Time-resolved Coherent Diffractive Imaging

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Timing and Dynamics Workshop
APS, Argonne
October 2013

Outline

- Coherent X-ray Diffraction Imaging
- Crystal strain as complex density
- Ultrafast CDI of nanocrystals
- Materials discovery in time domain?

CDI opportunities with MBA lattice

- High energy CDI.
  - same coherent fraction at a much higher energy,
  - in operando battery materials
- t-resolved CDI
  - phonon vibrations
  - materials discovery
  - modal analysis of fluctuations
- Smaller nanoparticle structures
- Magnetic CDI, orbital ordering
  - cross sections can be 10^{-4} of charge
- Quantum fluctuations
  - seen as loss of visibility, overlap with XPCS?
- Quick CDI by ptychography
  - Beat the beam stability by doing short scans

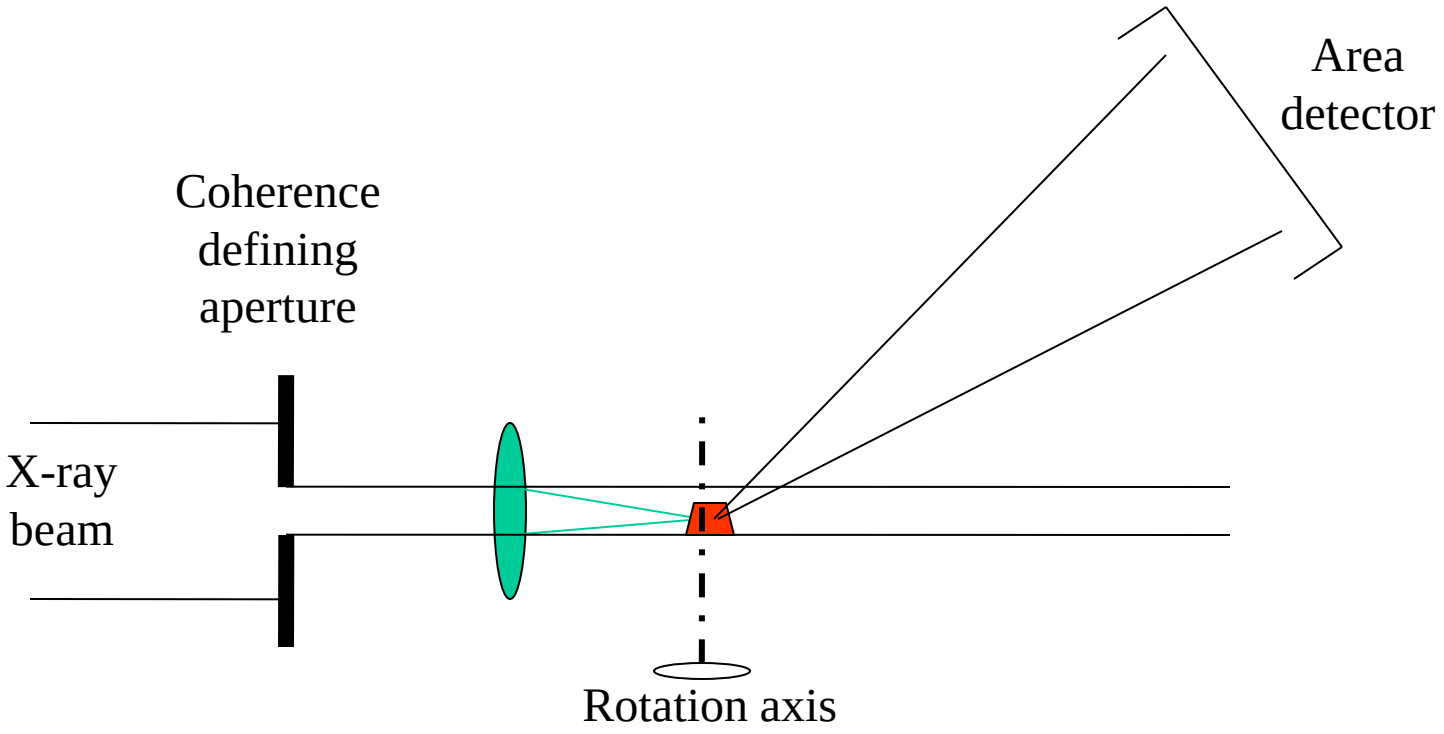
Challenges for MBA lattice

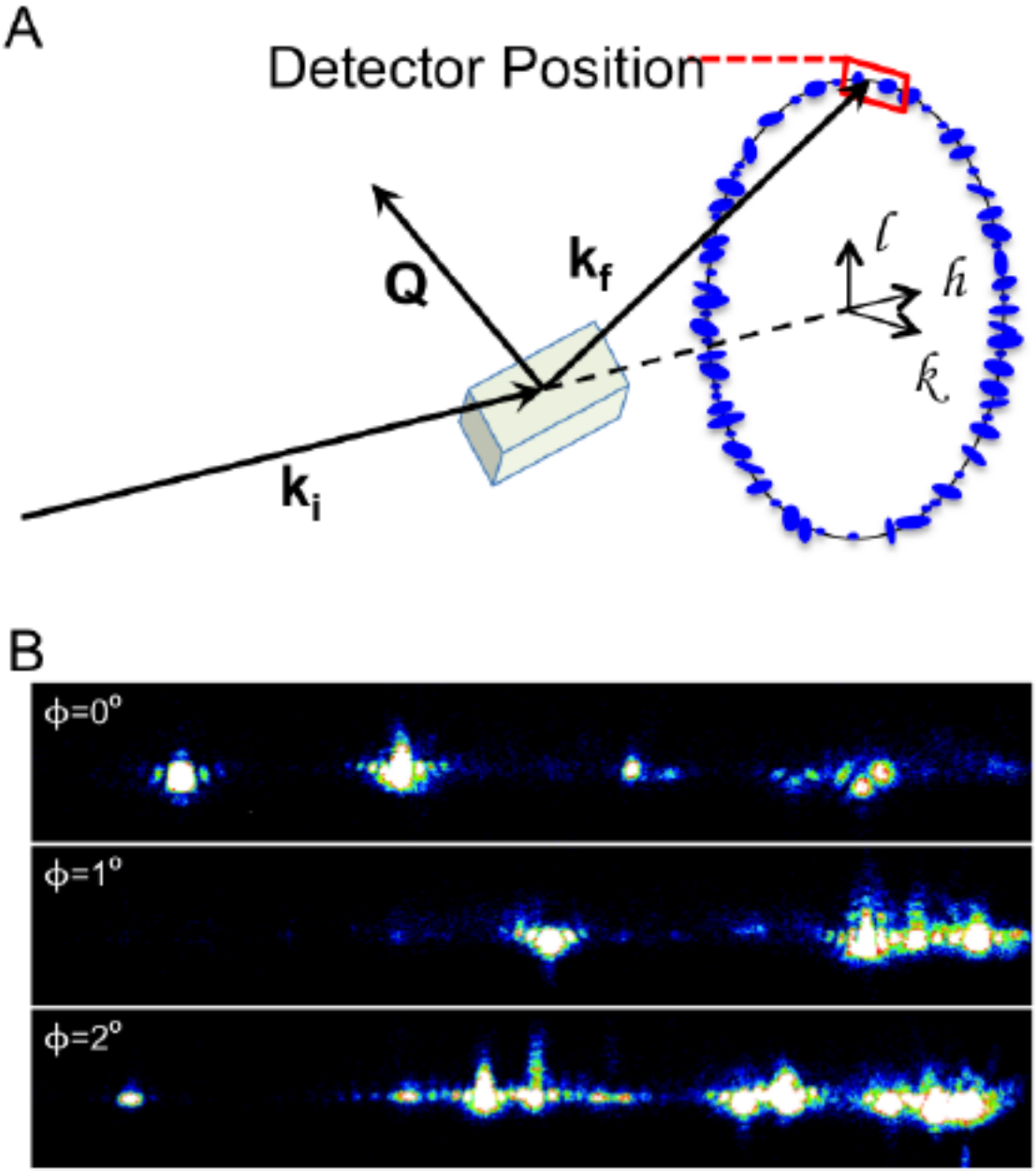
- New stability measures
- New optics, eg KB mirrors
- Brighter undulators
- Longer hutches (not long beamlines)
- Counting detectors
- Smaller detector pixels
- Real-time data analysis

