Direct Imaging of Phonon Modes in Gold Nano-Particles

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UK Free Electron Laser Forum
Imperial College, London
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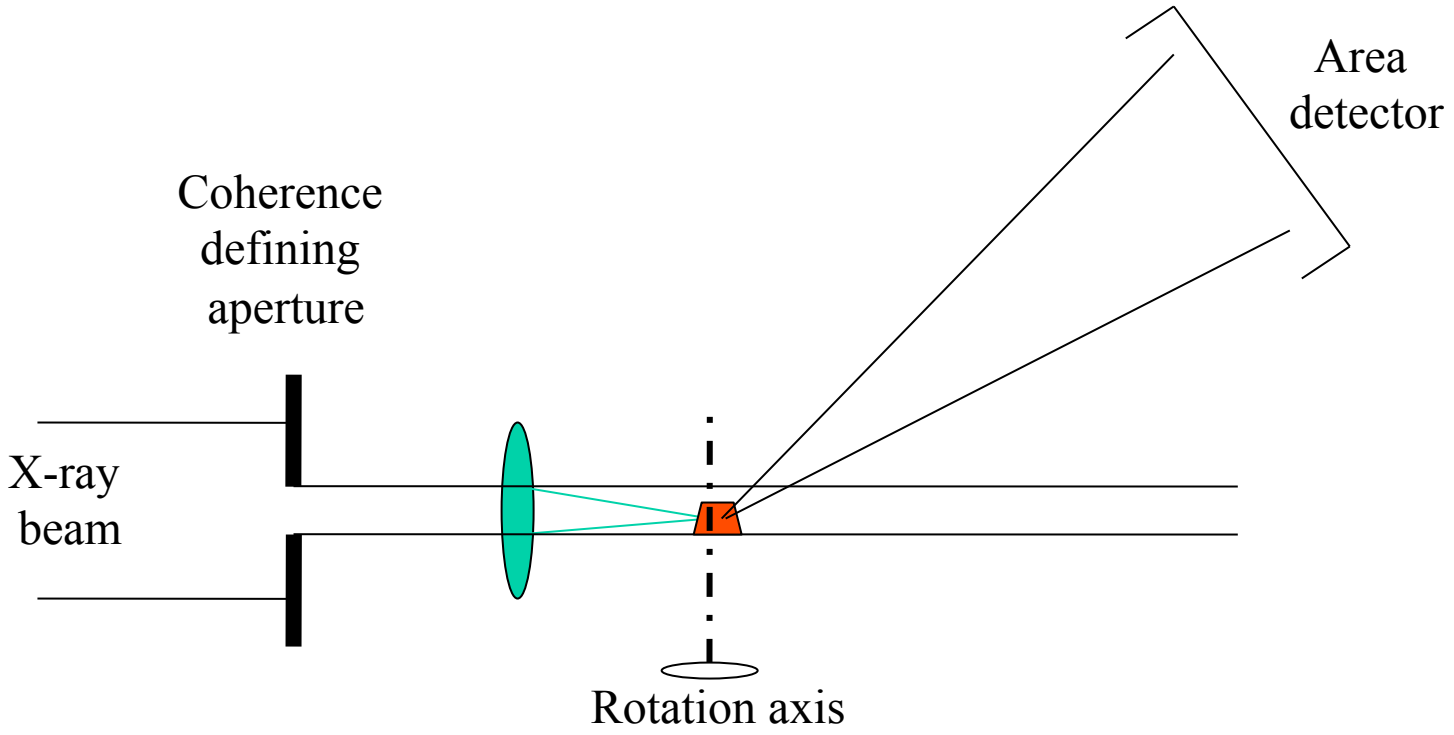
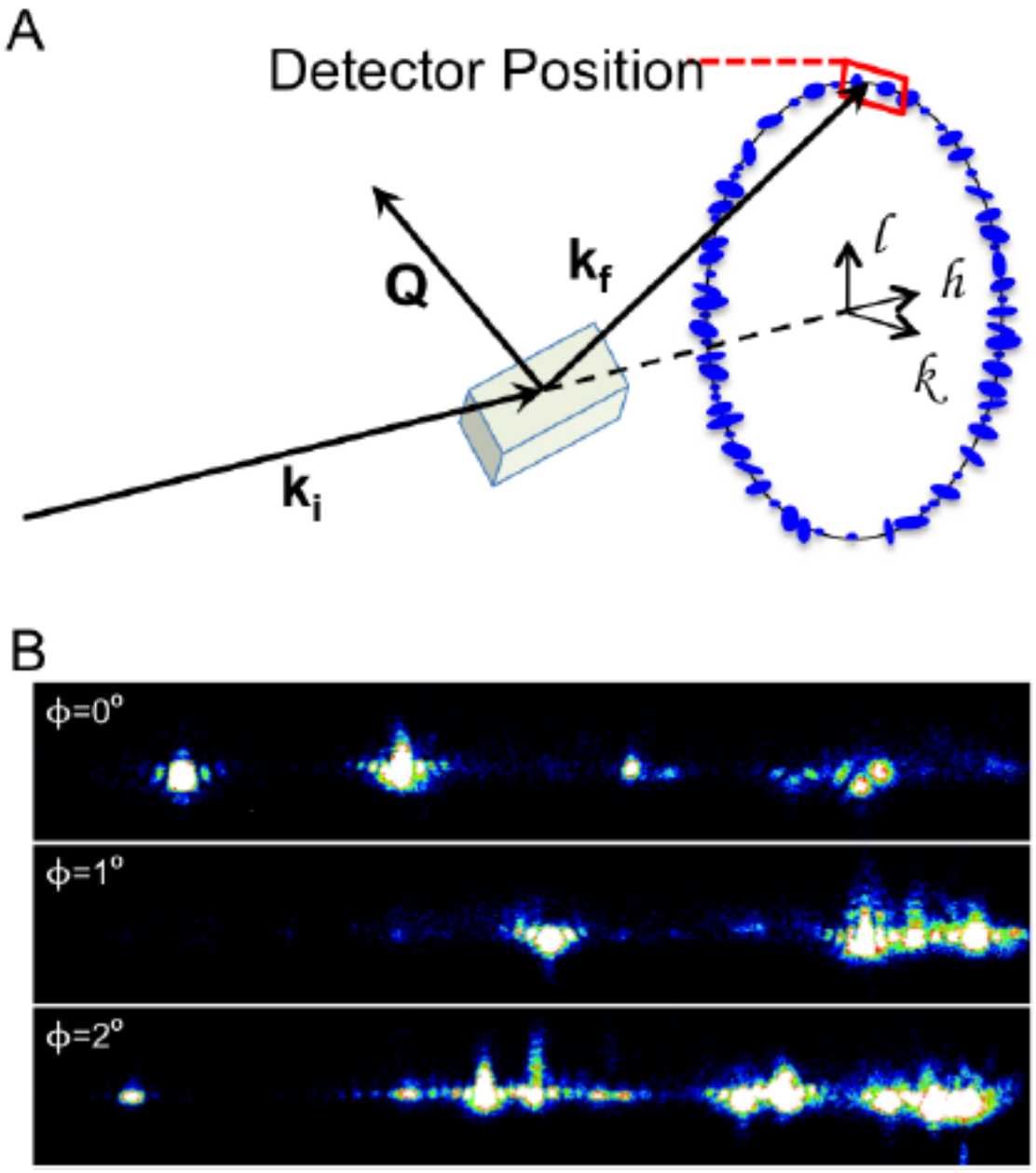
Outline

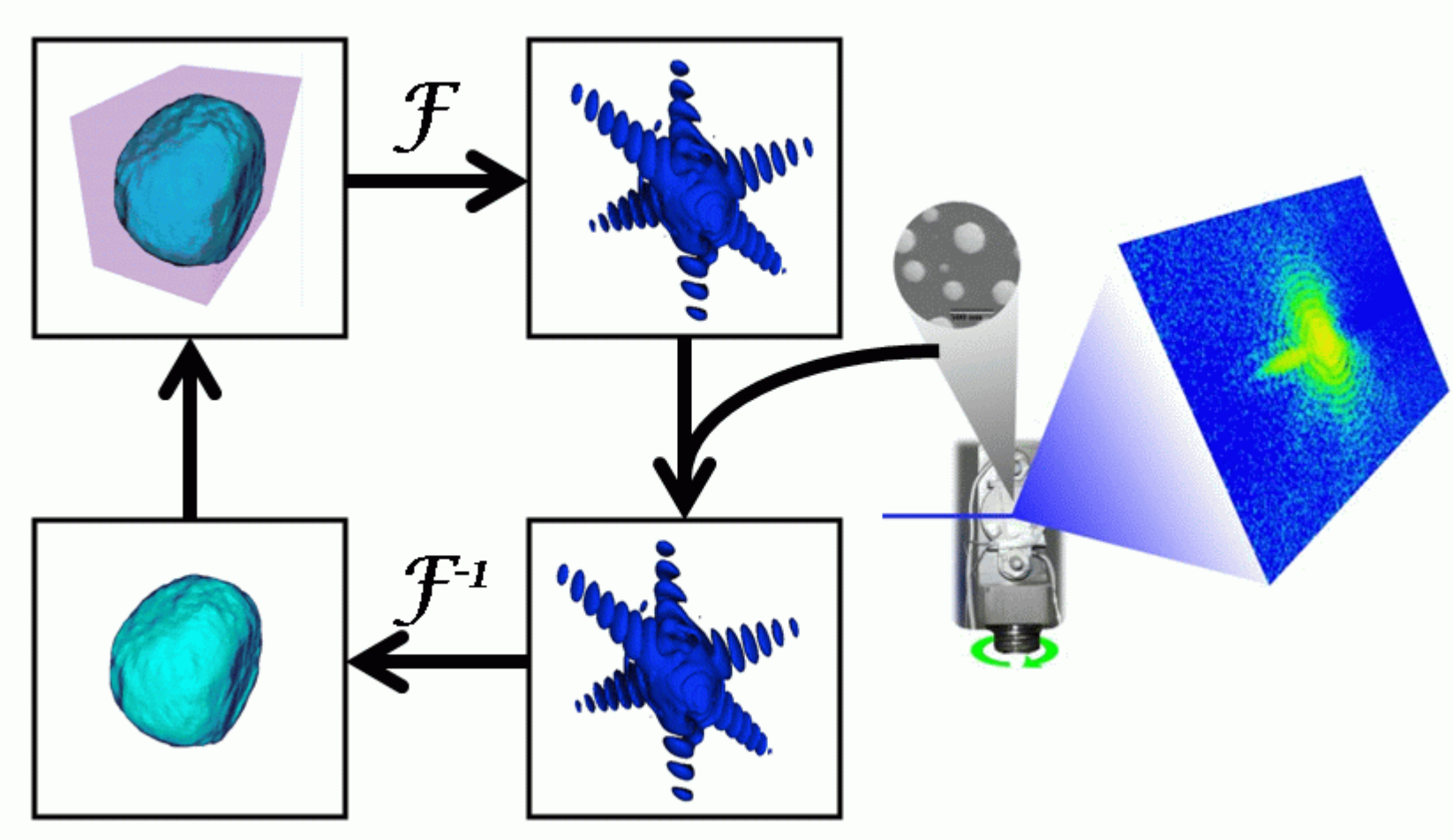
- Coherent X-ray Diffraction Imaging
- Crystal strain as complex density
- Ultrafast CDI of nanocrystals
- Materials Science by XFEL?

