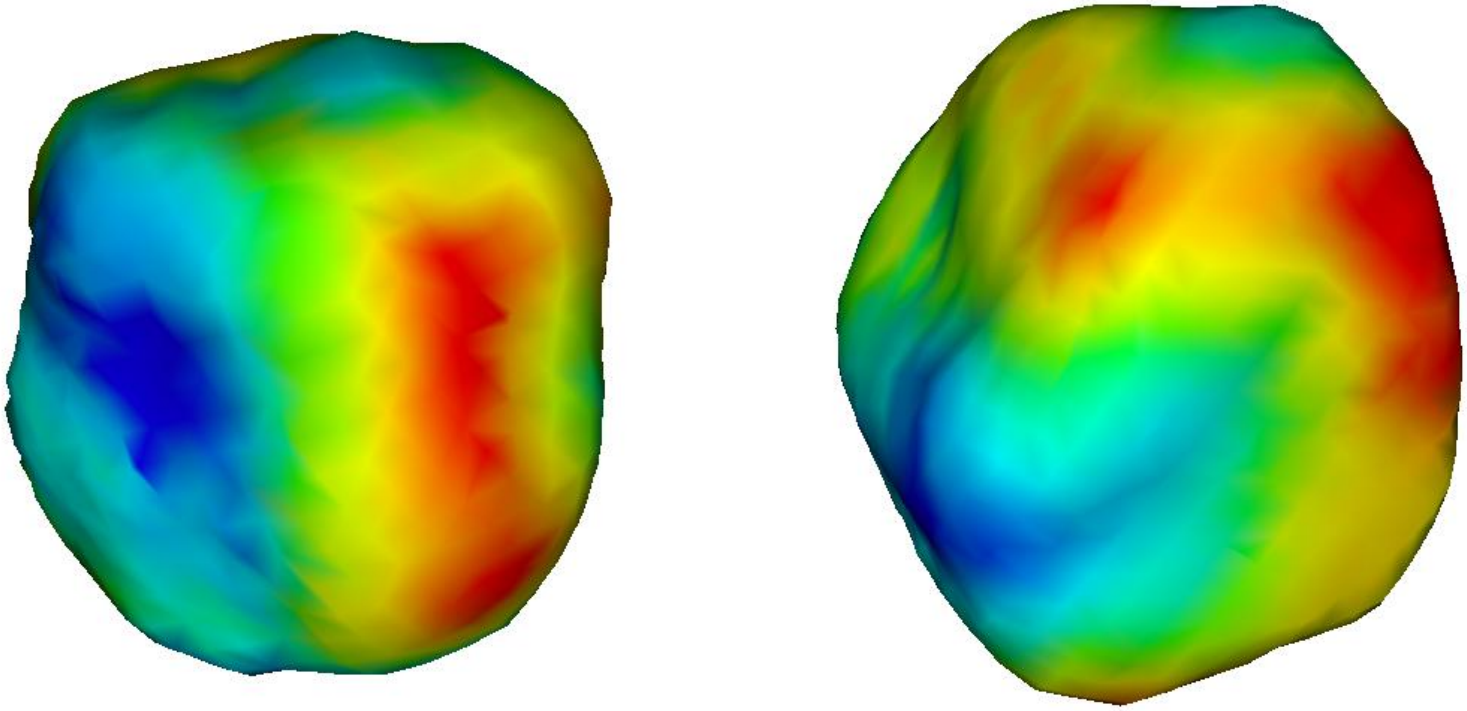
Laser induced transformation of CdS

J. Wittenberg…A. Lindenberg, Nano Lett. 14 1995 (2014)