New CDI methods with MBA lattice

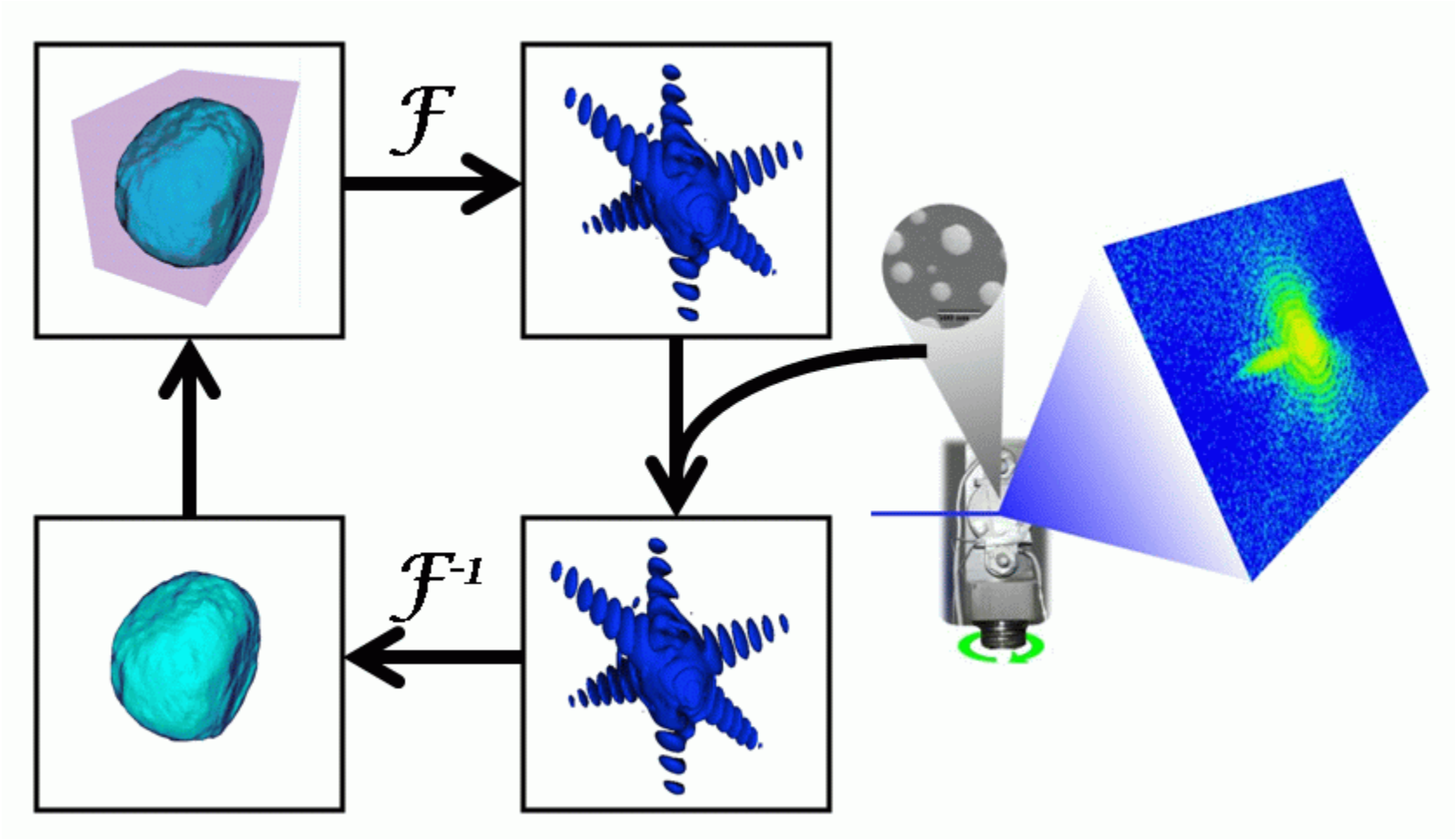
- Ptychography schemes
- Heterodyne (modulation schemes)
- Polarized beams
- Tools for higher energy beams
- In situ environments

Lensless X-ray Microscope, 2003




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

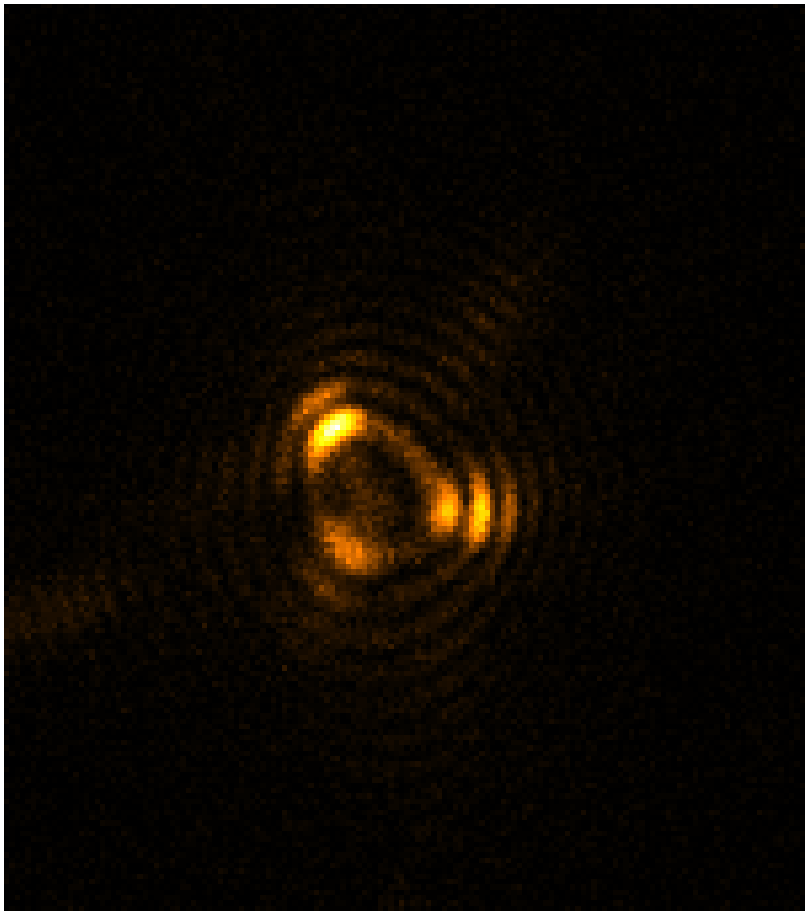
Generic "Error Reduction" method

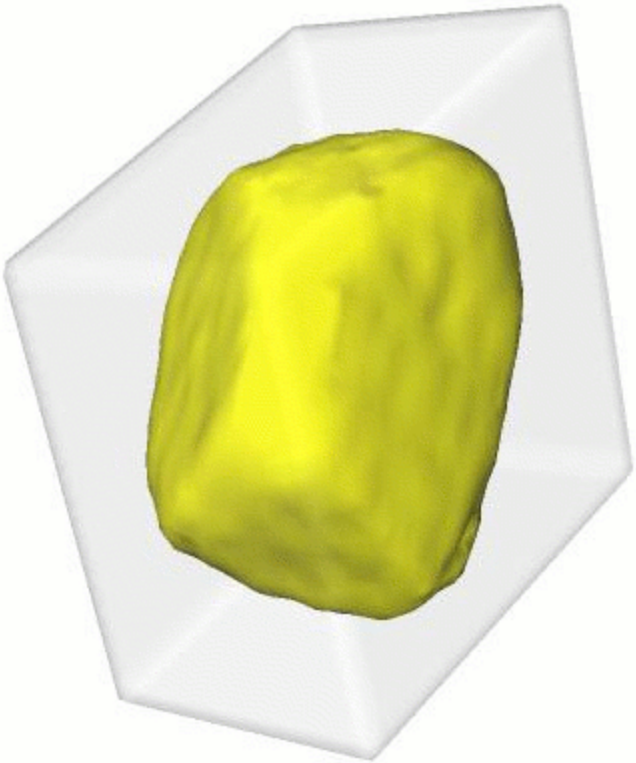


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

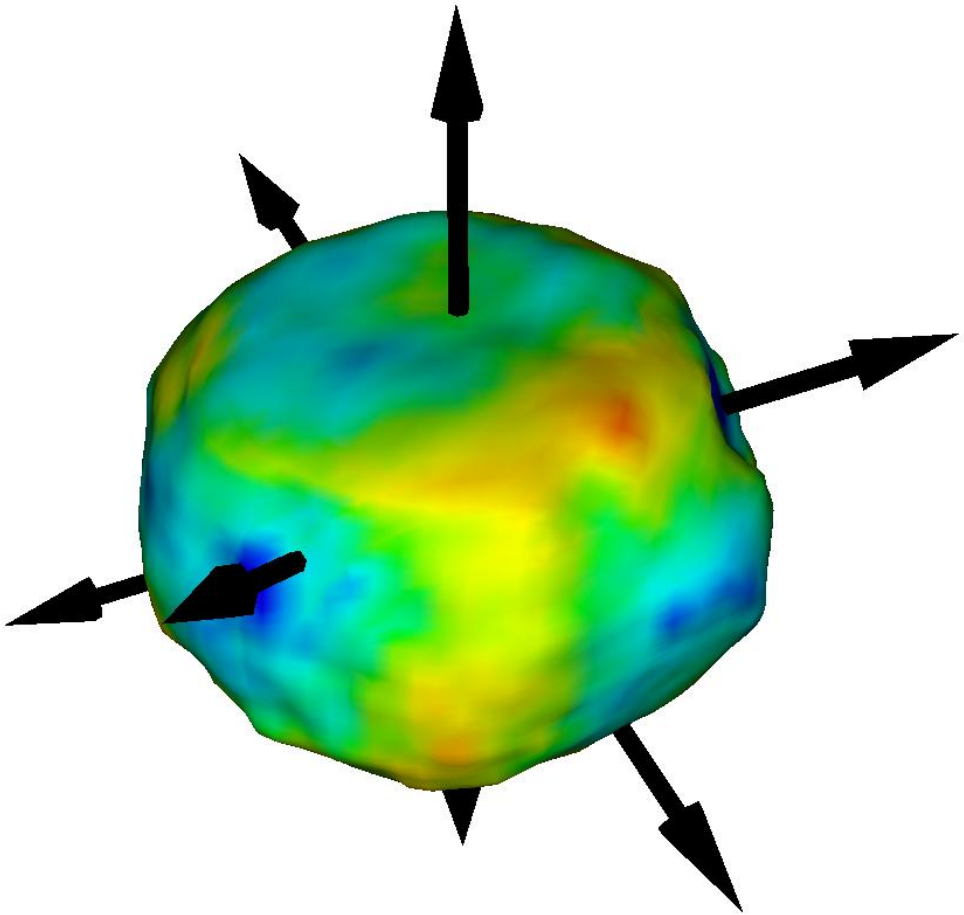
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