Lensless X-ray Microscope, 2003




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

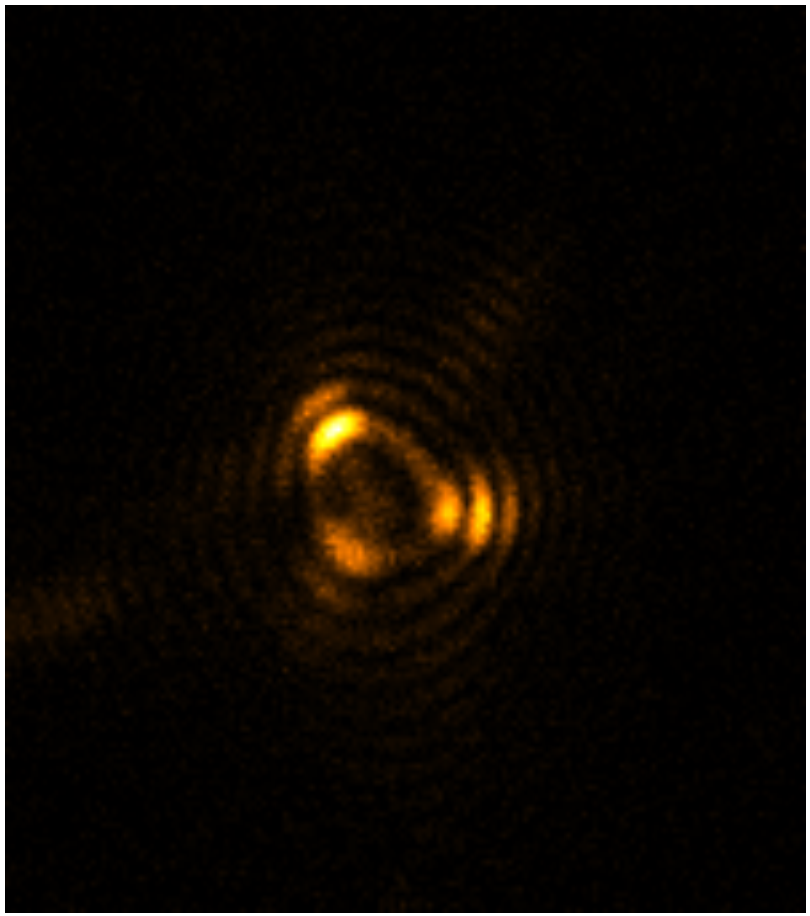
Generic "Error Reduction" method

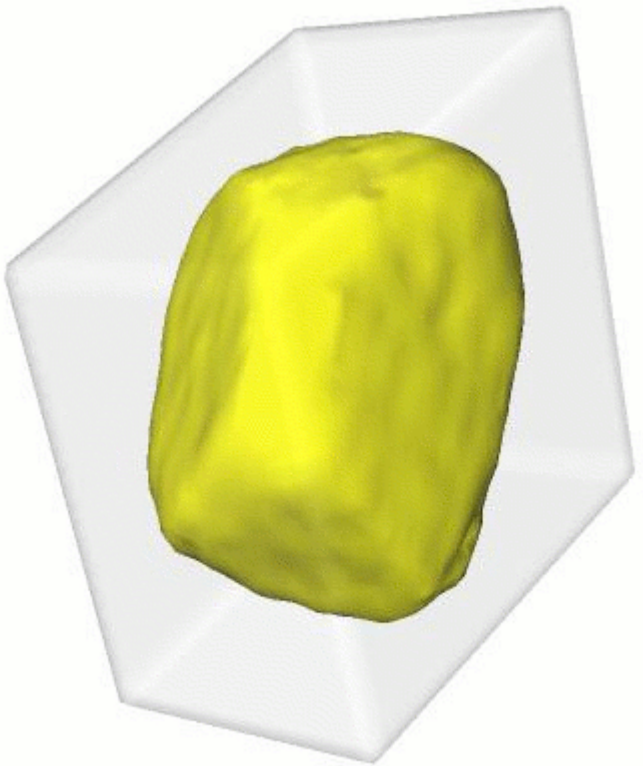


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

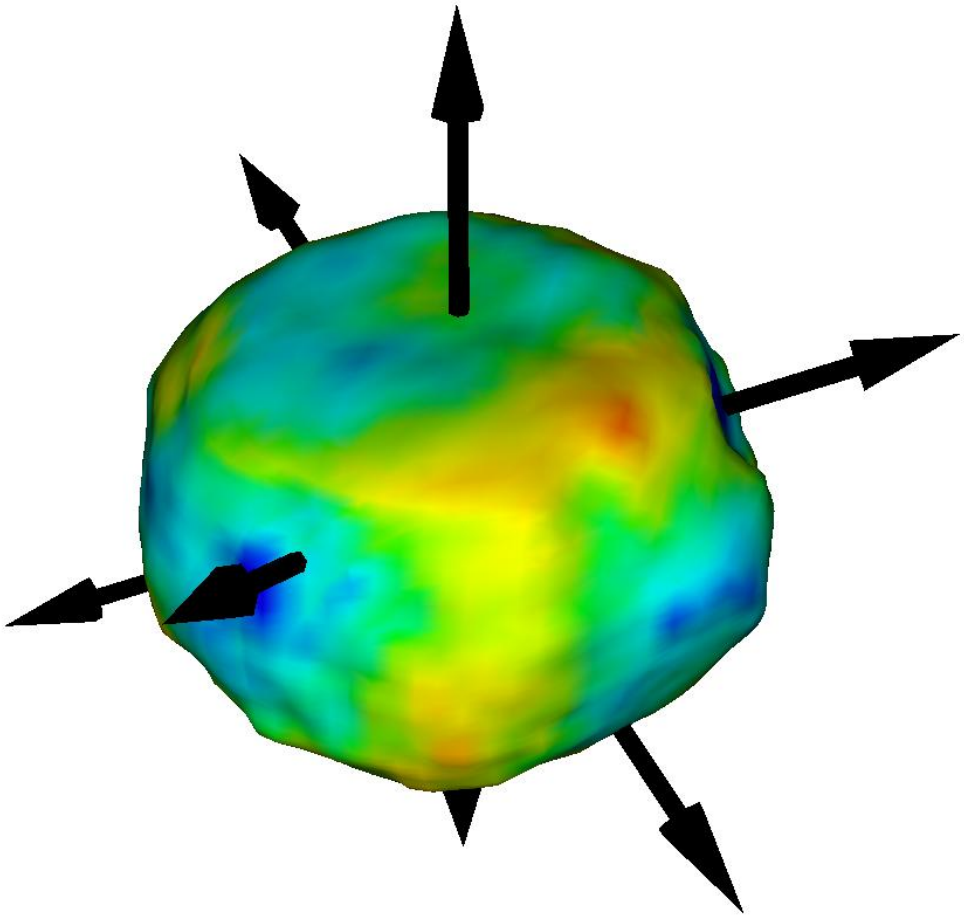
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



