

Ultrafast 3D Imaging in Gold Nanoparticles

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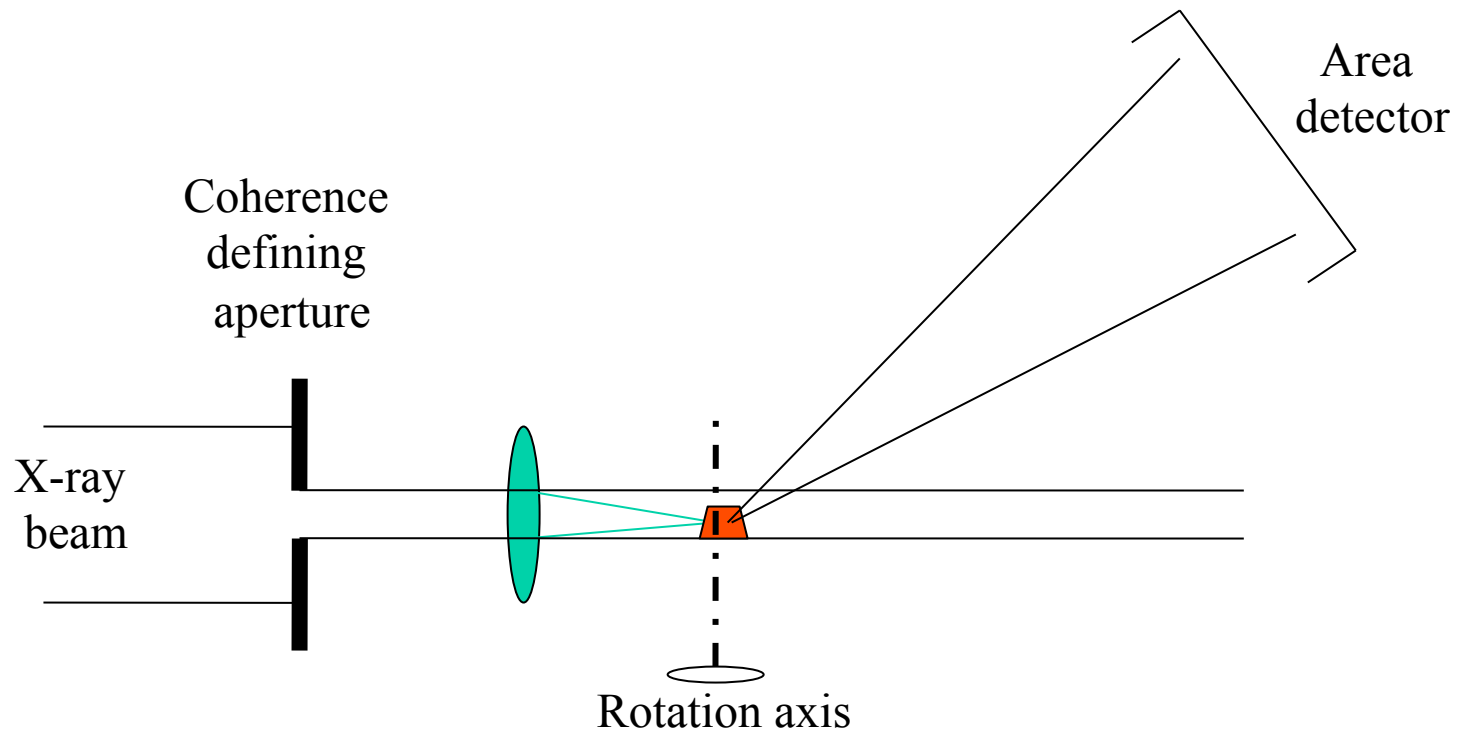
Hamburg