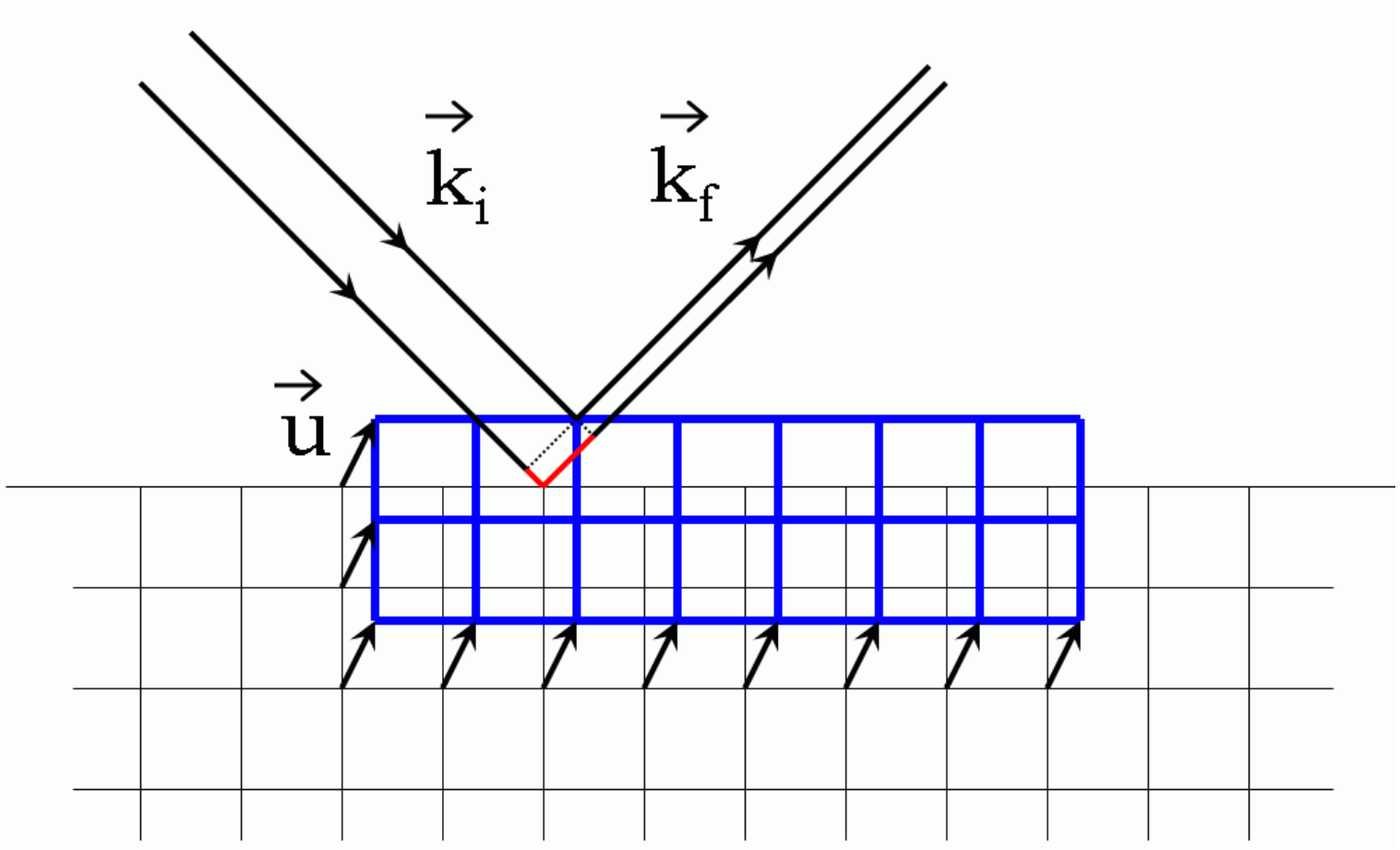


Phase isosurface of residual strain



Sensitivity to strain

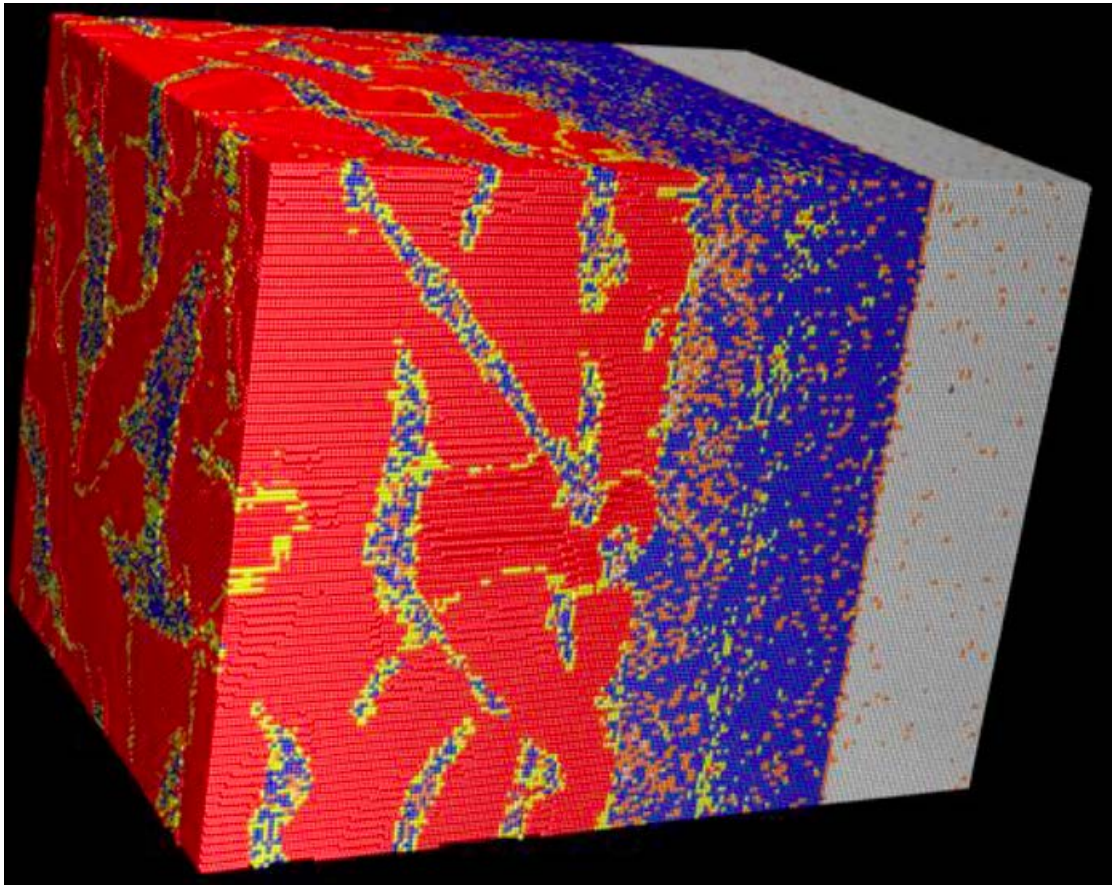
$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$