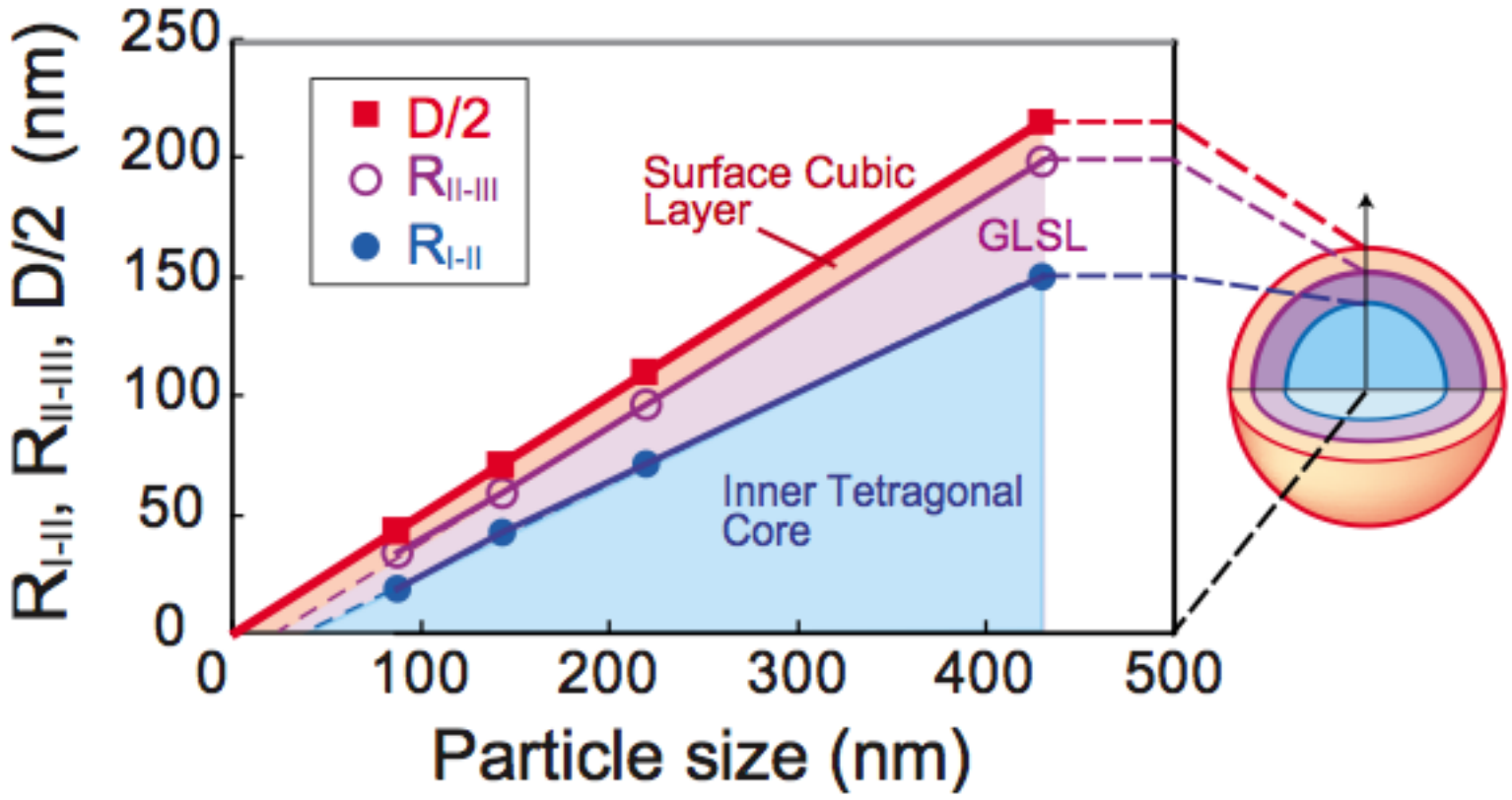
Phase isosurface of residual strain

200nm Barium Titanate (BTO) crystals