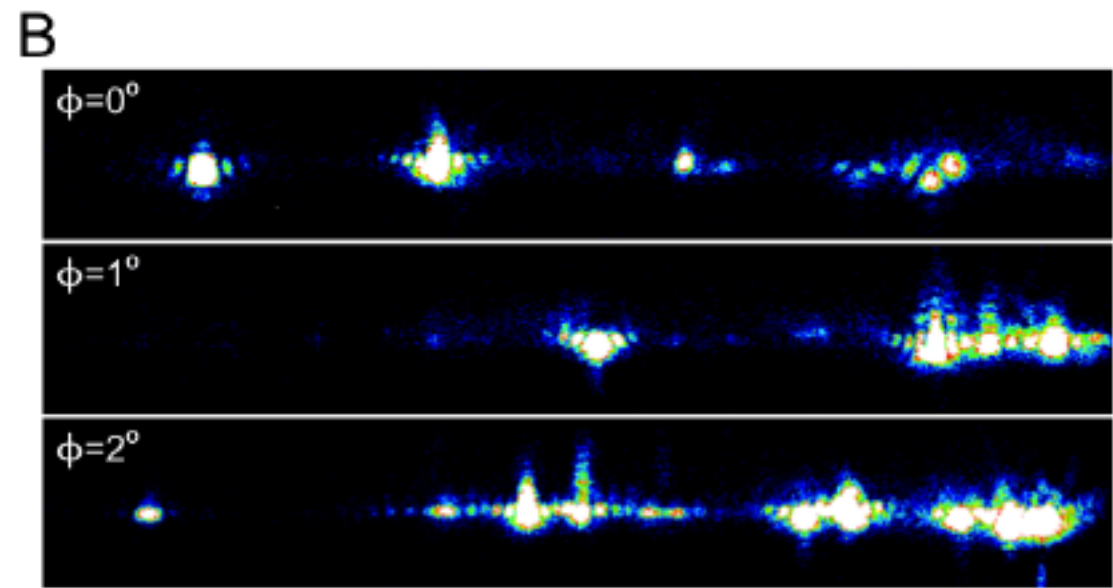
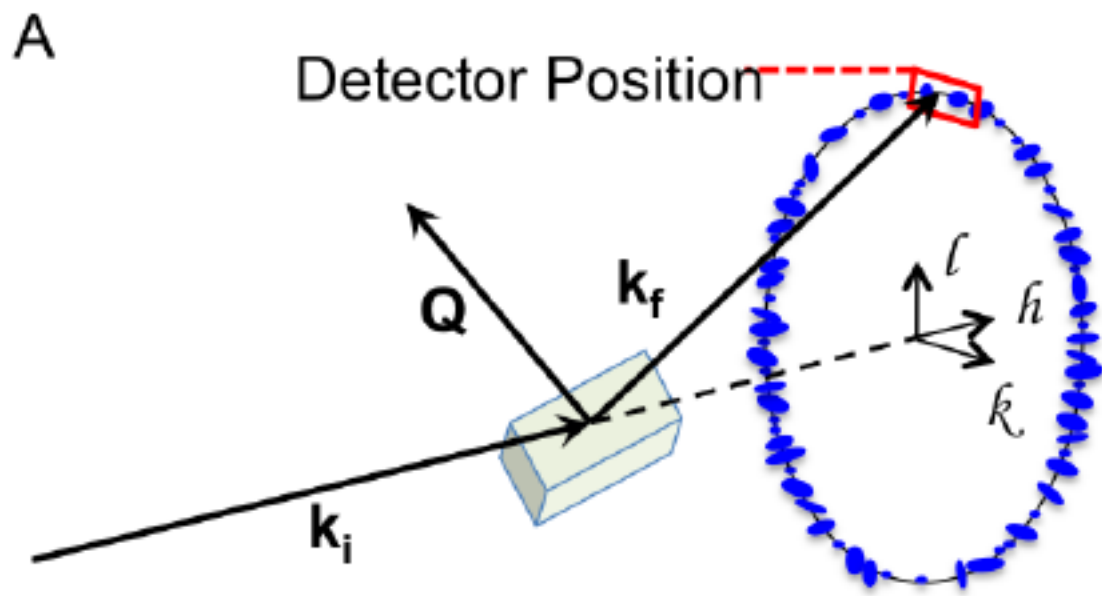
January 2014