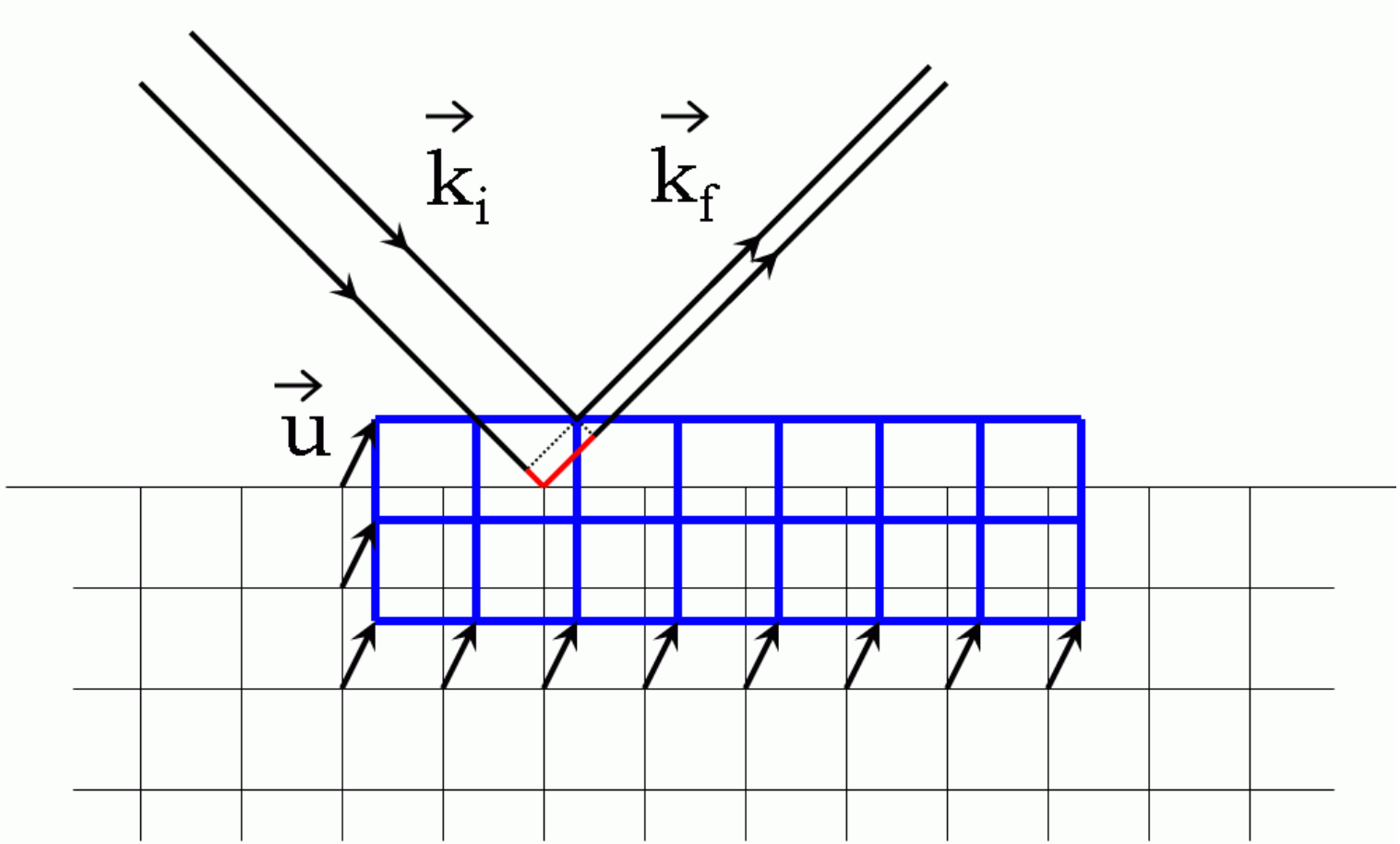


Phase isosurface of residual strain

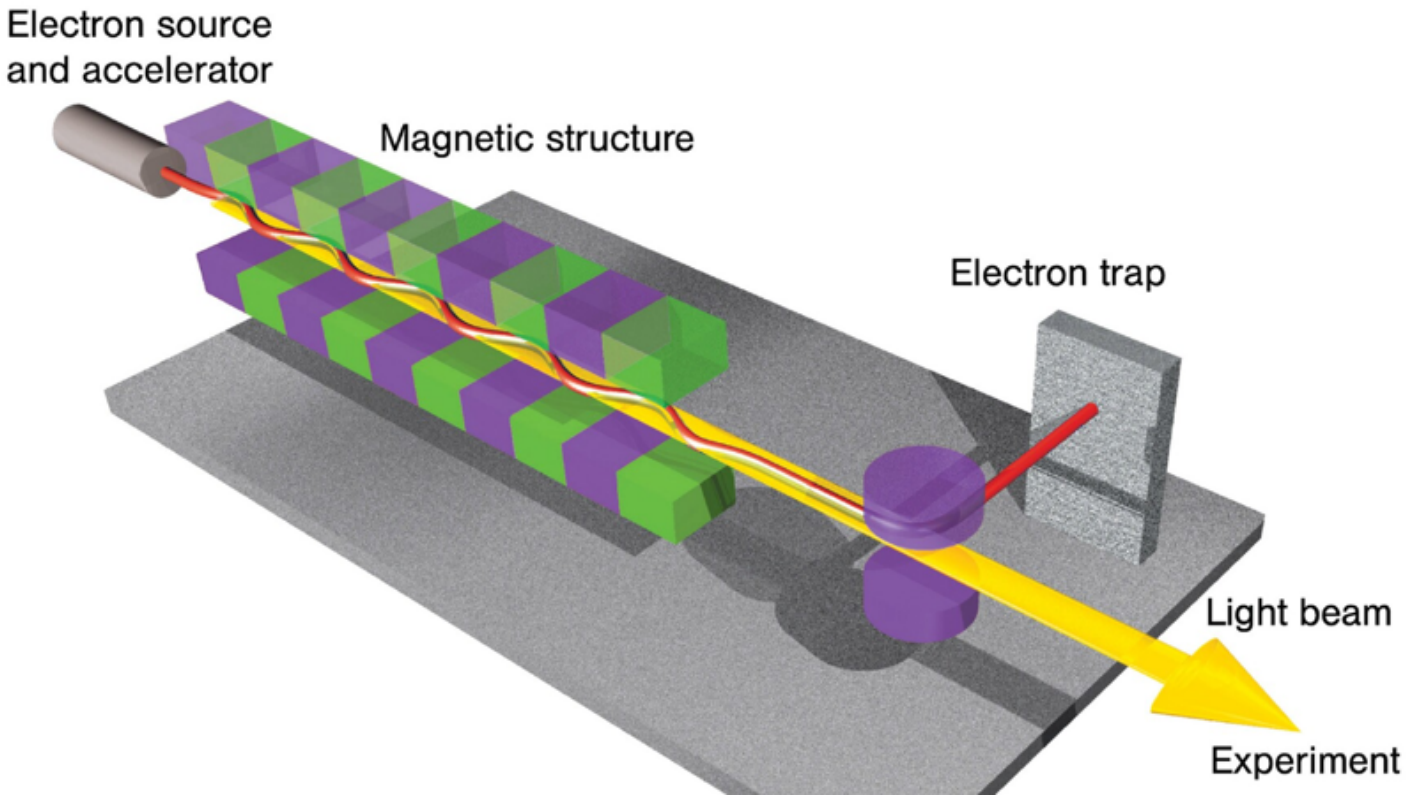


Sensitivity to strain

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

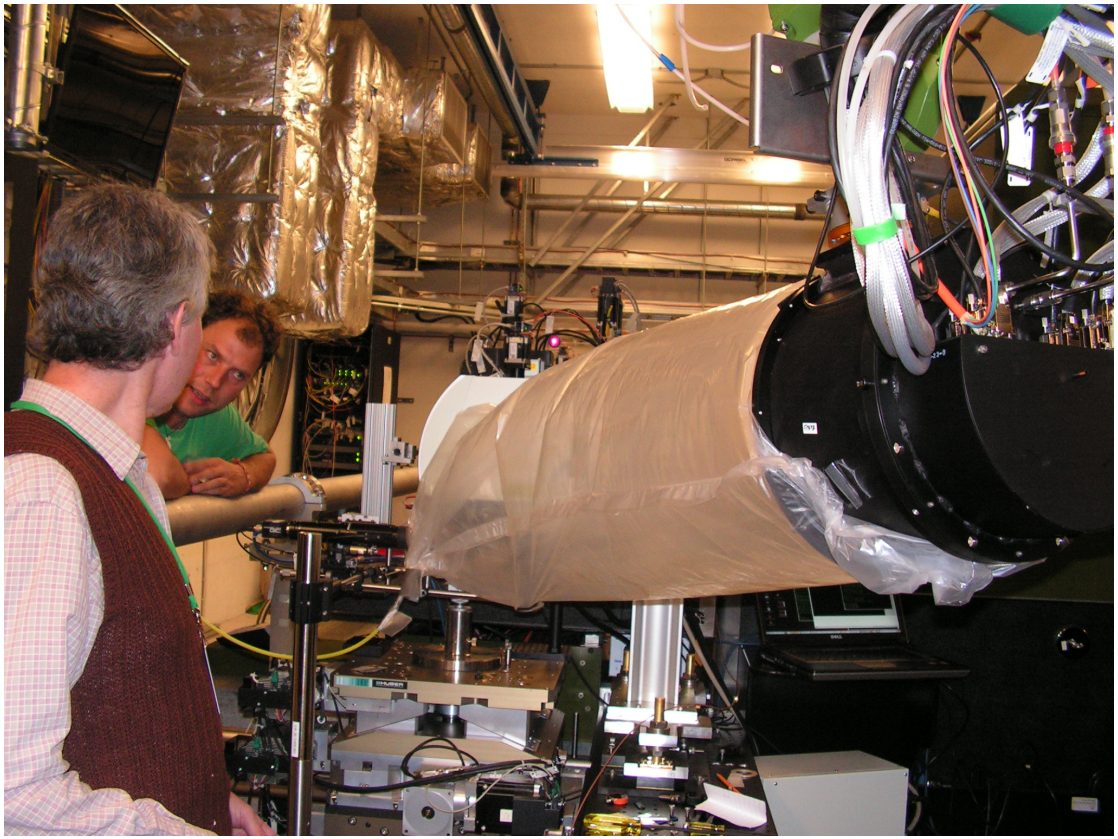


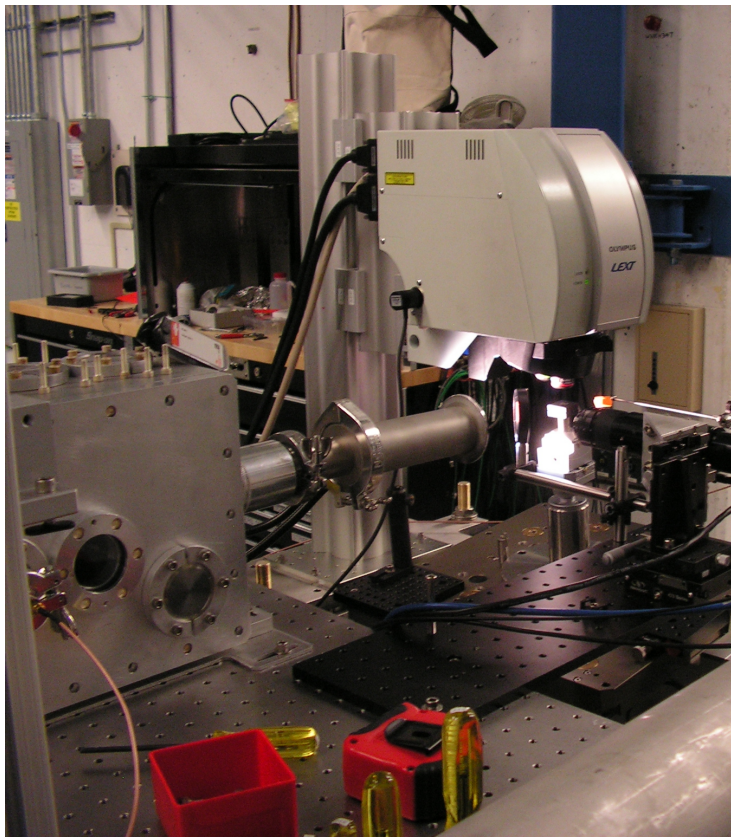
X-ray Free Electron Laser



Pump-probe at LCLS (XPP)