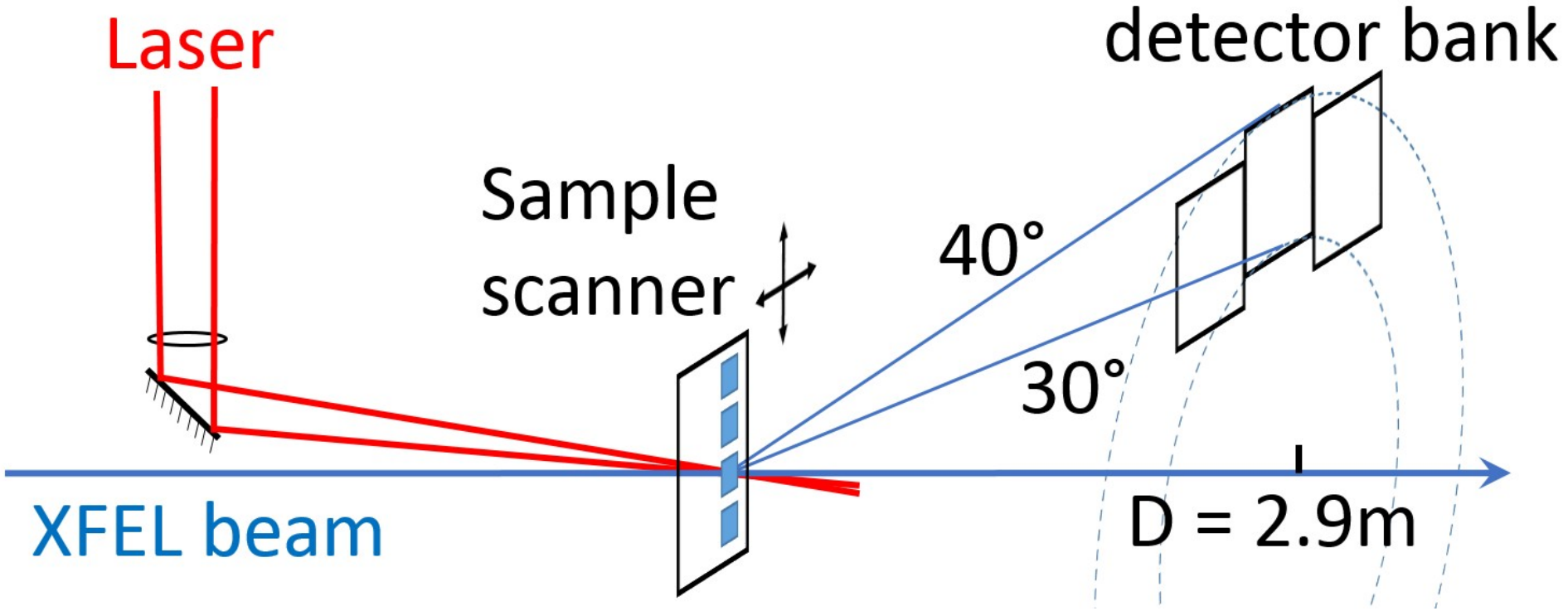


Core-shell structure of $BaTiO_3$

Takuya Hoshina, et al Appl. Phys. Lett. 93, 192914 (2008)