Outline

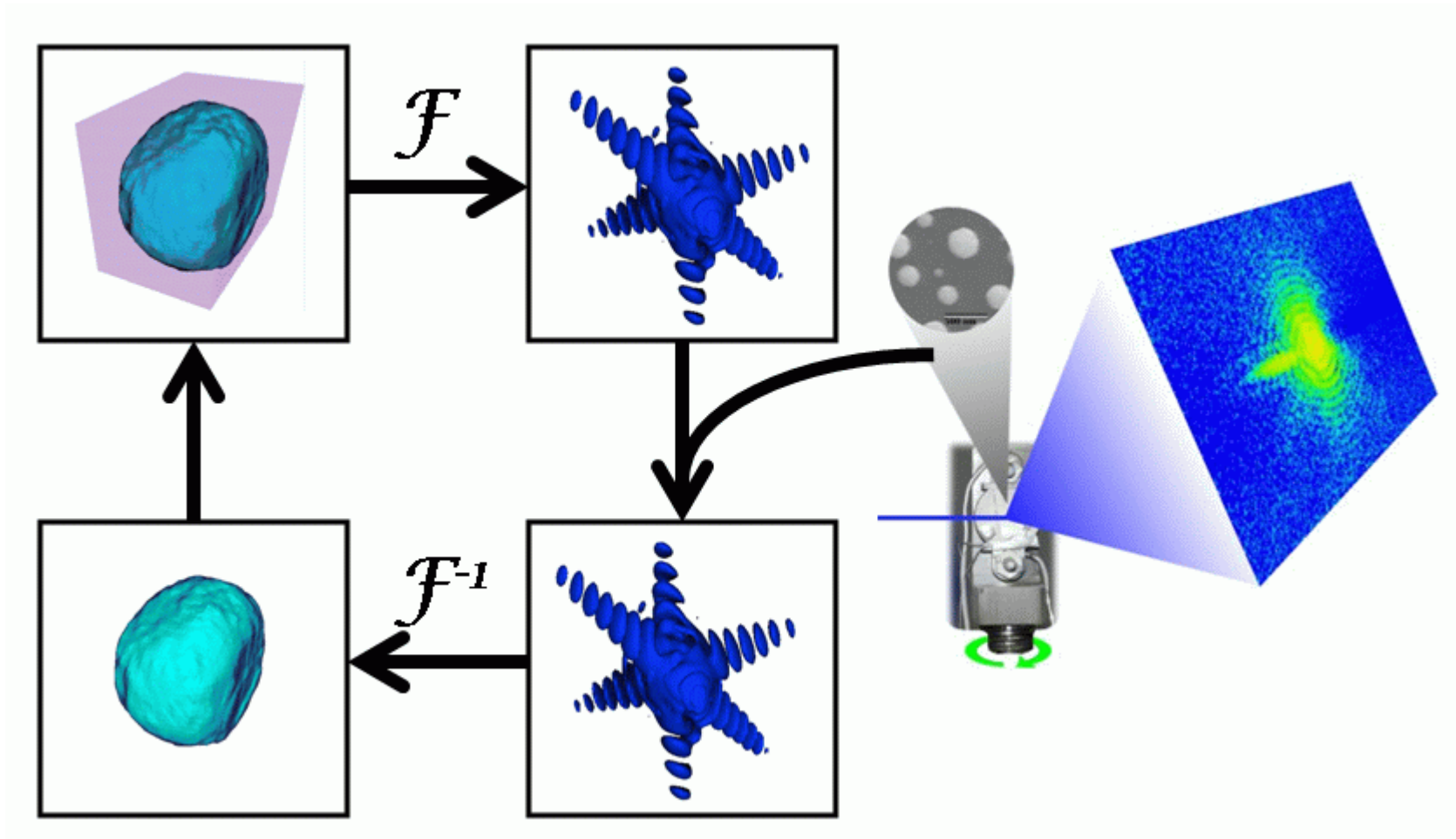
- Coherent X-ray Diffraction Imaging
- Crystal strain as complex density
- Ultrafast CDI of nanocrystals
- Materials Science by XFEL?