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

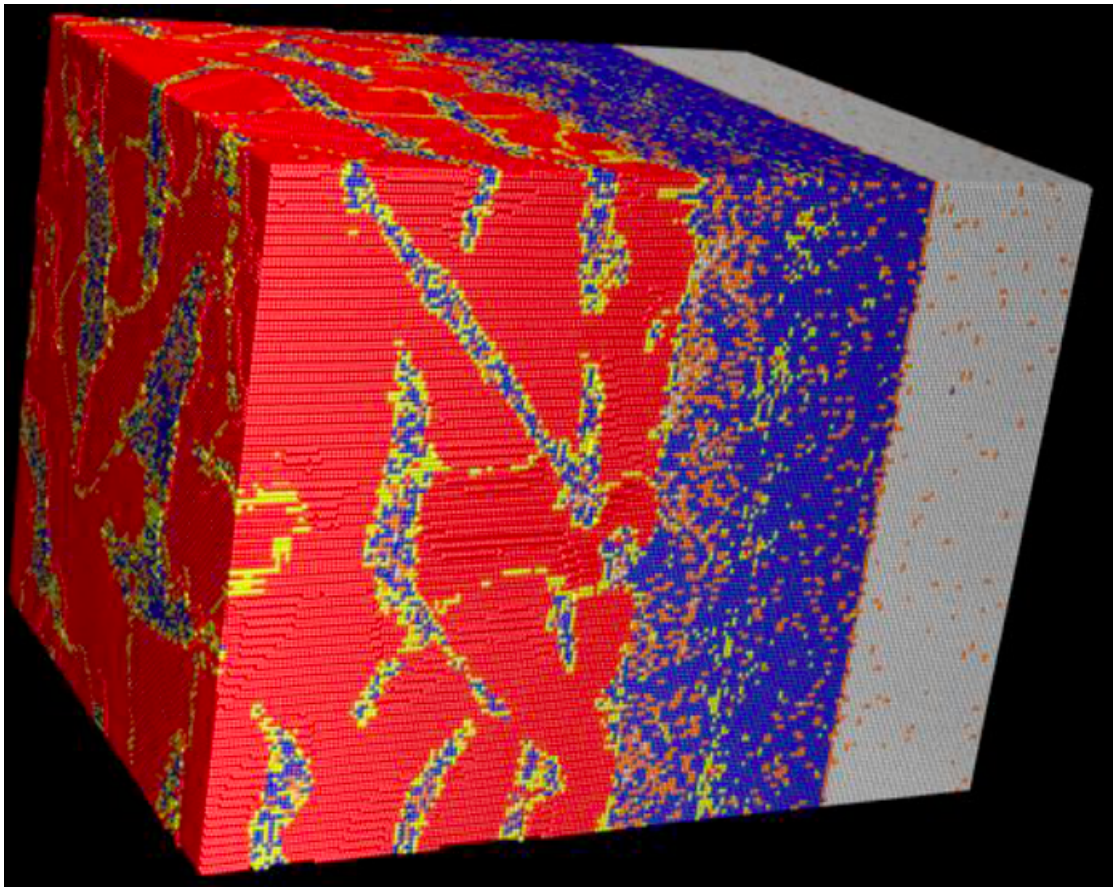




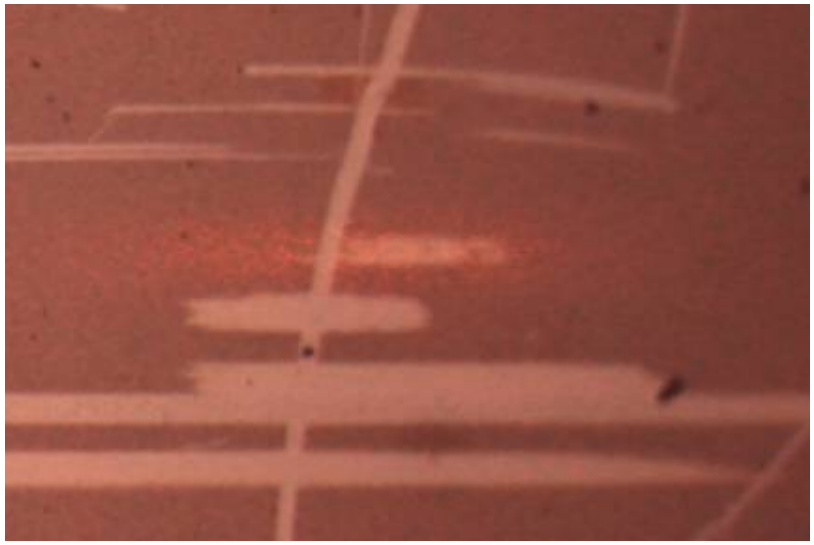
MD simulation of Shock Wave

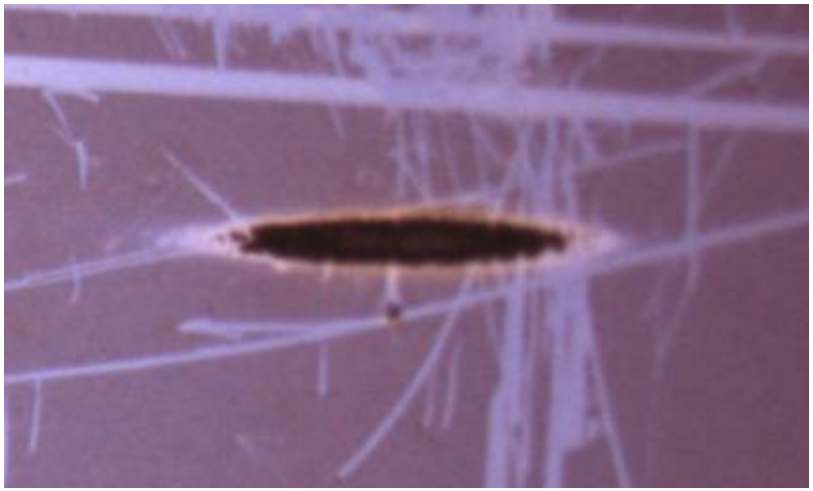
Damage in Fe along (001) direction

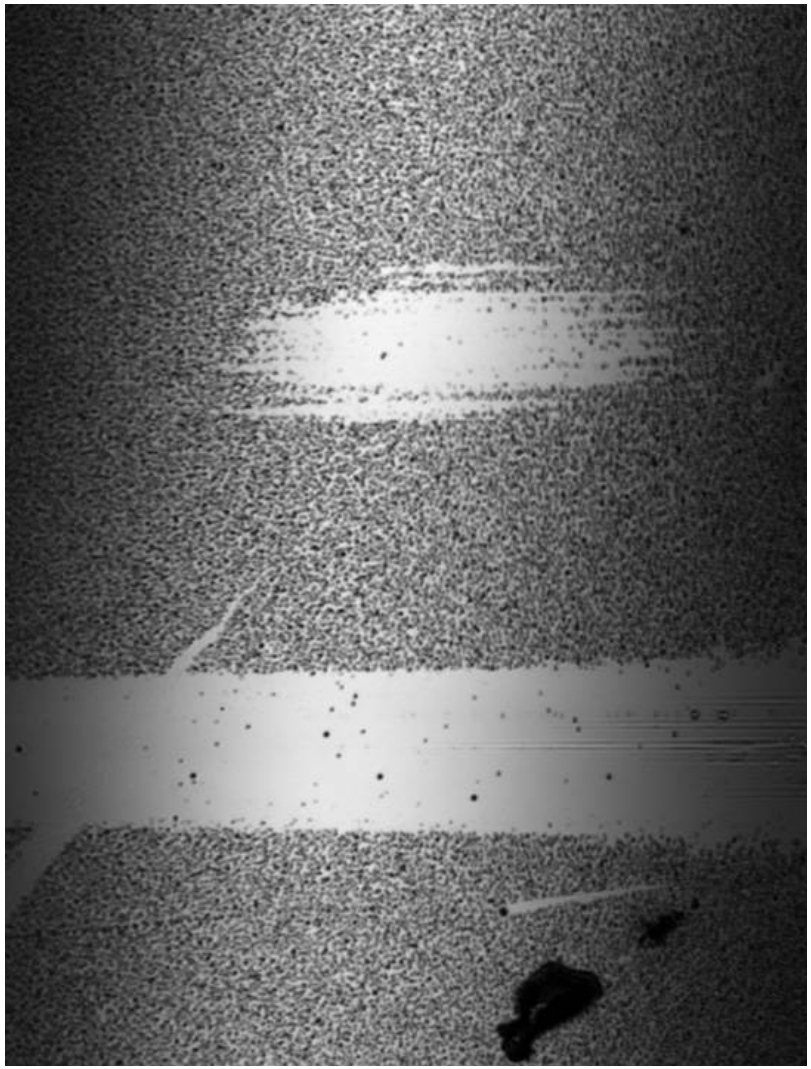
K Kadau, TC Germann, PS Lomdahl, and BL Holian. Science, 296 1681 2002



Visible and Confocal microscopy

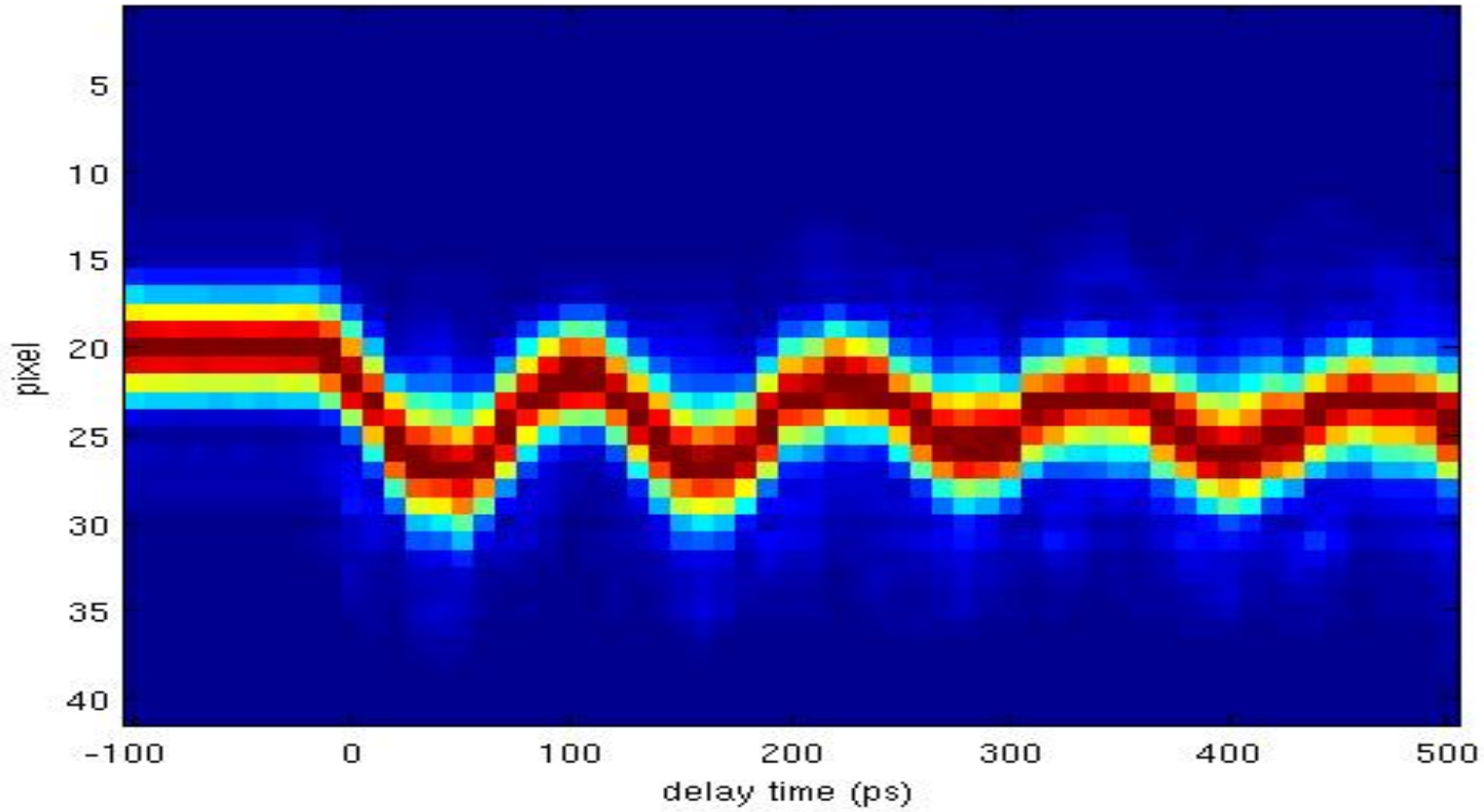






Pump-probe at LCLS (XPP)

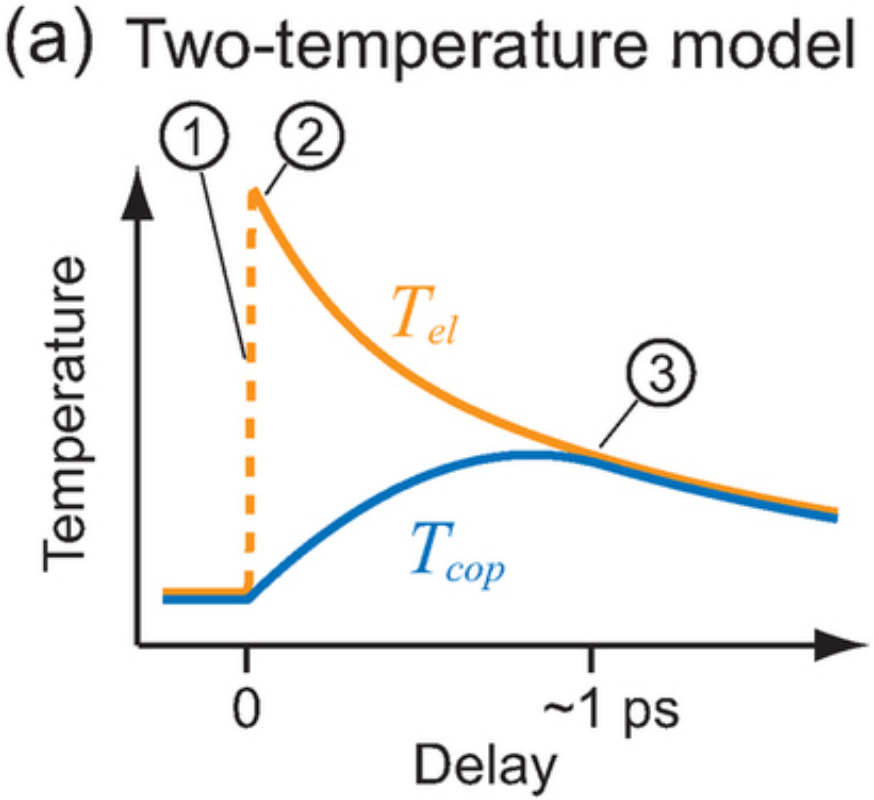
Jesse Clark, Gang Xiong, Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz, Garth Williams, Brian Abbey, Andy Higginbotham, Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt

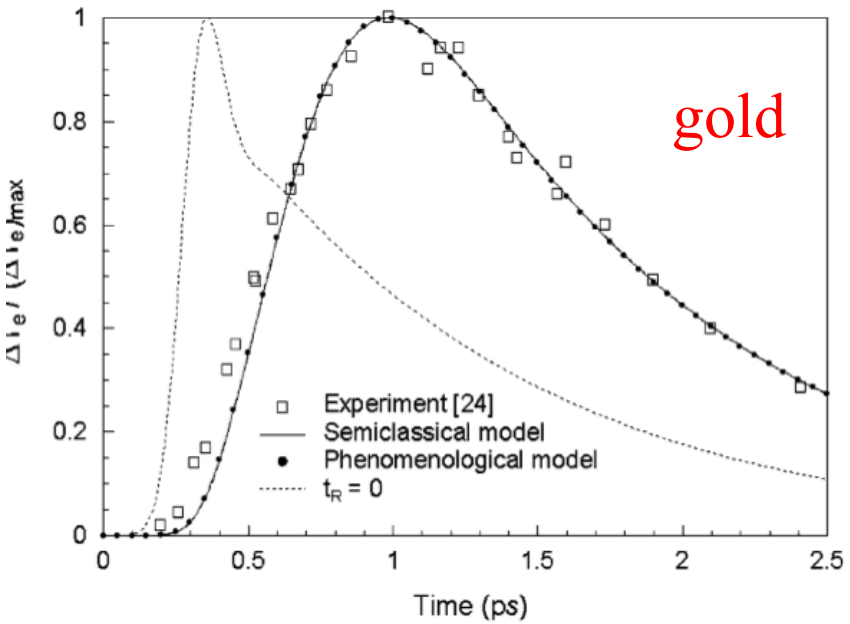


"Two-temperature" model

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

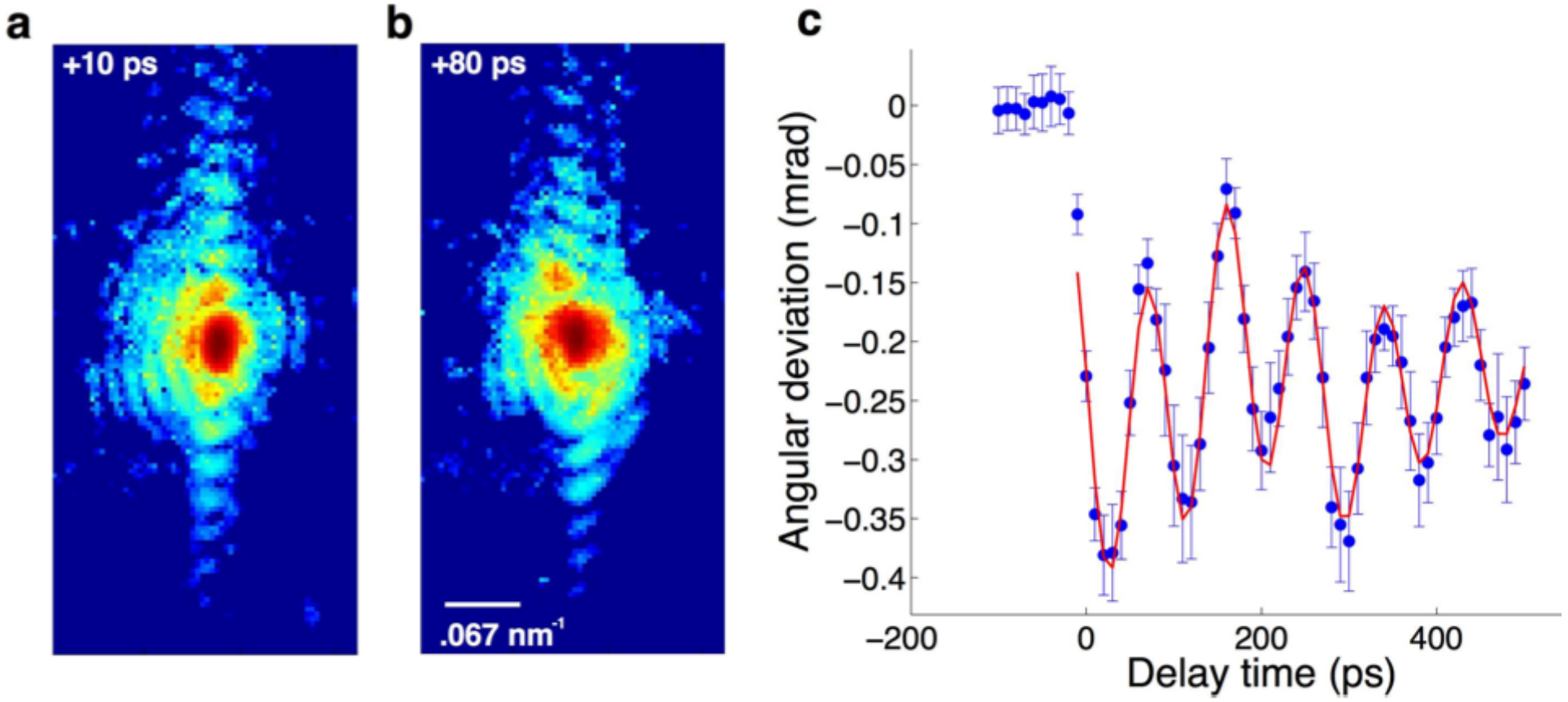
J.K. Chen et al, Int J. Heat Transfer 49 307 (2006)