MD simulation of Shock Wave

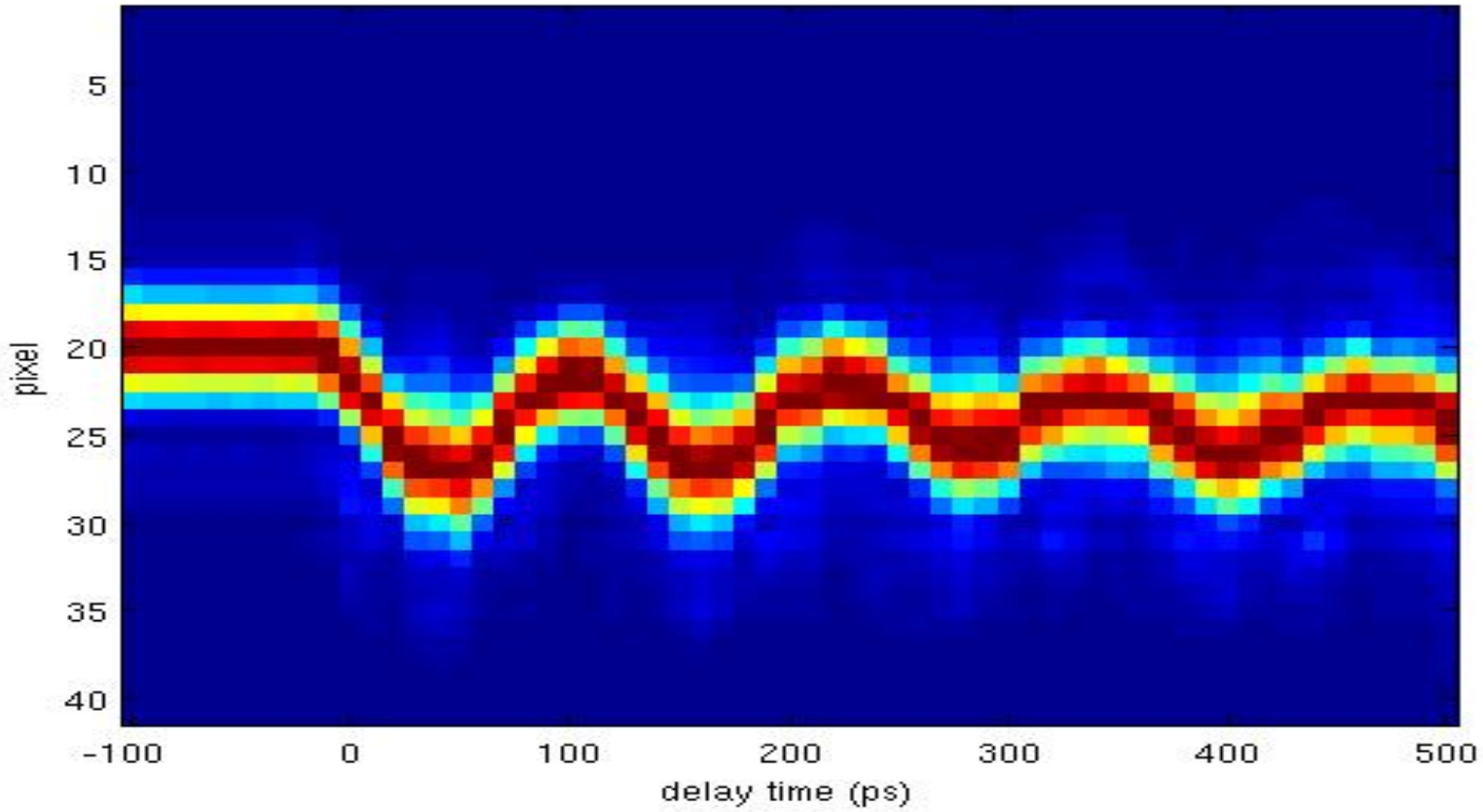
Damage in Fe along (001) direction

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



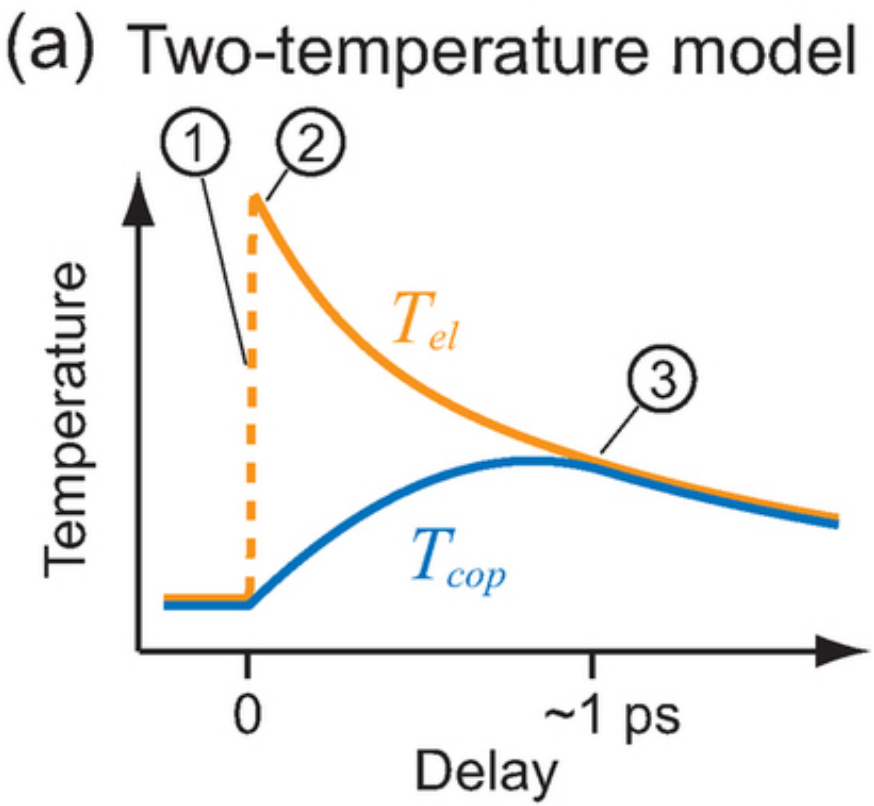
Pump-probe at LCLS (XPP)

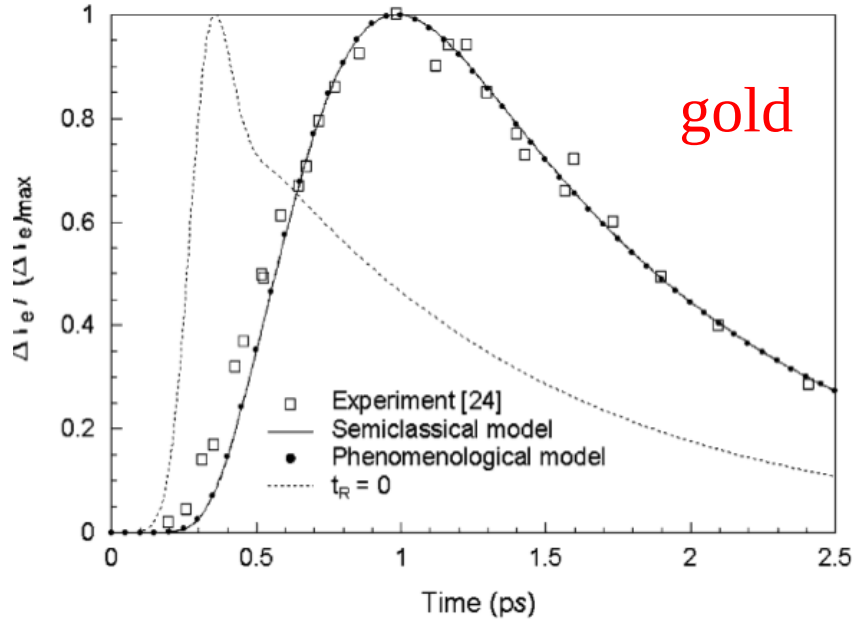
Jesse Clark, Gang Xiong, Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz, Garth Williams, Brian Abbey, Andy Higginbotham, Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt



“Two-temperature” model

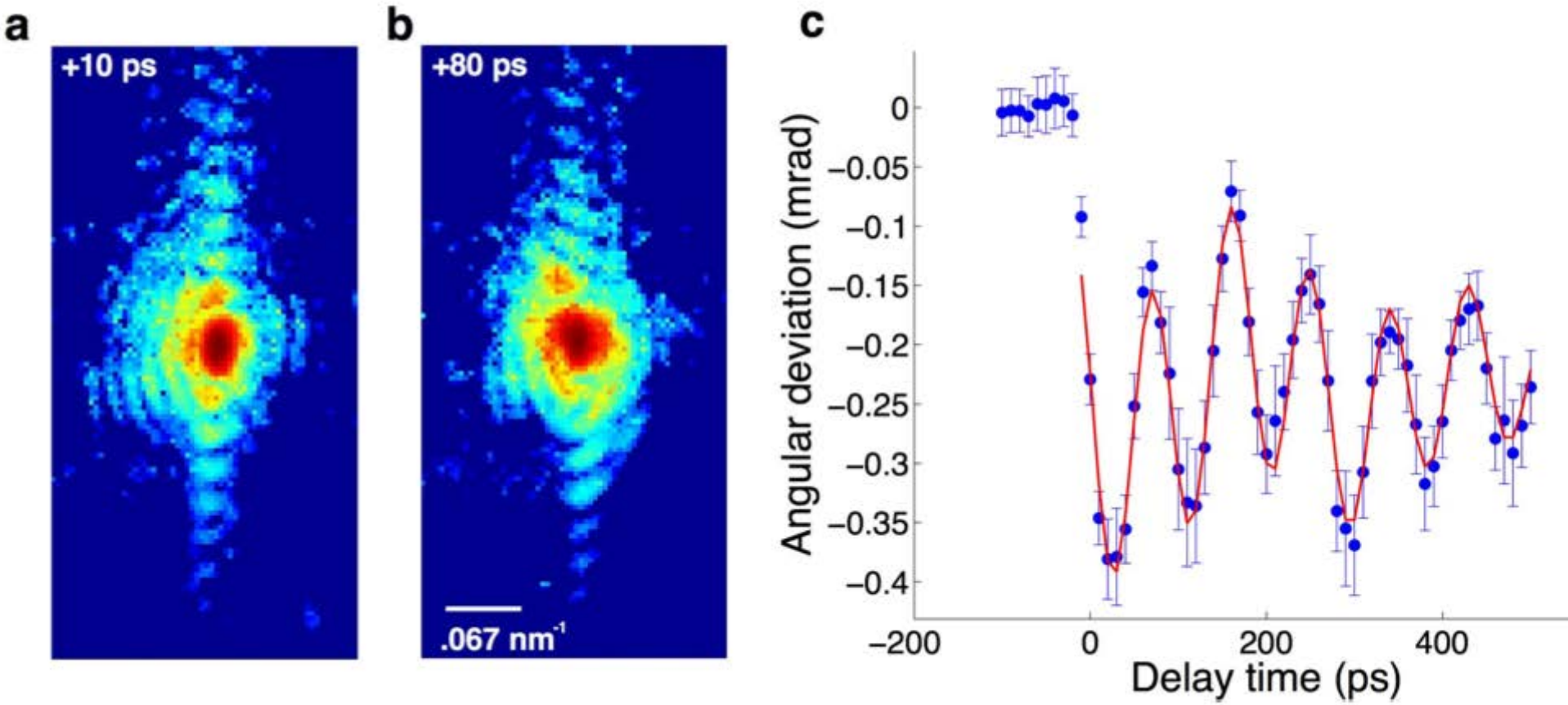
Y. Ishida et al, Nature Scientific Reports 1 64 (2011)
J.K. Chen et al, Int J. Heat Transfer 49 307 (2006)





ig. 2. Comparison of the change in electron temperature at 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