Lensless X-ray Microscope, 2003





Generic “Error Reduction” method

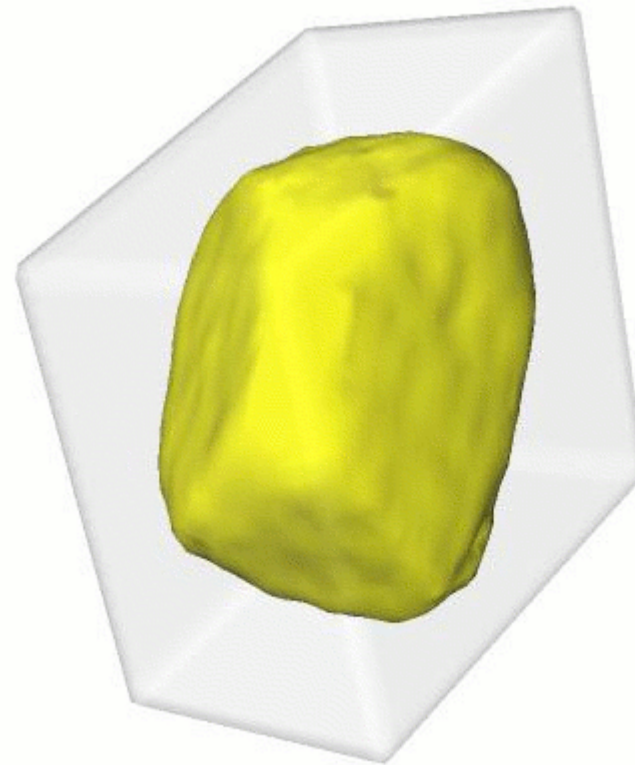
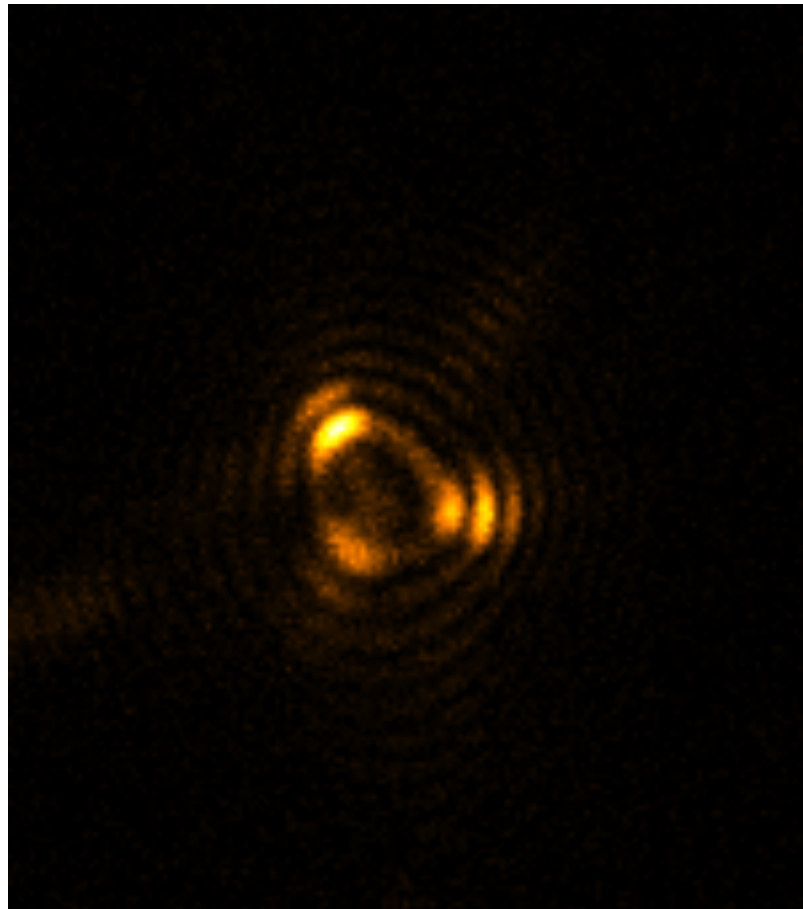