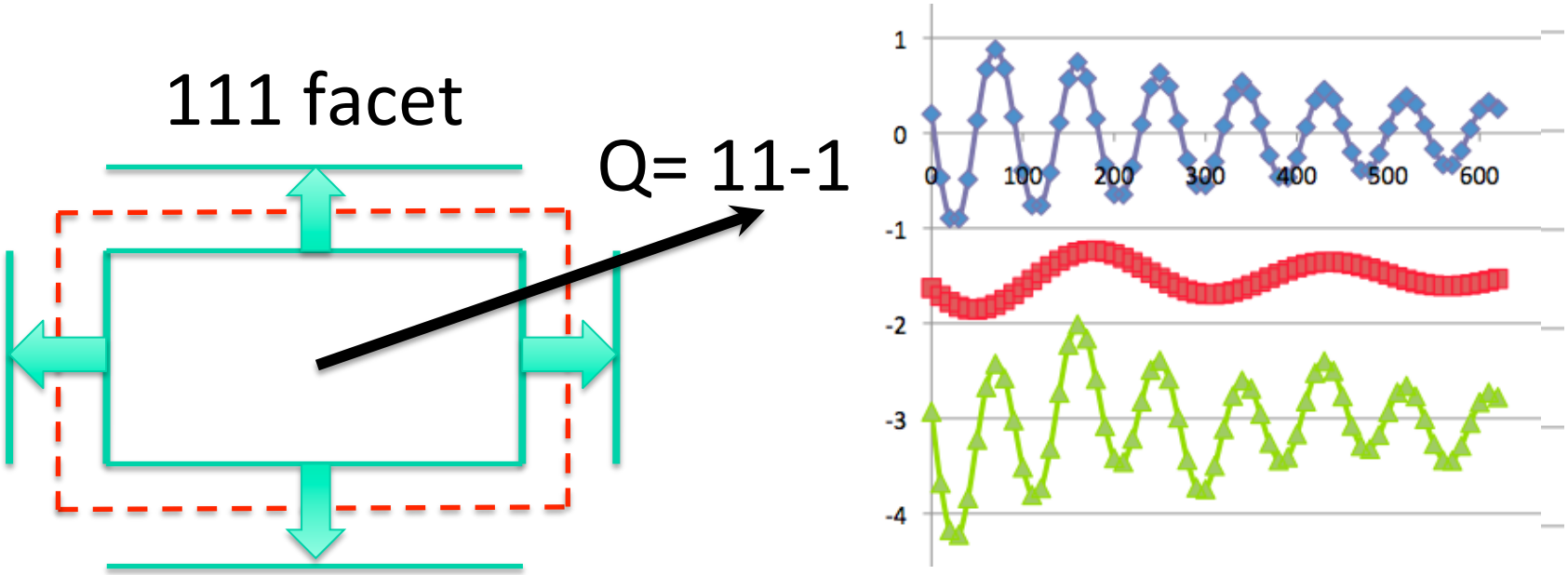
ig. 2. Comparison of the change in electron temperature at
e front surface of an 80-nm gold film irradiated by a 2.8 mJ/
n^2, 800 nm, 150-fs laser pulse.

Time resolved Bragg peak position



Two Normal Modes of Vibration

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



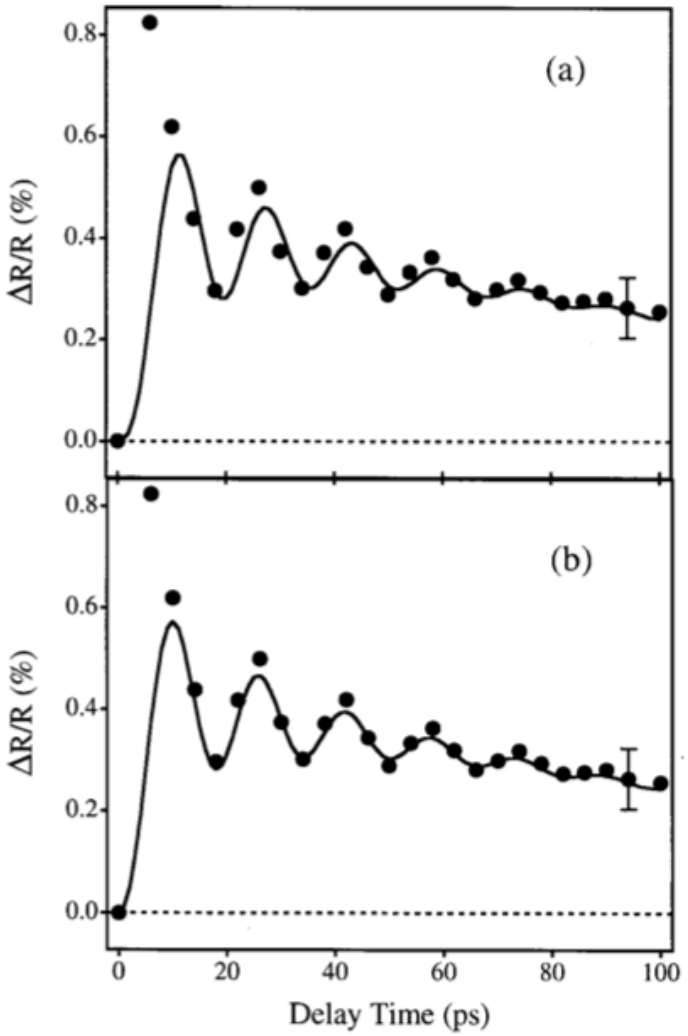
T_1 = 90ps h_1 = 145nm c_s = 3240 m/s

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)

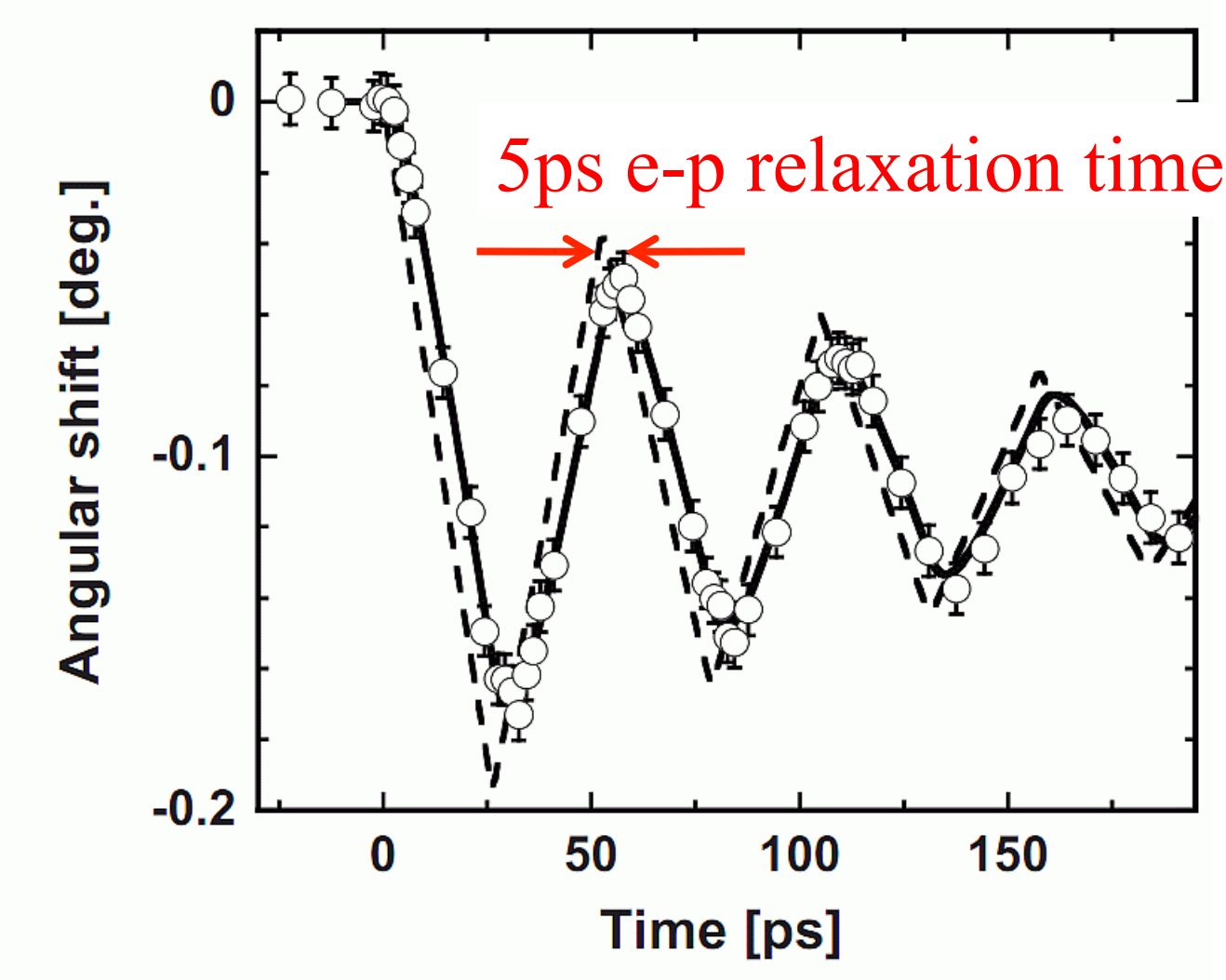


(a) Simple normal mode analysis with impulse heating.

(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)