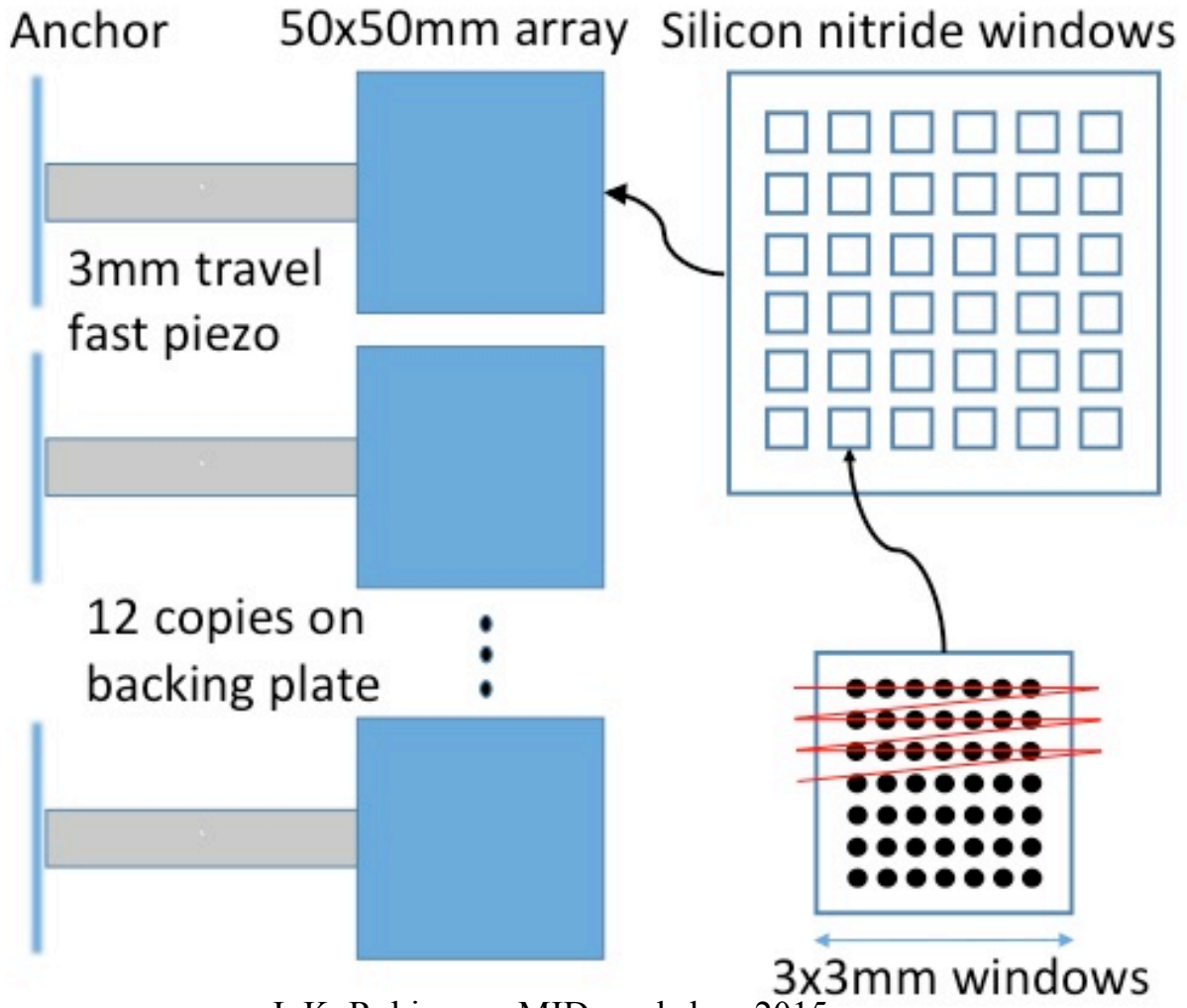


Proposed Fixed Geometry Setup



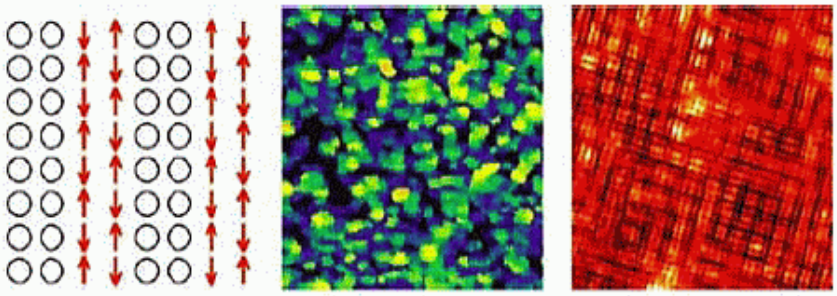
Scannable sample arrays

multiple windows reduces risk of fracture



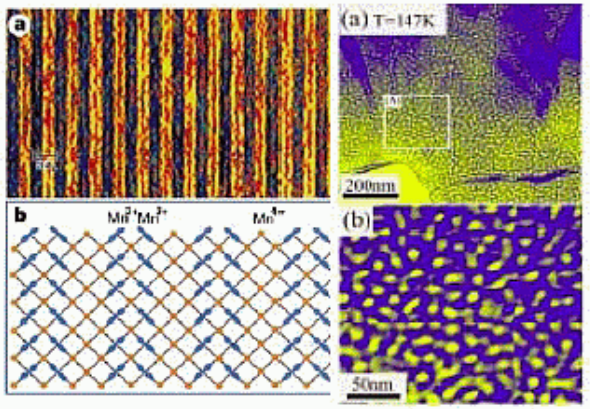
Stripes, checkerboards and zig-zags

High-Tc cuprates



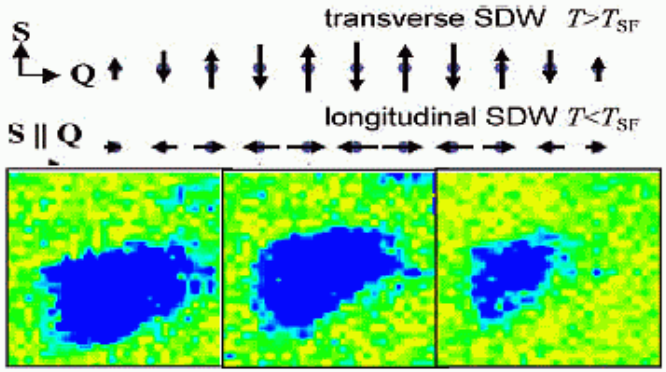
E. Dagotto, T. M. Rice, *Science* **271**, 618 (1996).
T. Hanaguri et al., *Nature* **430**, 1001 (2004).