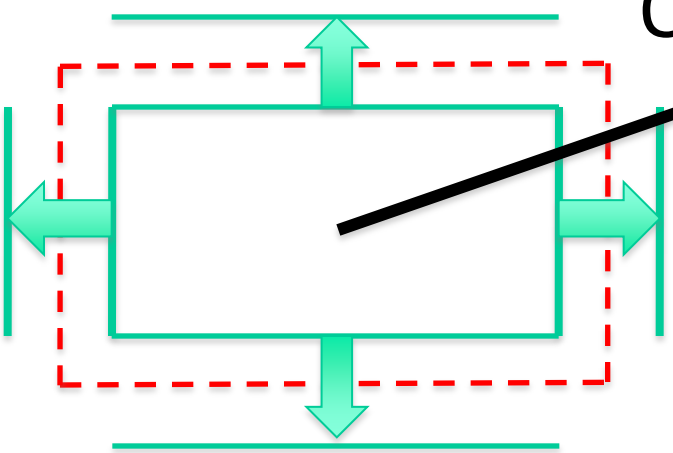


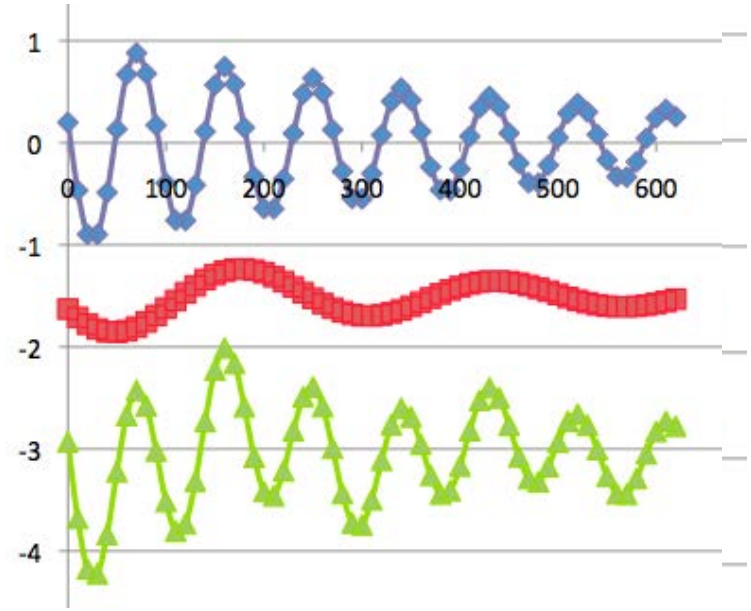
Two Normal Modes of Vibration

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

111 facet

Q= 11-1





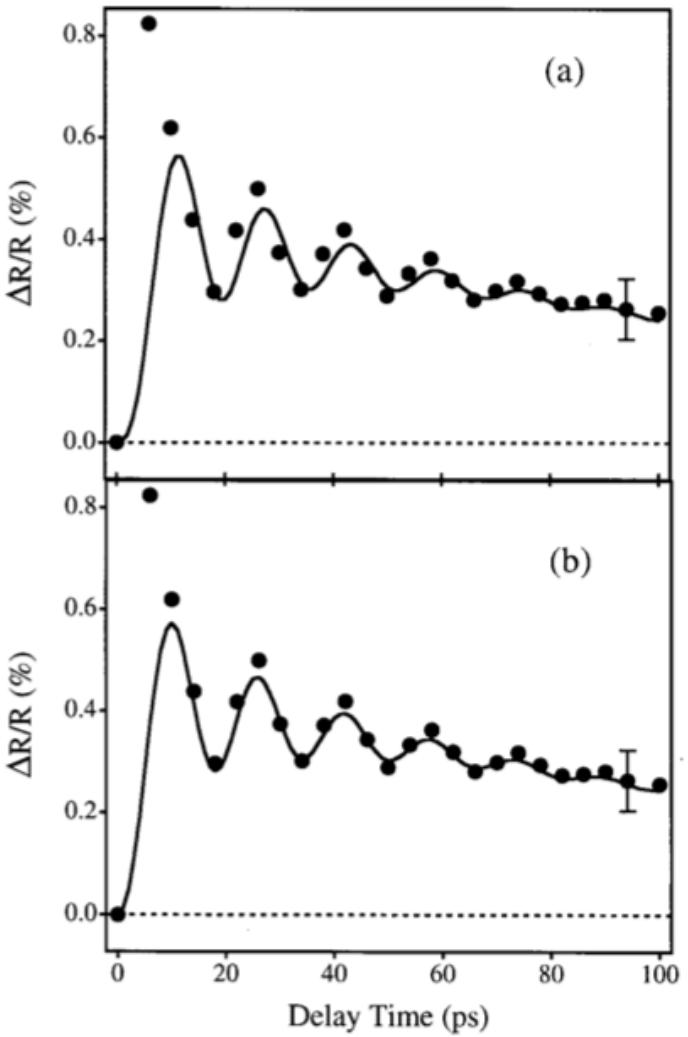
T_1 = 90ps h_1 = 145nm c_S = 3240 m/s

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)

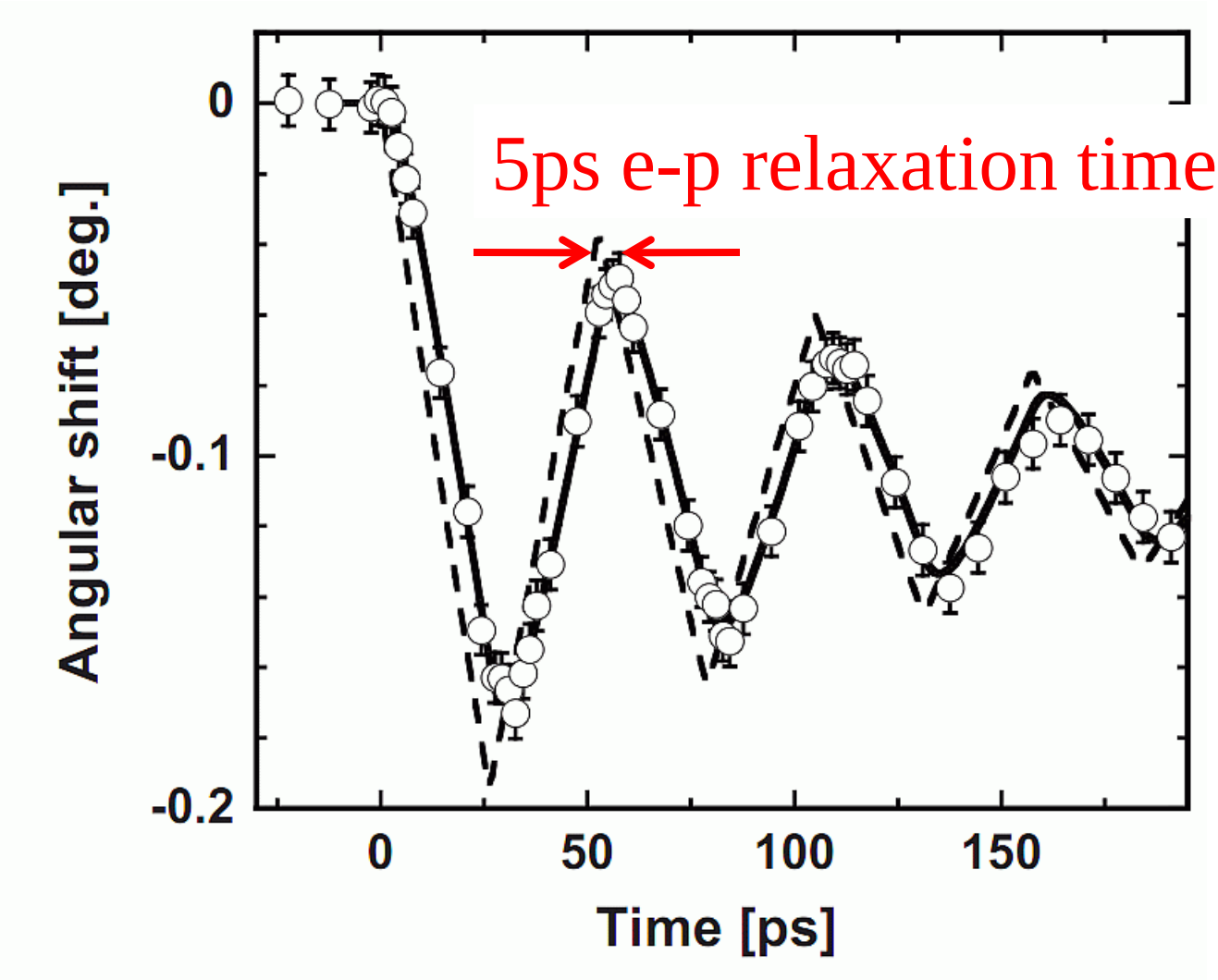


(a) Simple normal mode analysis with impulse heating.

(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)

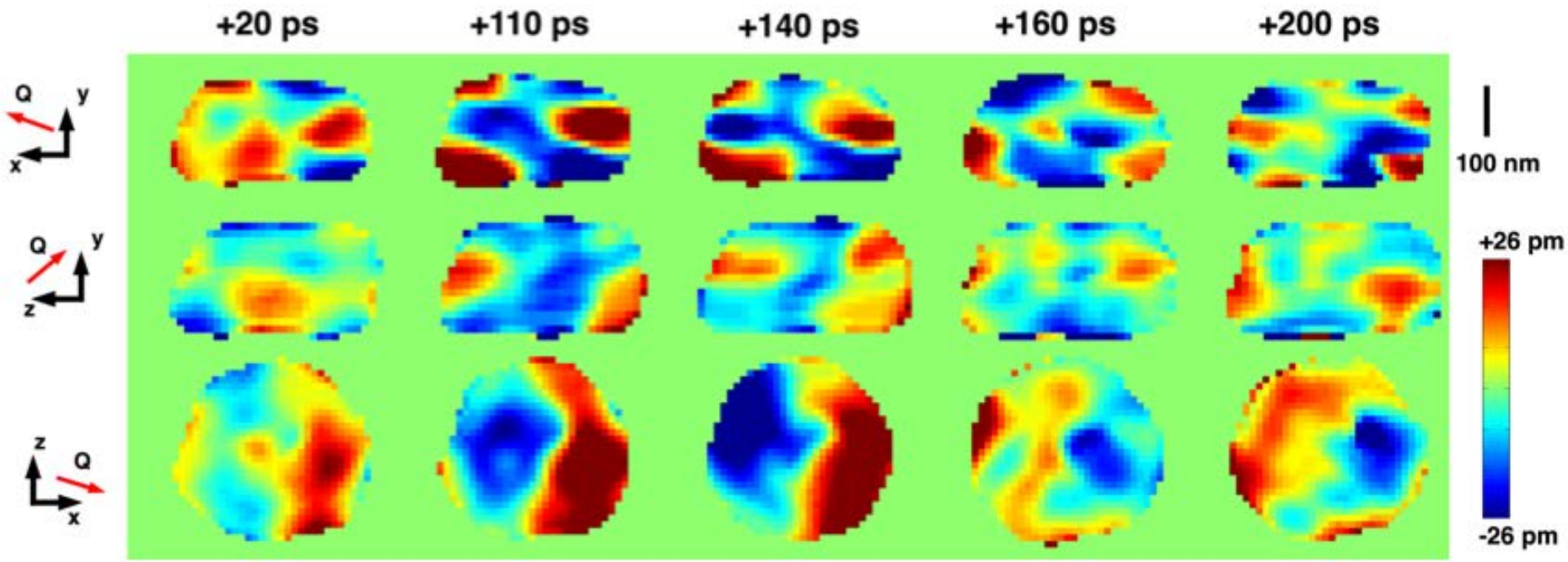


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

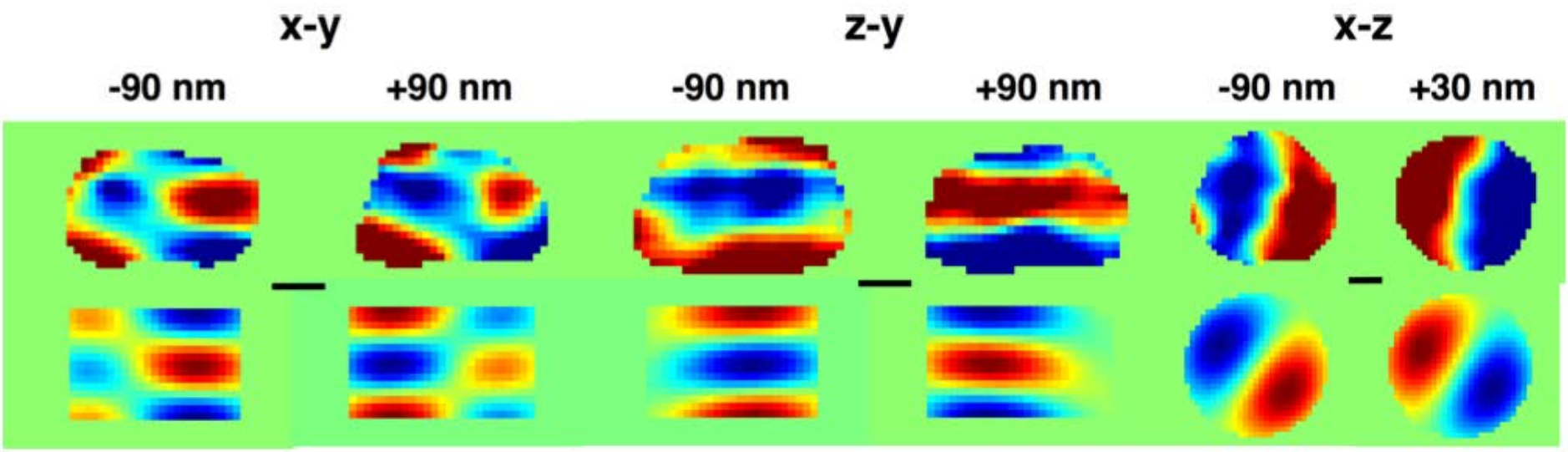
1000 frames averaged at each point of rocking curve