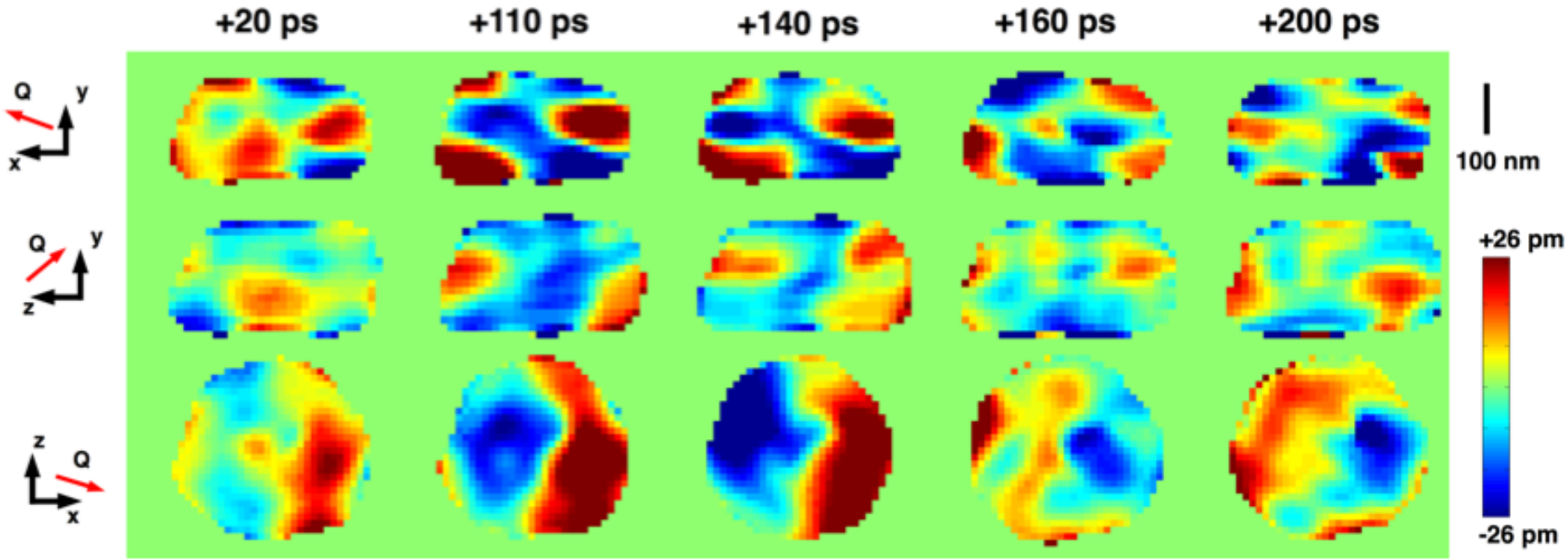


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

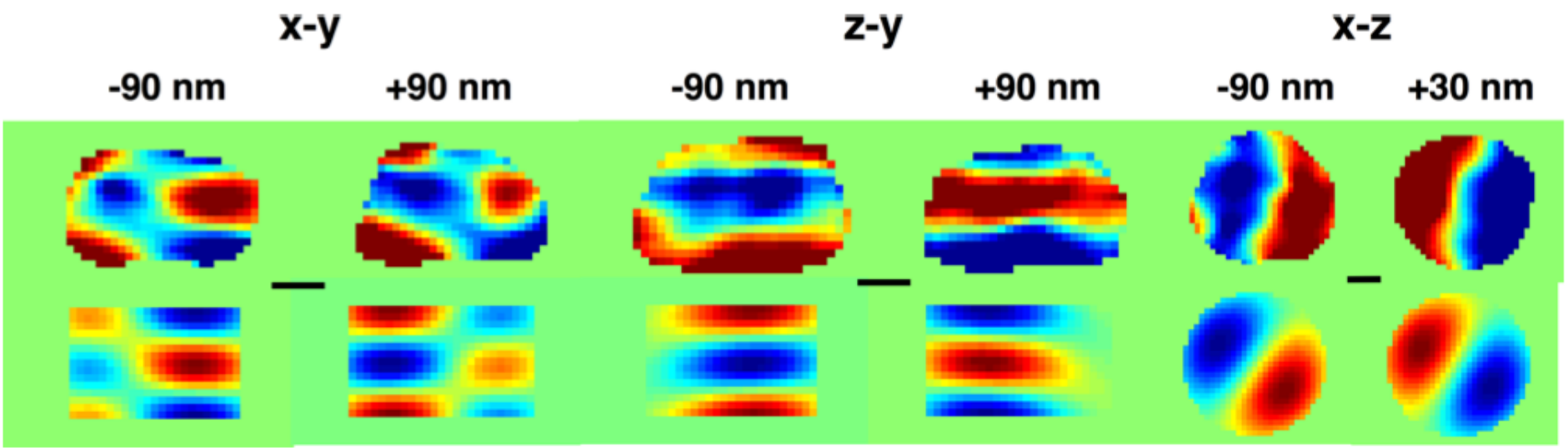
1000 frames averaged at each point of rocking curve

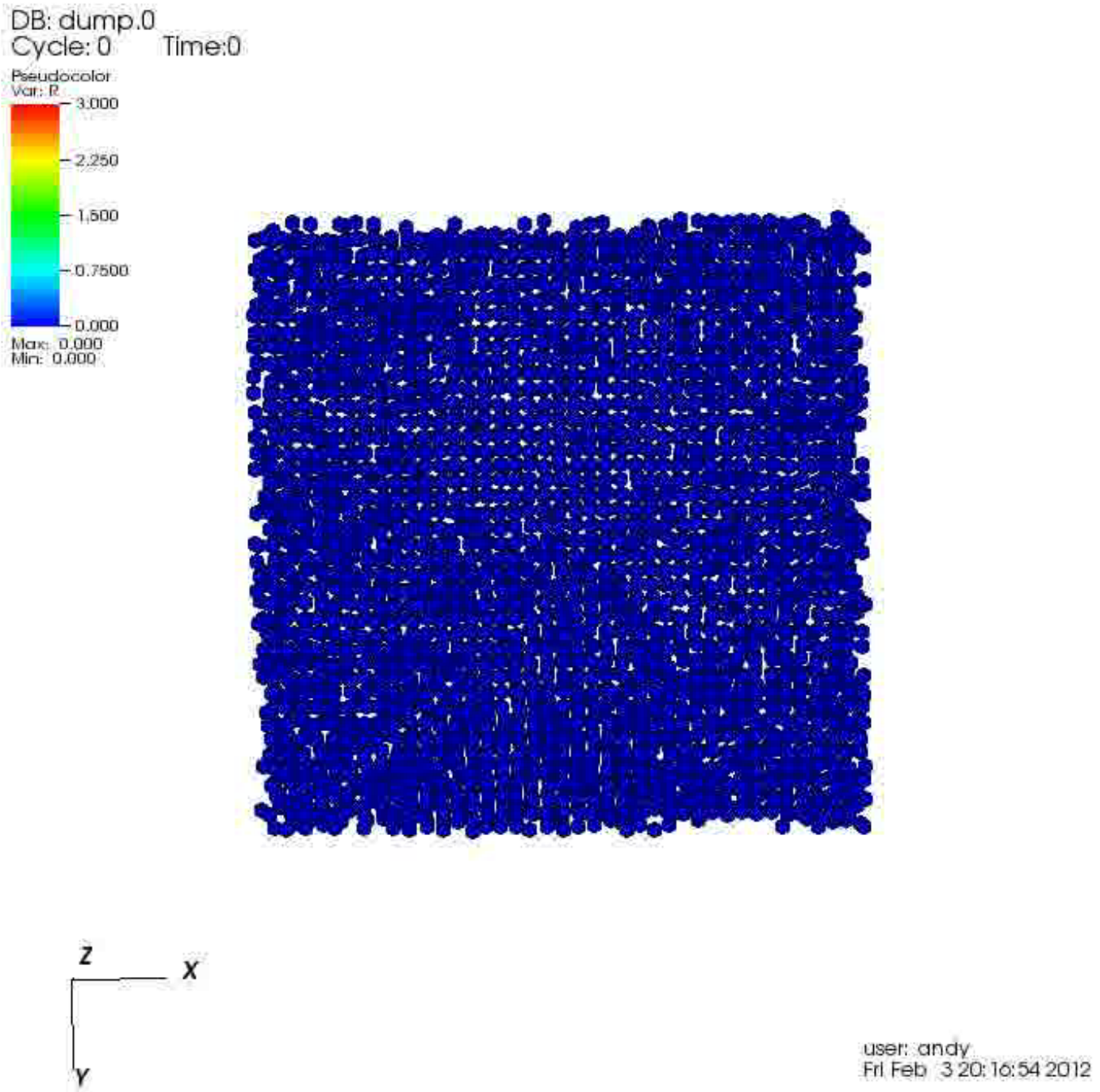
Jesse Clark et al Science (2013)



Dynamic imaging of displacements

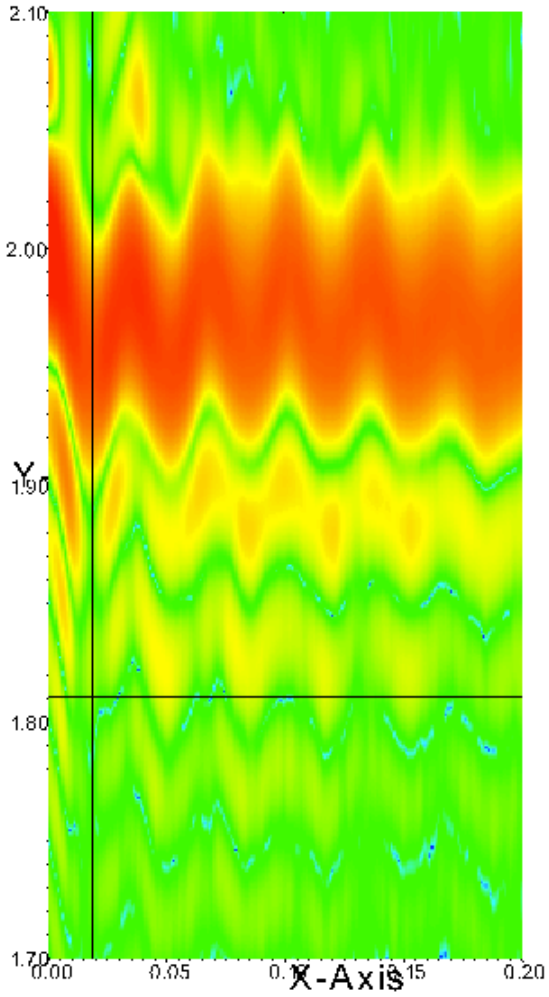
CDI inversion of 3D diffraction patterns
Comparison with (1,1) normal mode of cylinder
Jesse Clark et al Science (2013)

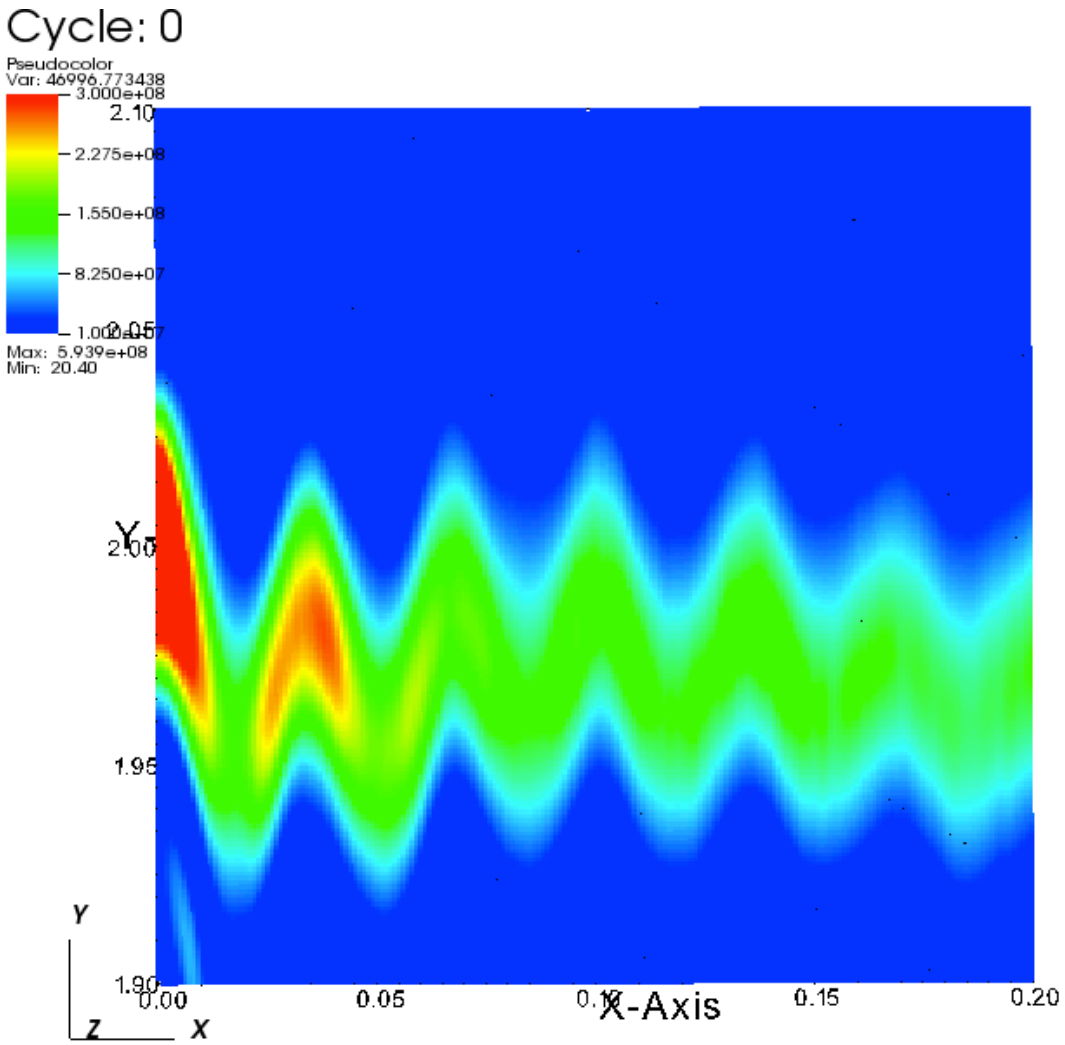



DB: dump.0
Cycle: 0 Time:0
Pseudocolor
Var: R
3.000
2.250
1.500
0.7500
0.000
Max: 0.000
Min: 0.000
Z
X
Y
user: andy
Fri Feb 3 20:16:54 2012