CMR manganites

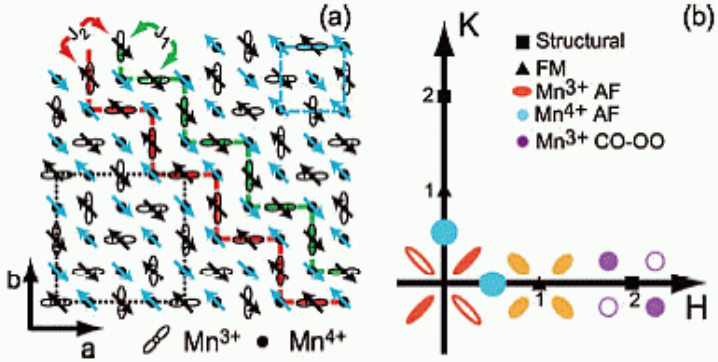


S. Mori et al., *Nature* **392**, 473 (1998)
M. Uehara et al., *Nature* **399**, 560 (1999)

AFM chromium



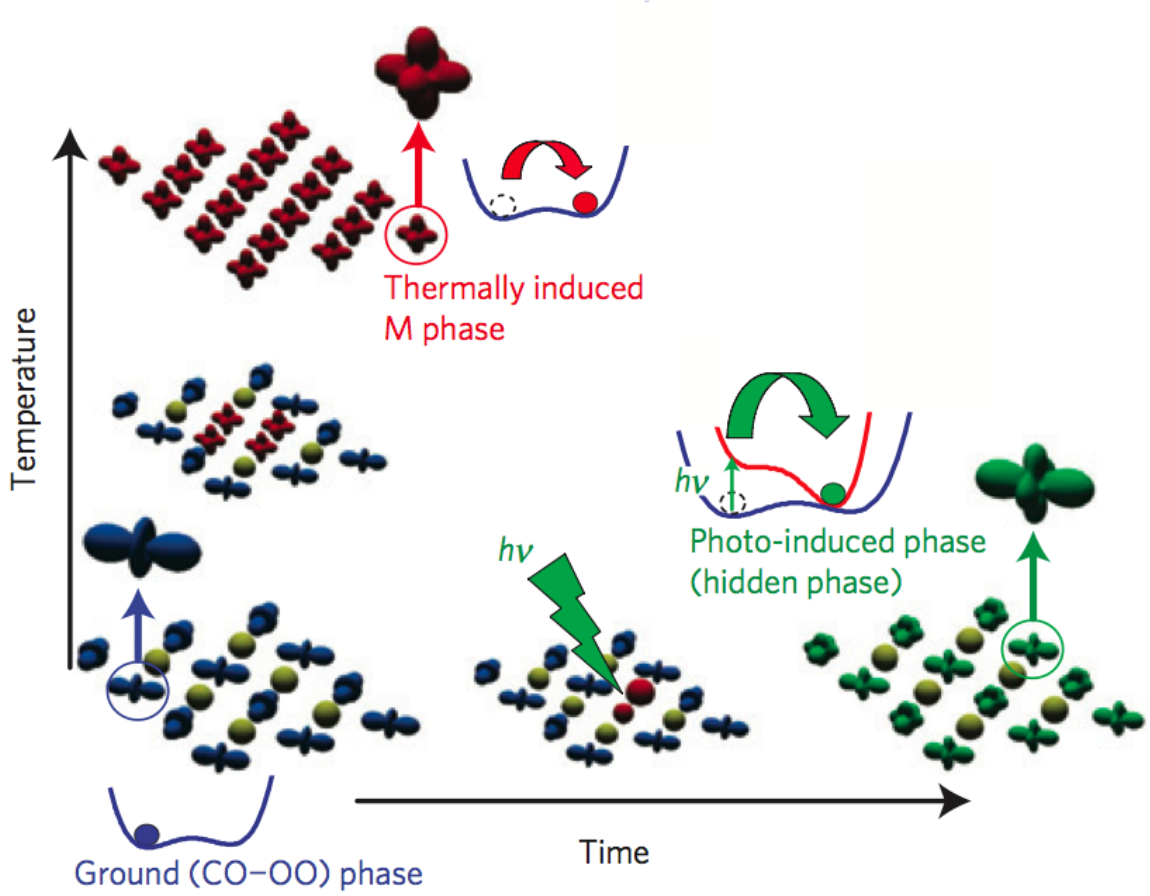
P. G. Evans et al., *Science* (2002)