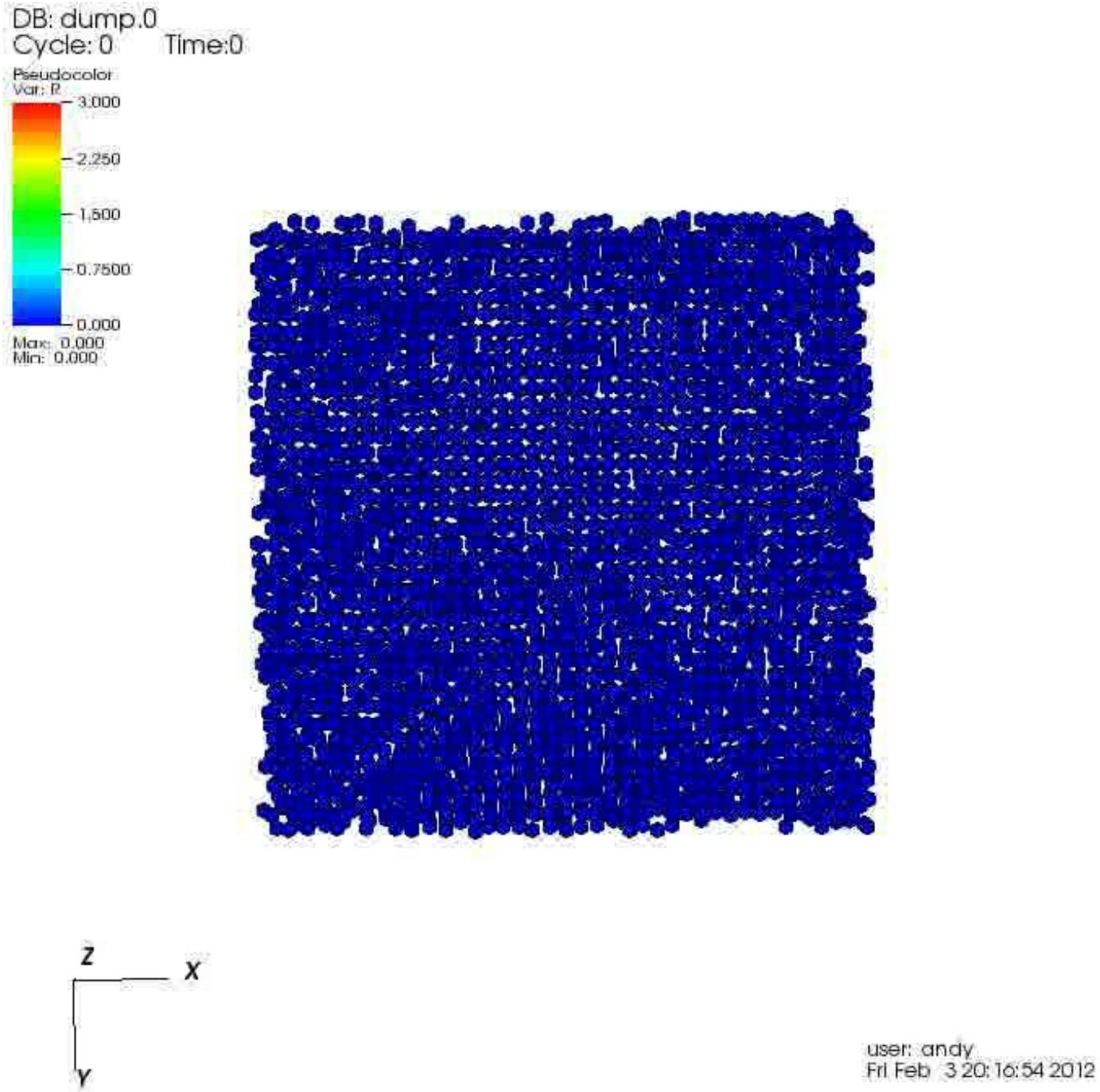
Jesse Clark et al Science (2013)



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
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Var: R
3.000
2.250
1.500
0.7500
0.000
Max: 0.000
Min: 0.000
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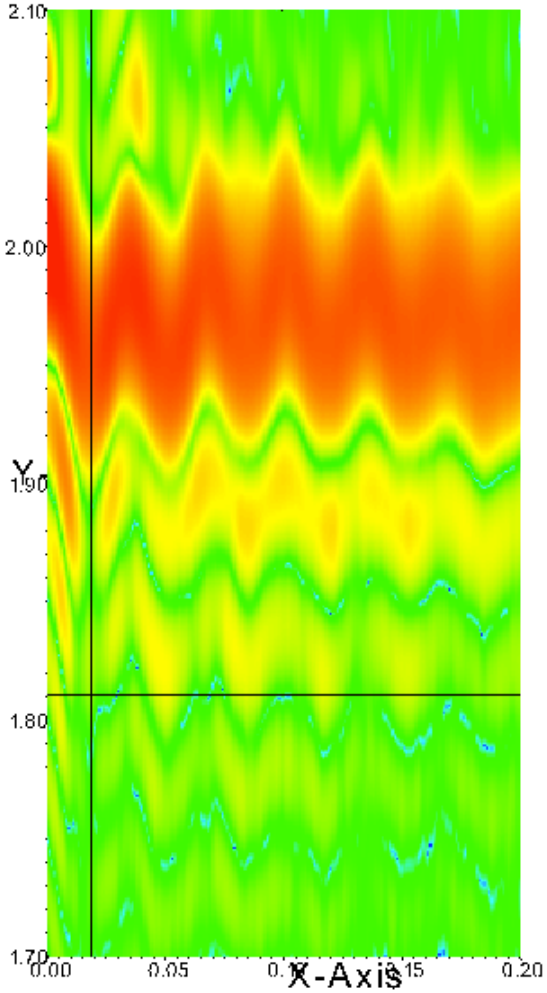
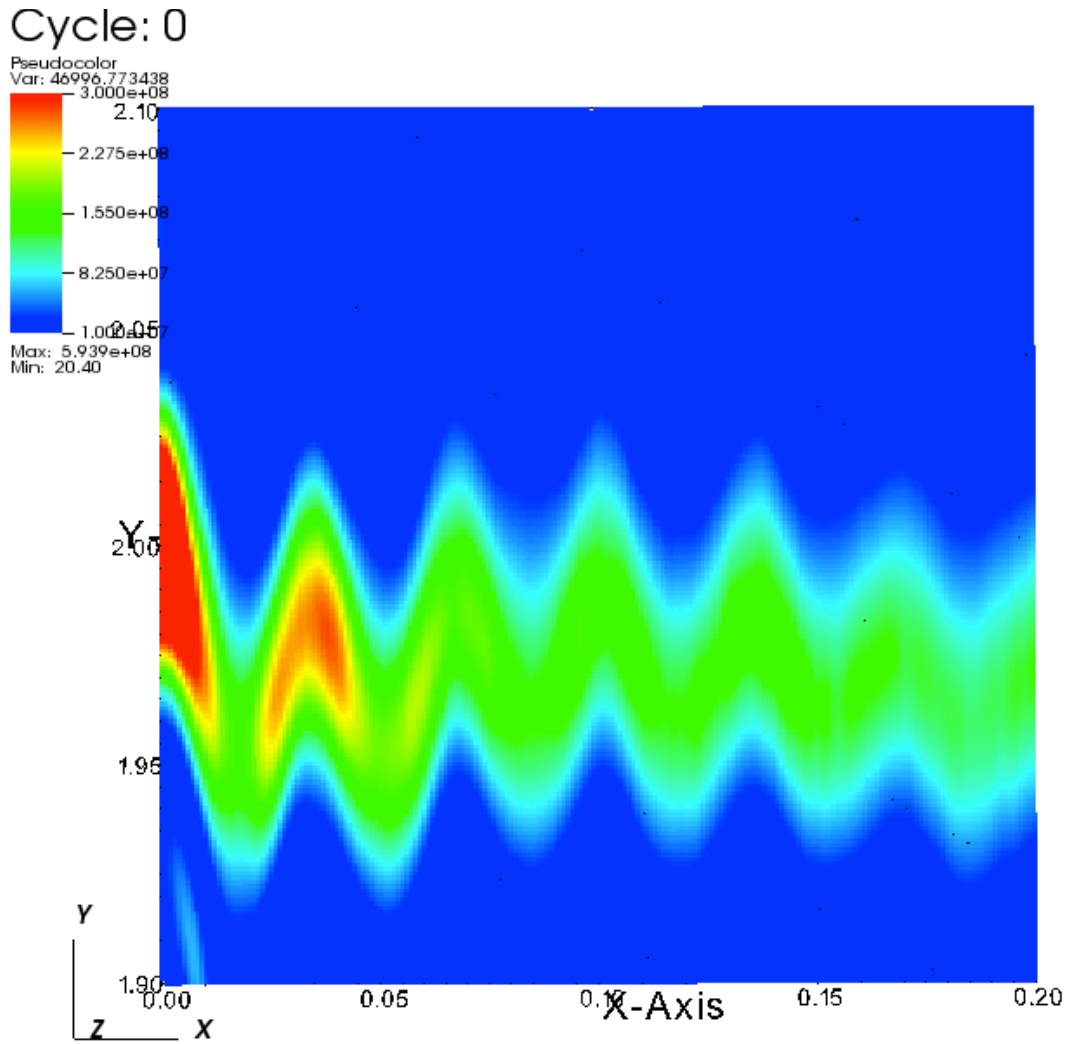
Y
user: andy
Fri Feb 3 20:16:54 2012