MD Simulation (LAMMPS)

Andy Higginbotham and Loren Beitra



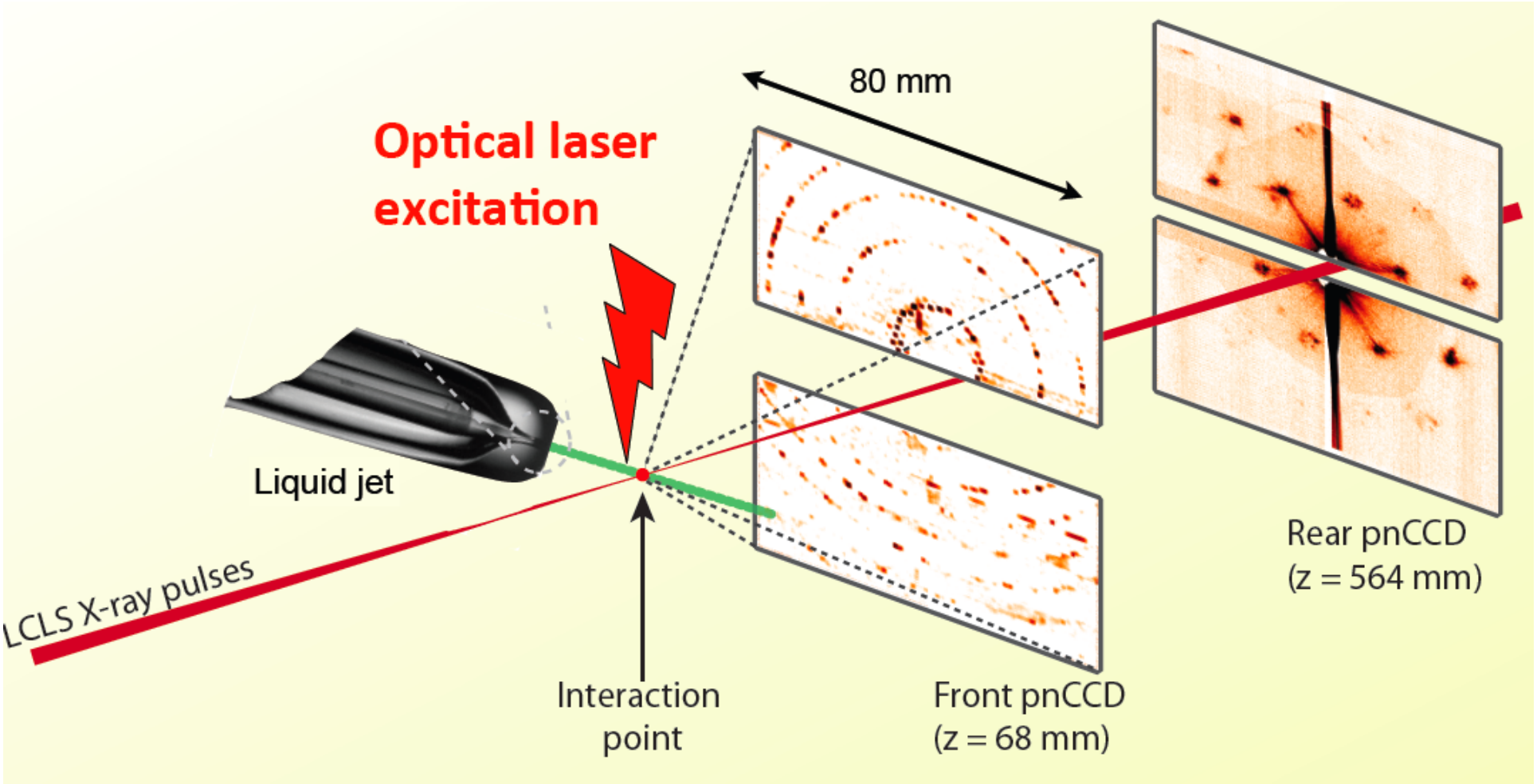


Materials Science using XFELs

- Ground rule #1: €13,000 per hour
- Ground rule #2: fully automated experiment
- Ground rule #3: non-toxic, safe samples
- Ground rule #4: nanoparticles by the kg
- 27,000 pulses/sec at XFEL.EU, 2700x10
- up to 2000 frames/sec data rate = TB/hr

Pump-probe schematic

Henry Chapman, Bio-XFEL workshop Jan 2011

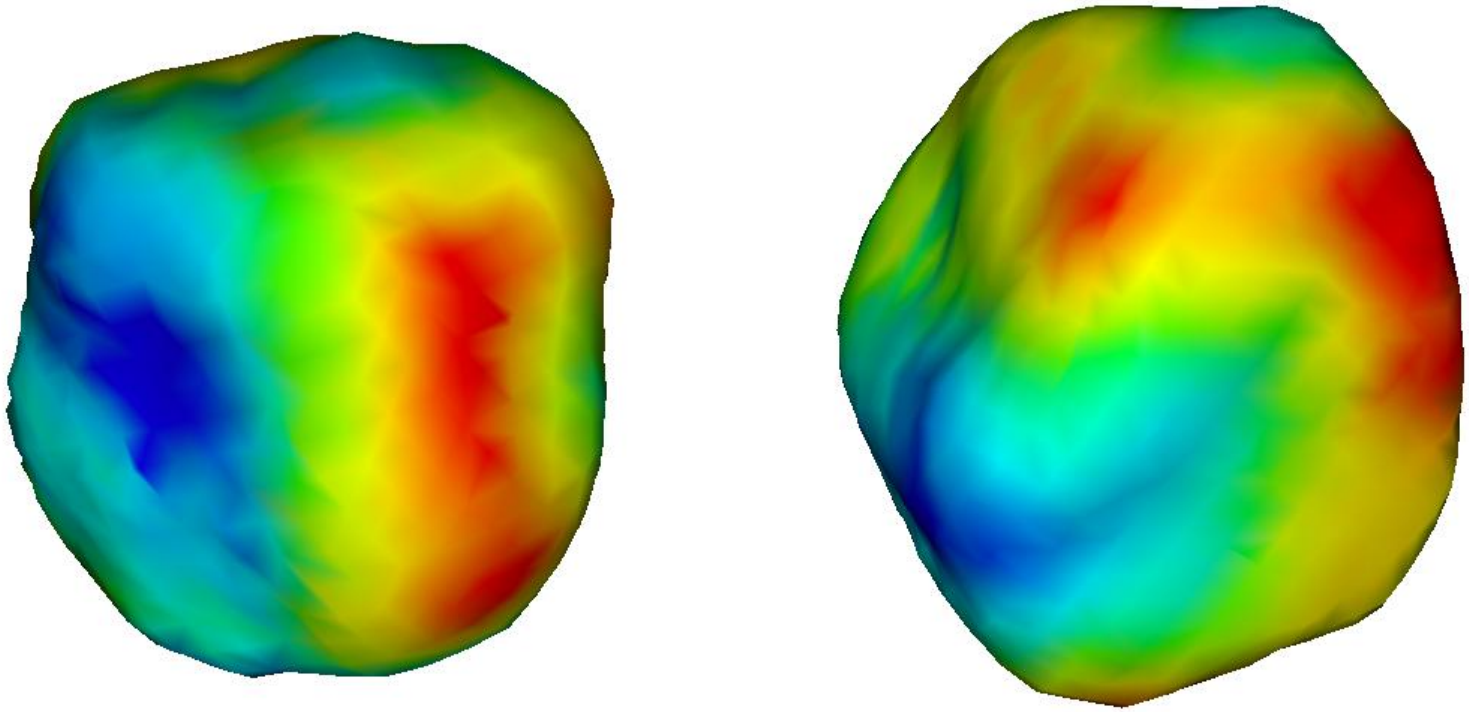


Materials Science using XFELs

- Nanoparticles injected into X-ray beam
- Synthesize samples in nanoparticle format
- Veto frames where no "hit" or diffraction
- 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