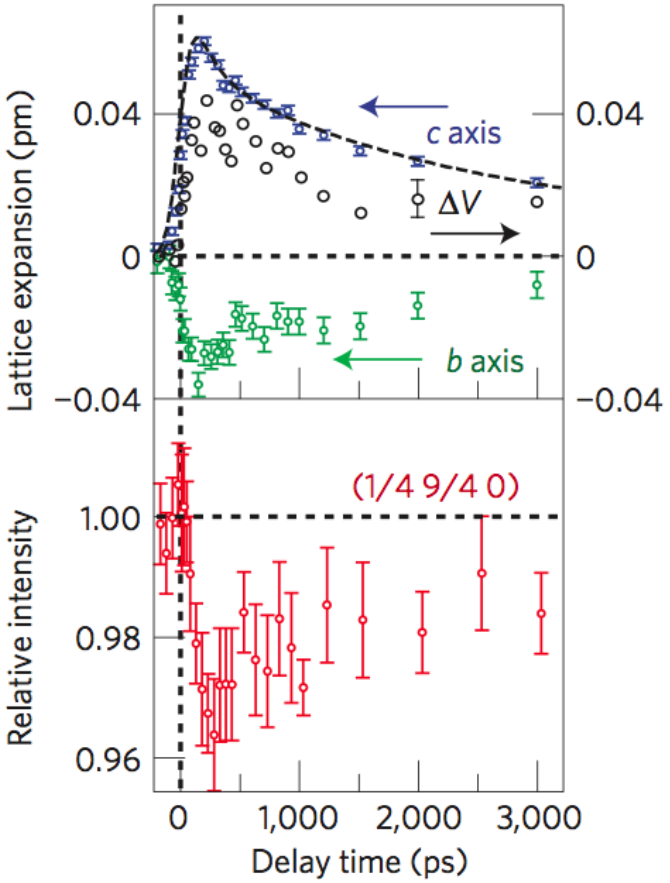


Transient "Hidden" Phase in Manganite

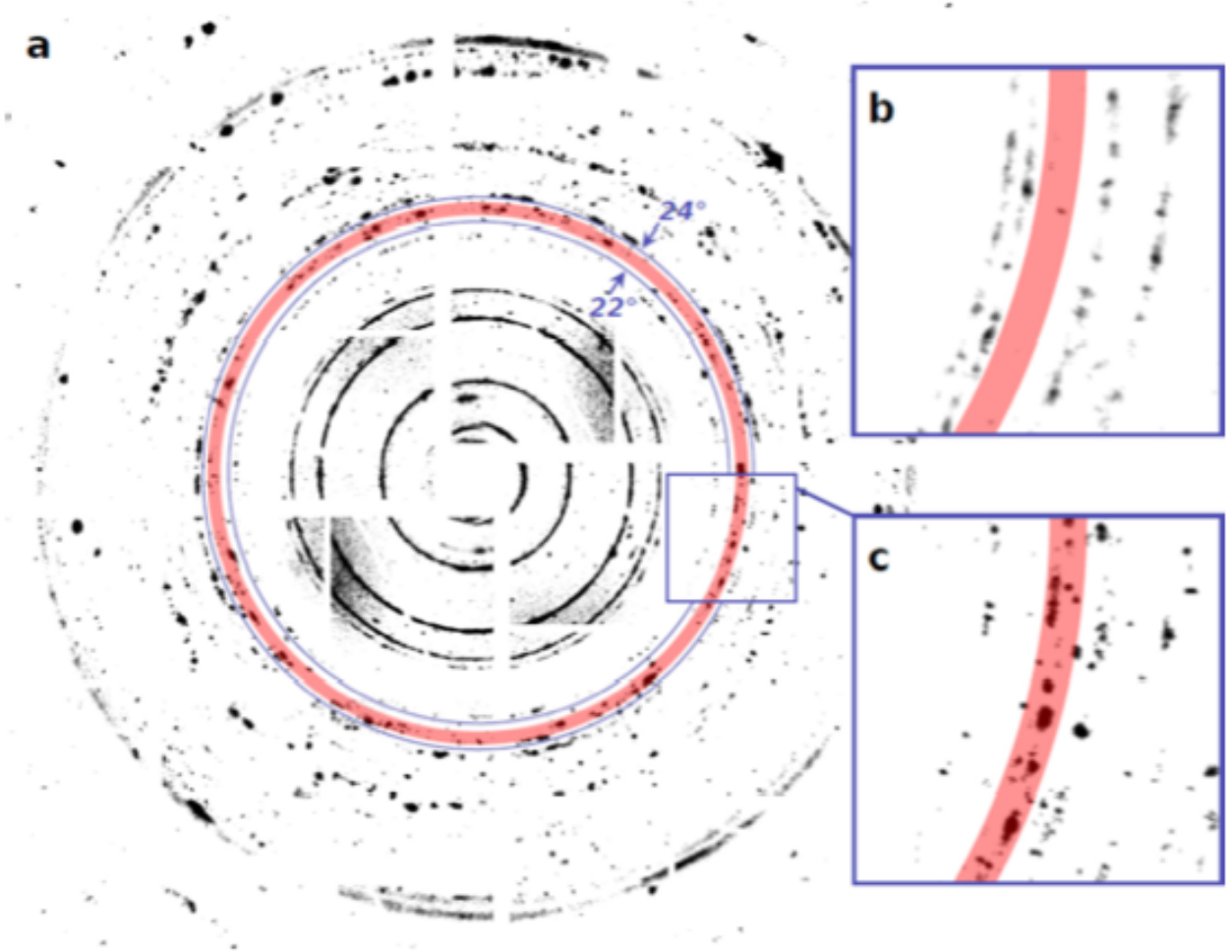
Hirohiko Ichikawa et al, Nature Materials **10** 101 (2011)

$Nd_{0.5}Sr_{0.5}MnO_3$ (NSMO) film on STO





"Femtosecond X-ray Laser induced transient electronic phase change observed in fullerene C_{60}"
B Abbey and H. Quiney, archive preprint (2013)



Bragg Coherent Diffraction Imaging

- Nanoparticle imaging by BCDI
- Complex density can image strain
- Strain associated with nano-shape
- Dislocations during crystal growth
- Ultrafast snapshots of vibrations
- Transient melting
- Materials science in the time domain