MD Simulation (LAMMPS)

Andy Higginbotham and Loren Beitra



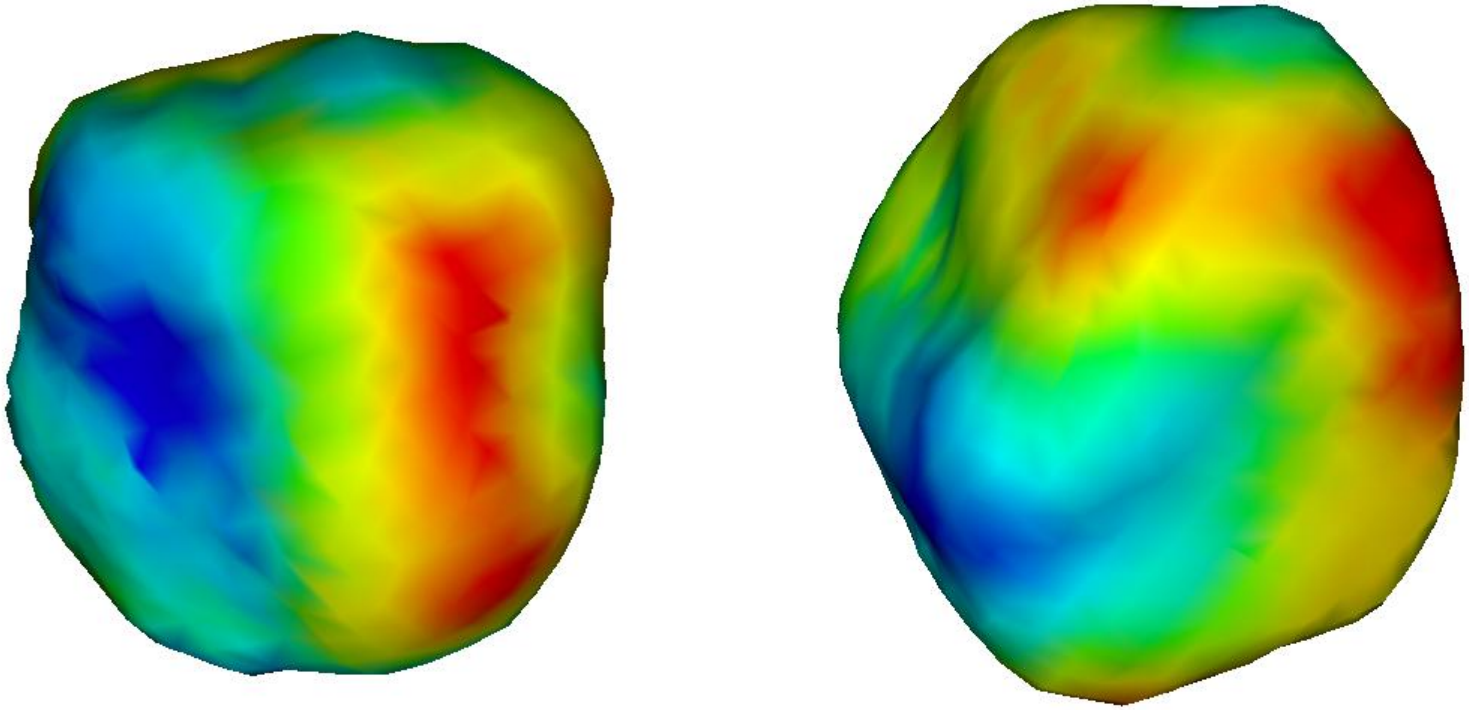


Materials Science using 1ps beam

- 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

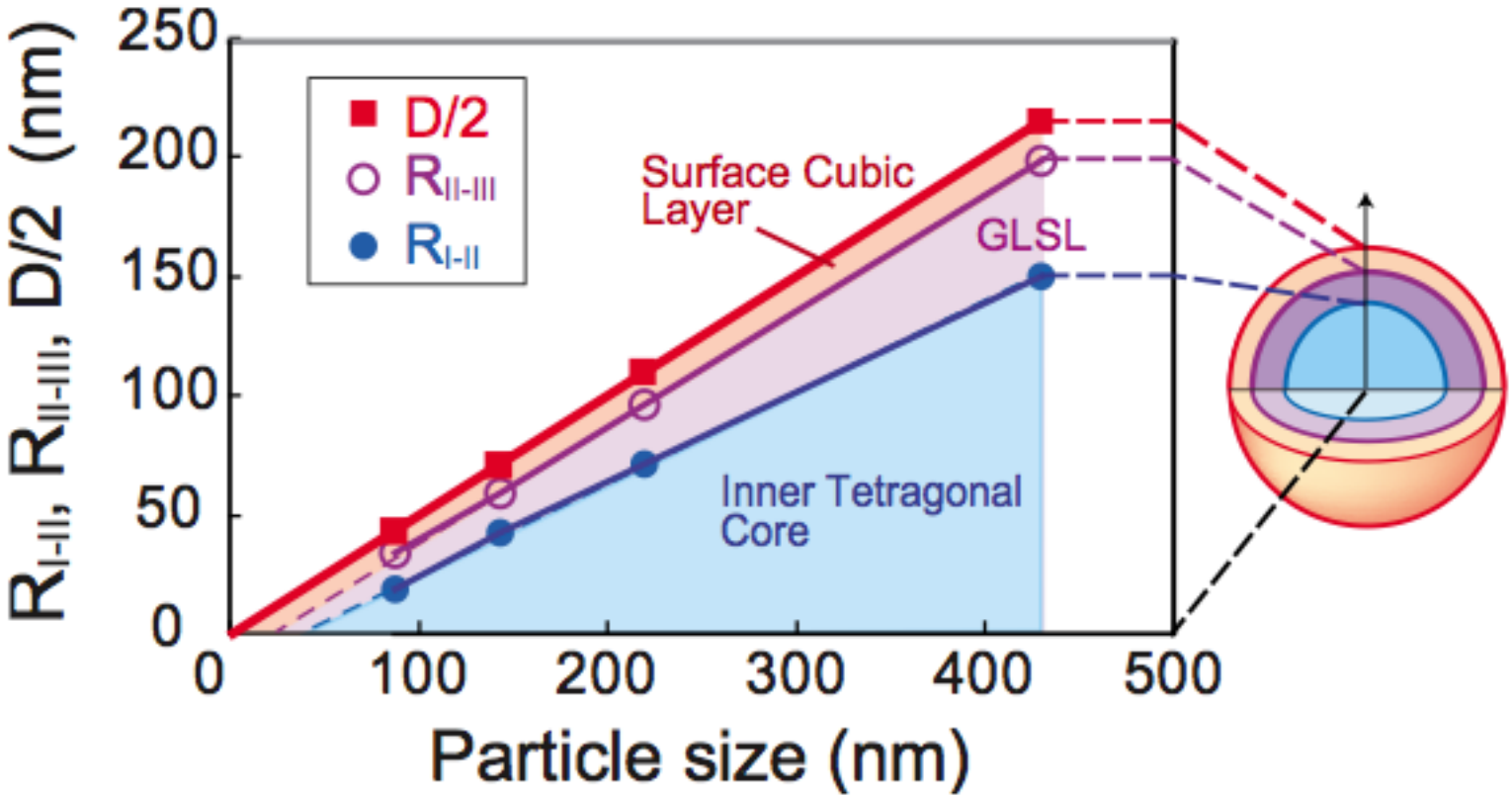
Phase isosurface of residual strain

200nm Barium Titanate (BTO) crystals



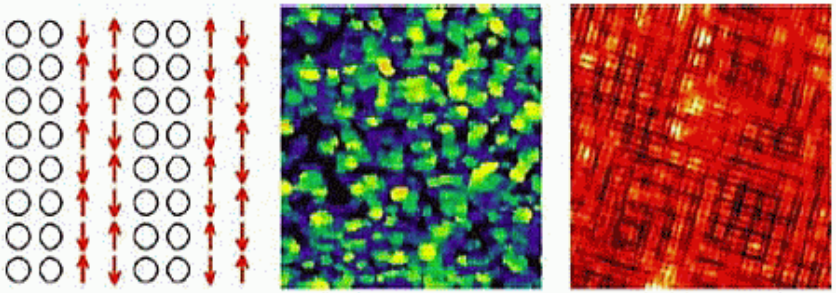
Core-shell structure of BTO

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



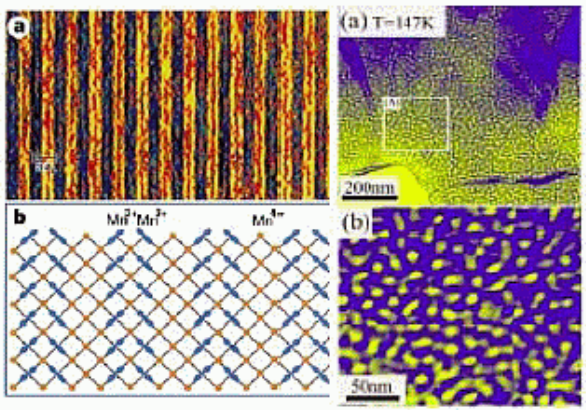
Stripes, checkerboards and zig-zags

High-Tc cuprates



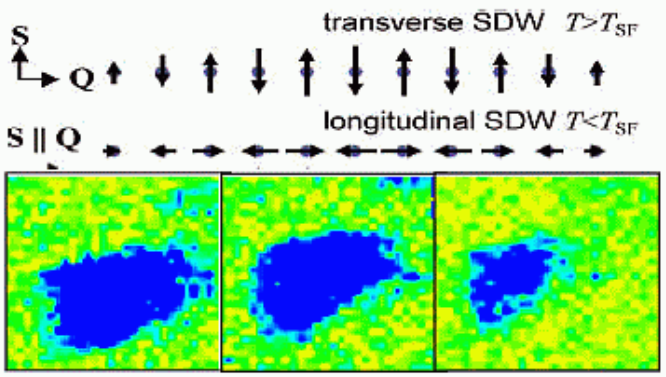
E. Dagotto, T. M. Rice, *Science* **271**, 618 (1996).
T. Hanaguri et al., *Nature* **430**, 1001 (2004).