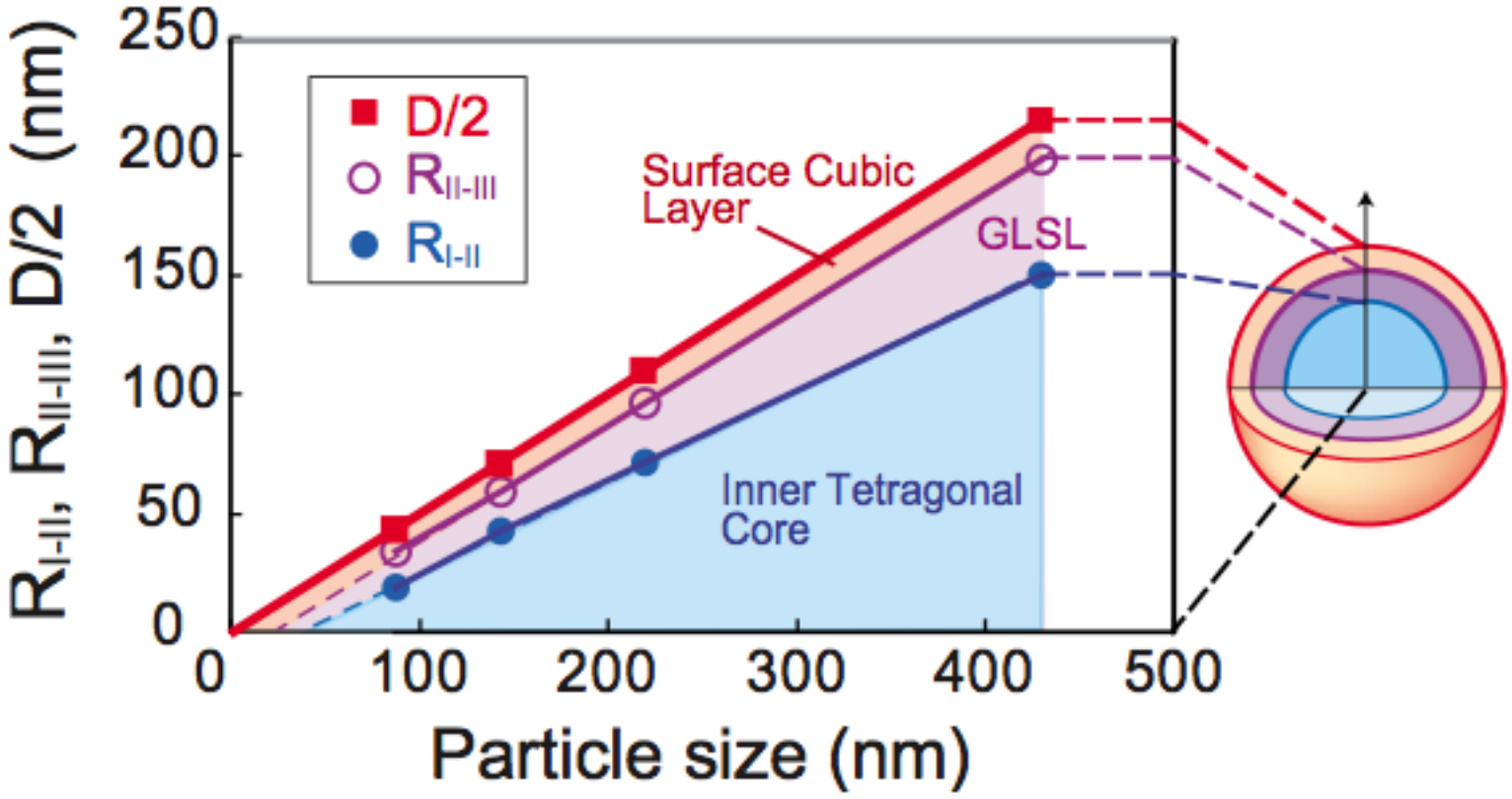
Phase isosurface of residual strain

200nm Barium Titanate (BTO) crystals



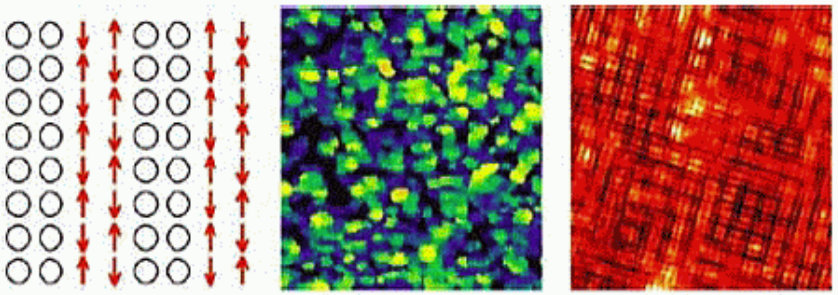
Core-shell structure of BTO

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



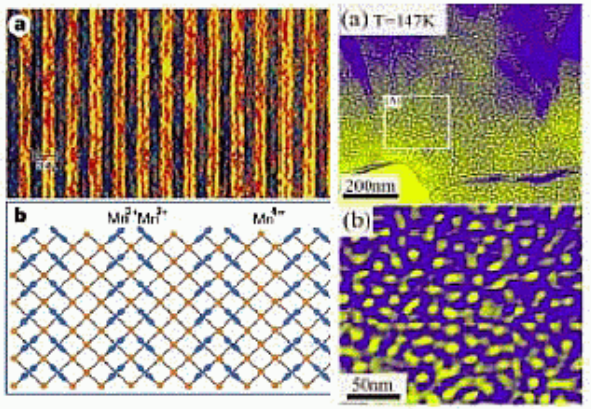
Stripes, checkerboards and zig-zags

High-Tc cuprates



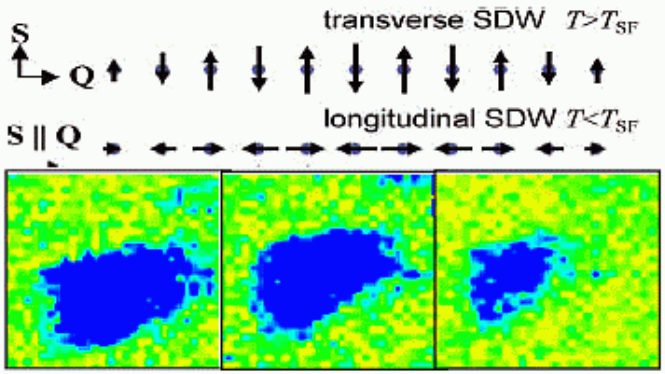
E. Dagotto, T. M. Rice, *Science* **271**, 618 (1996).
T. Hanaguri et al., *Nature* **430**, 1001 (2004).

CMR manganites

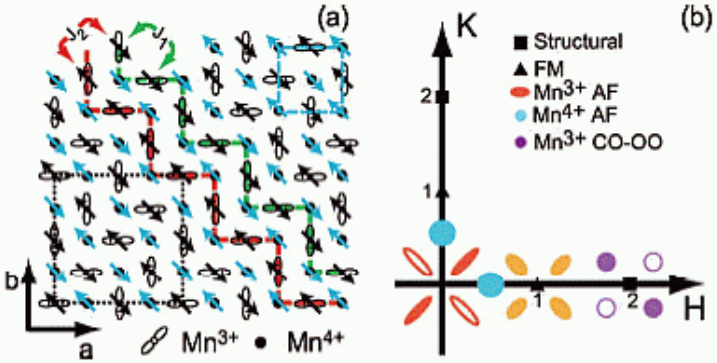


S. Mori et al., *Nature* **392**, 473 (1998)
M. Uehara et al., *Nature* **399**, 560 (1999)

AFM chromium



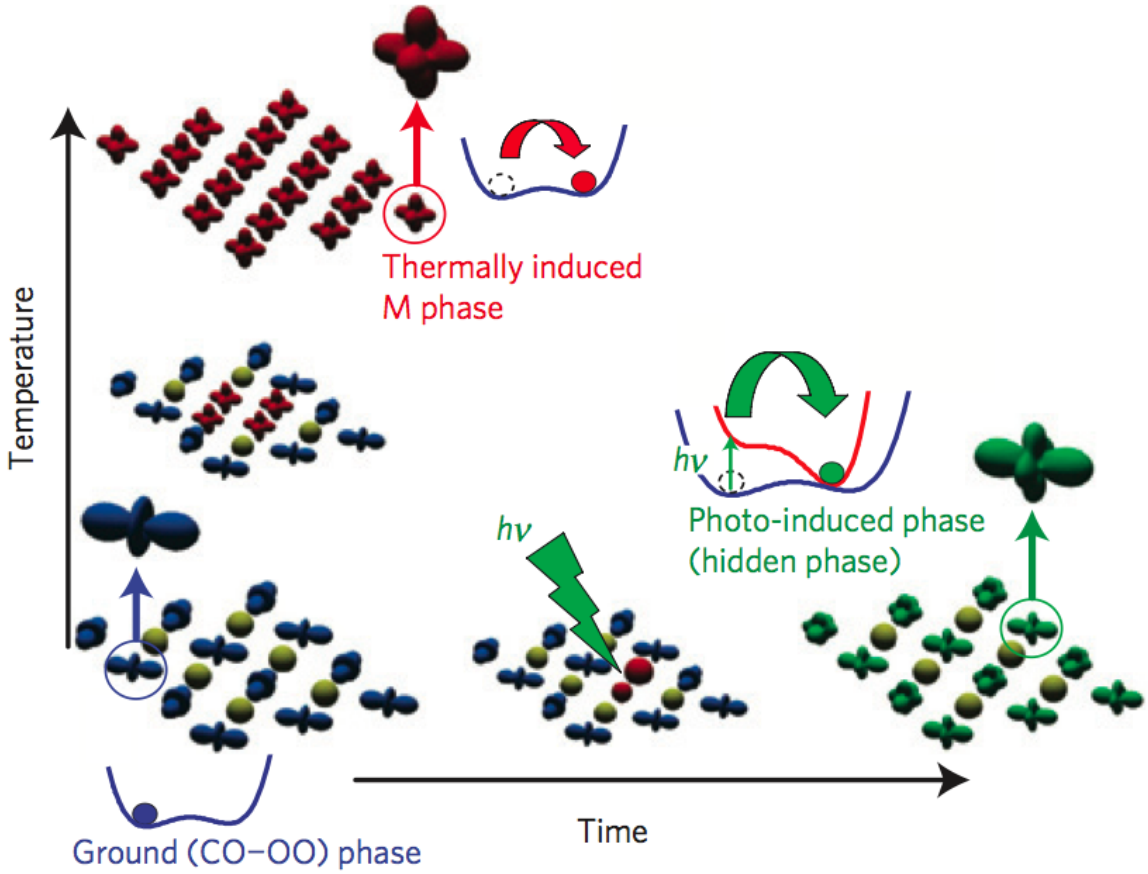
P. G. Evans et al., *Science* (2002)

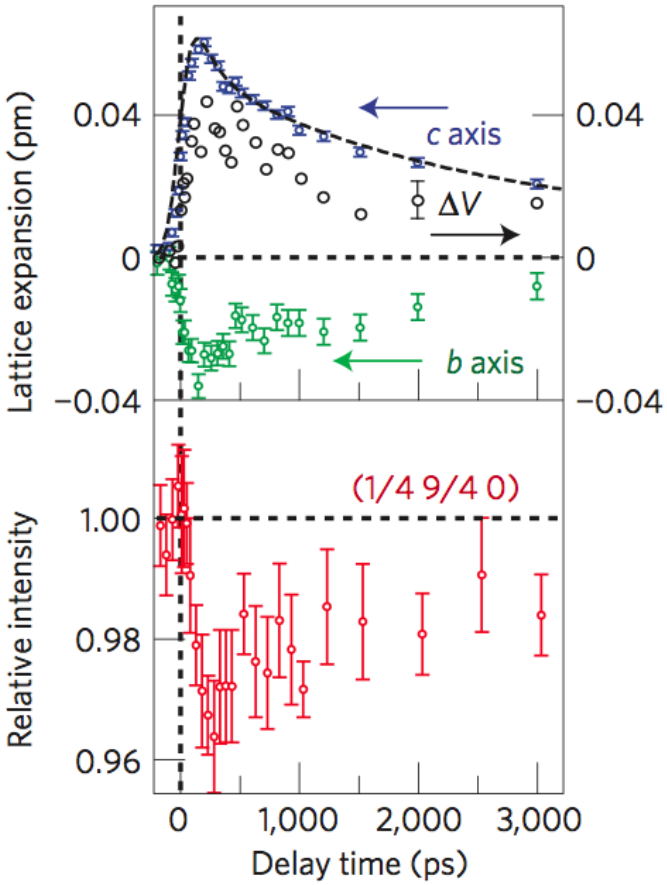


Transient "Hidden" Phase in Manganite

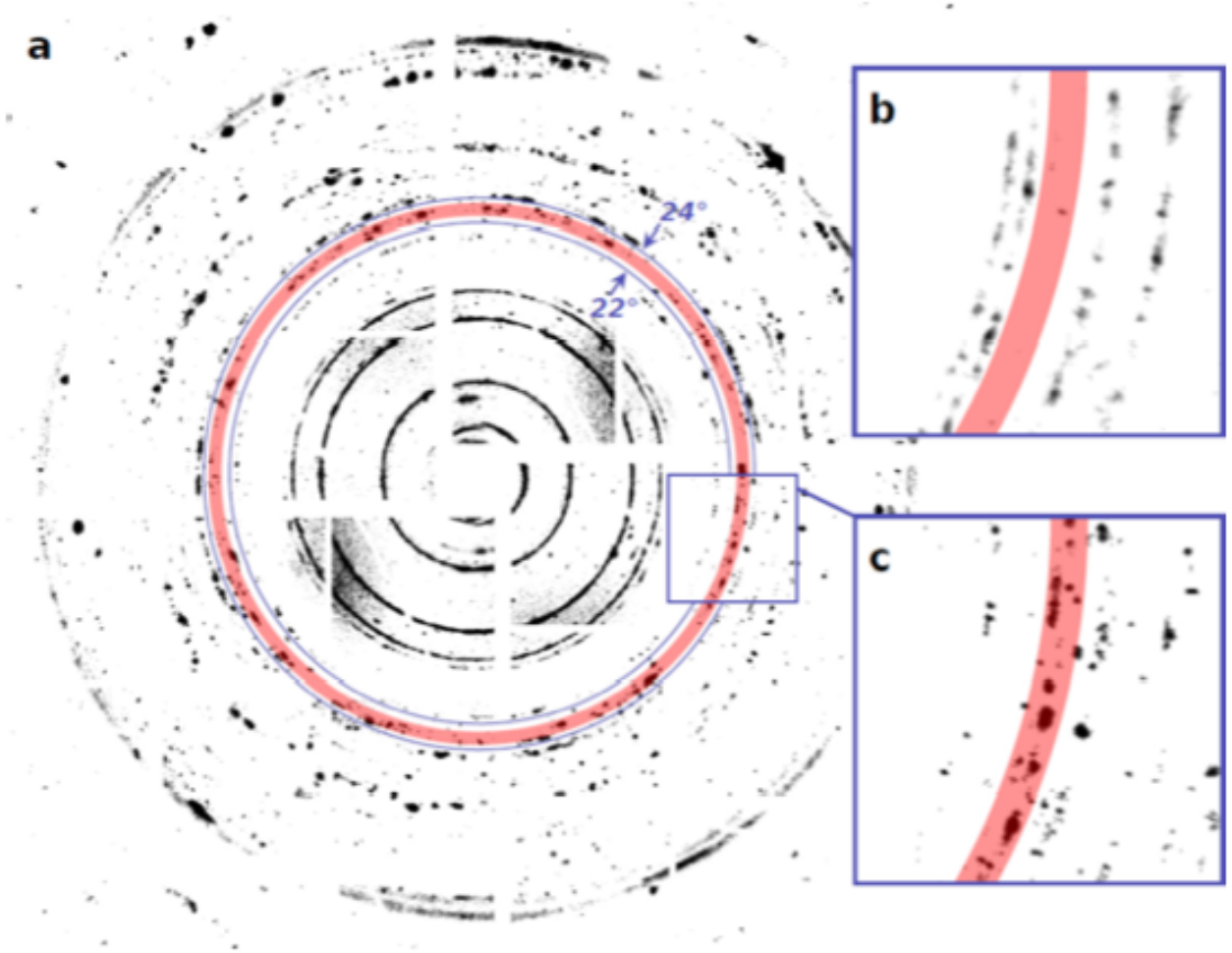
Hirohiko Ichikawa et al, Nature Materials **10** 101 (2011)

$Nd_{0.5}Sr_{0.5}MnO_3$ (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)



Coherent x-ray diffraction (CXD)

- Complex density can image strain
- Strain associated with nano-shape
- Time resolved strain patterns
- New transient materials using lasers
- Materials Science by XFEL?