CMR manganites

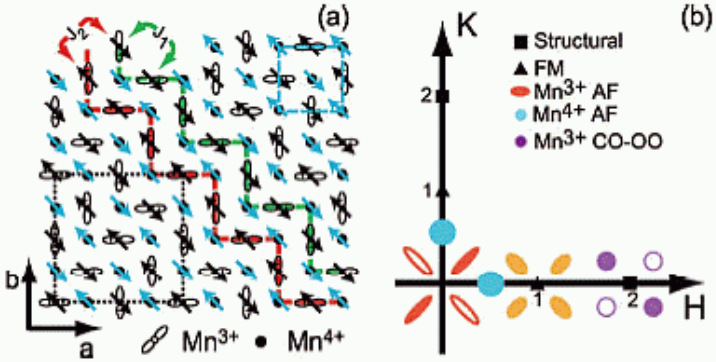


S. Mori et al., *Nature* **392**, 473 (1998)
M. Uehara et al., *Nature* **399**, 560 (1999)

AFM chromium



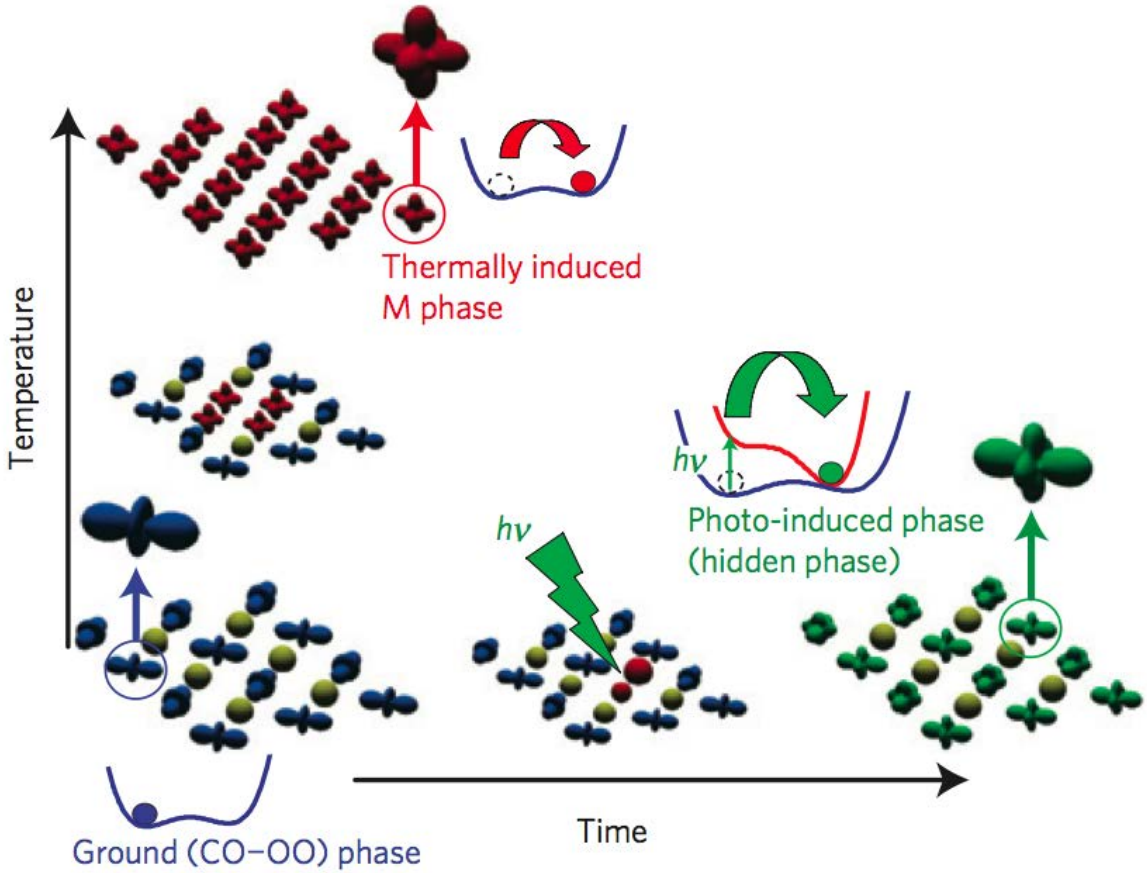
P. G. Evans et al., *Science* (2002)

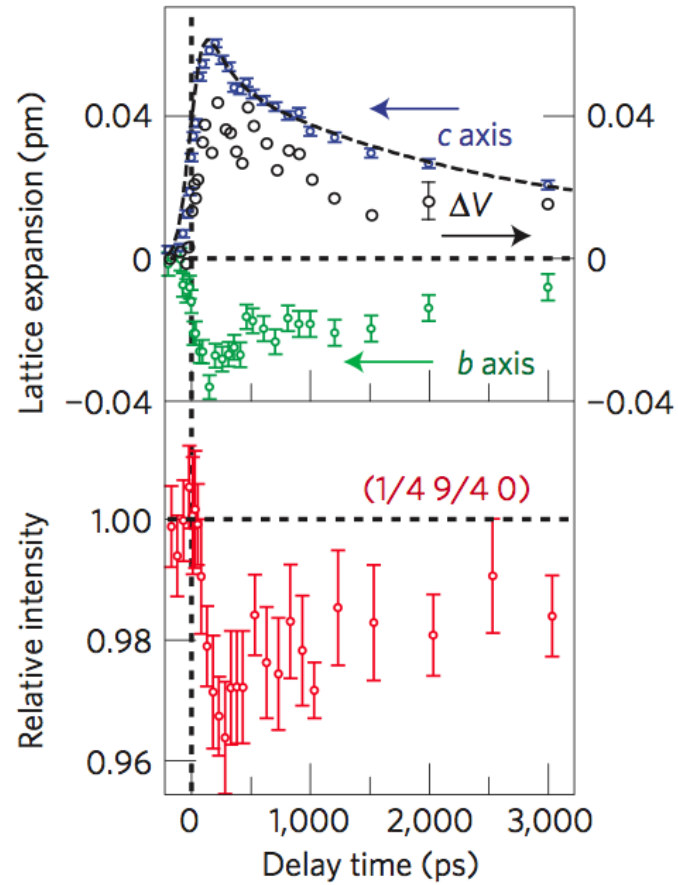


Transient "Hidden" Phase in Manganite

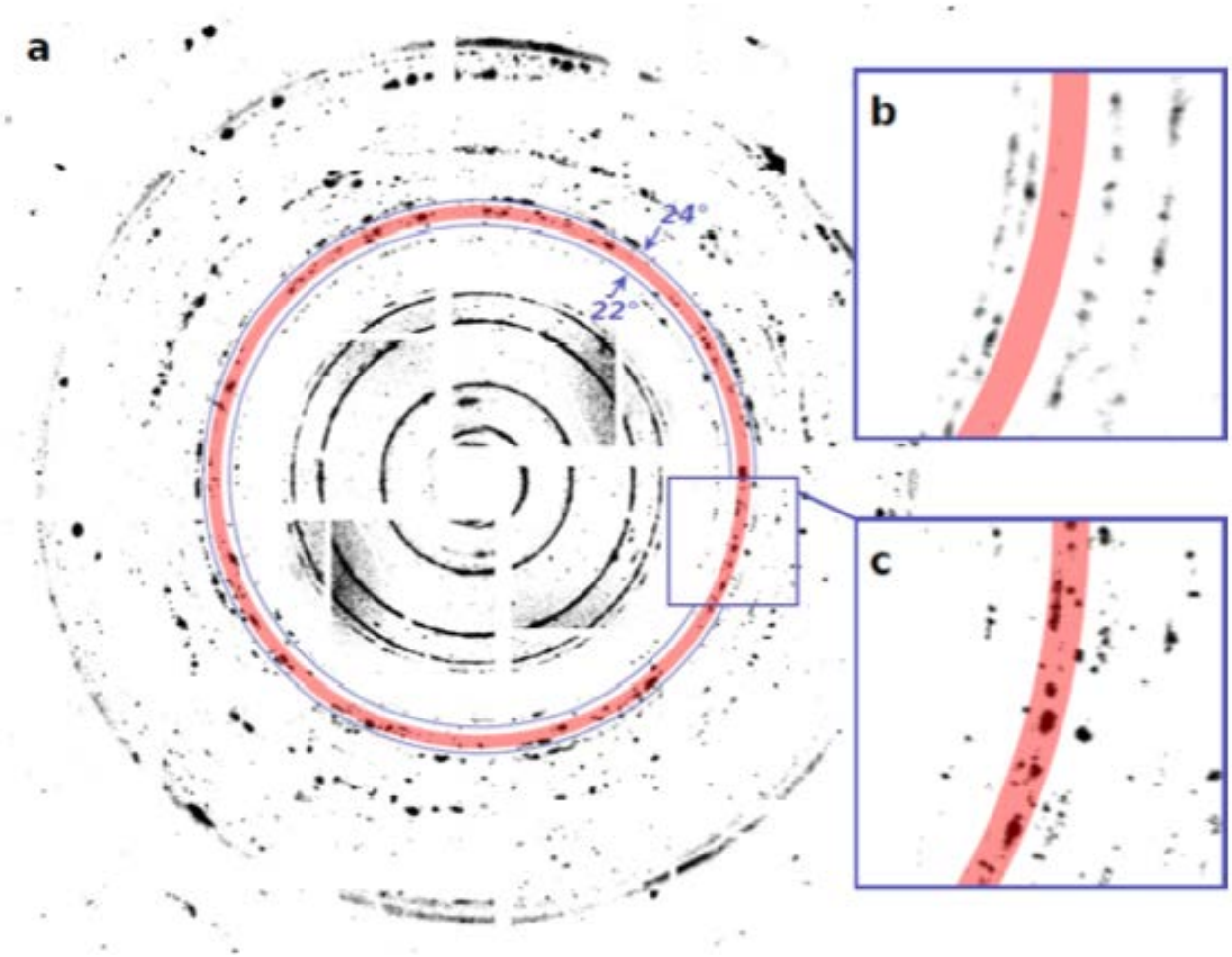
Hirohiko Ichikawa et al, Nature Materials **10** 101 (2011)

$Nd_{0.5}Sr_{0.5}MnO_3$ (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 exploration in time domain?