J. R. Fienup *Appl. Opt.* 21 2758 (1982)

R. W. Gerchberg and W. O. Saxton *Optik* 35 237 (1972)

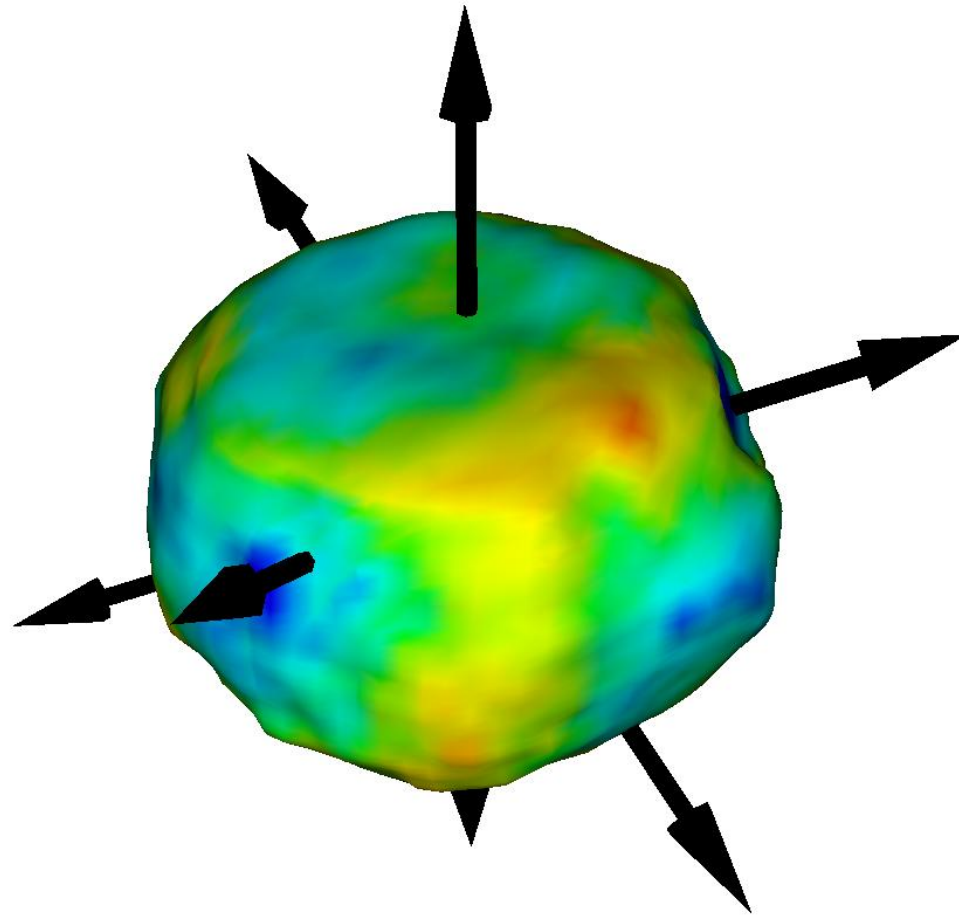
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER

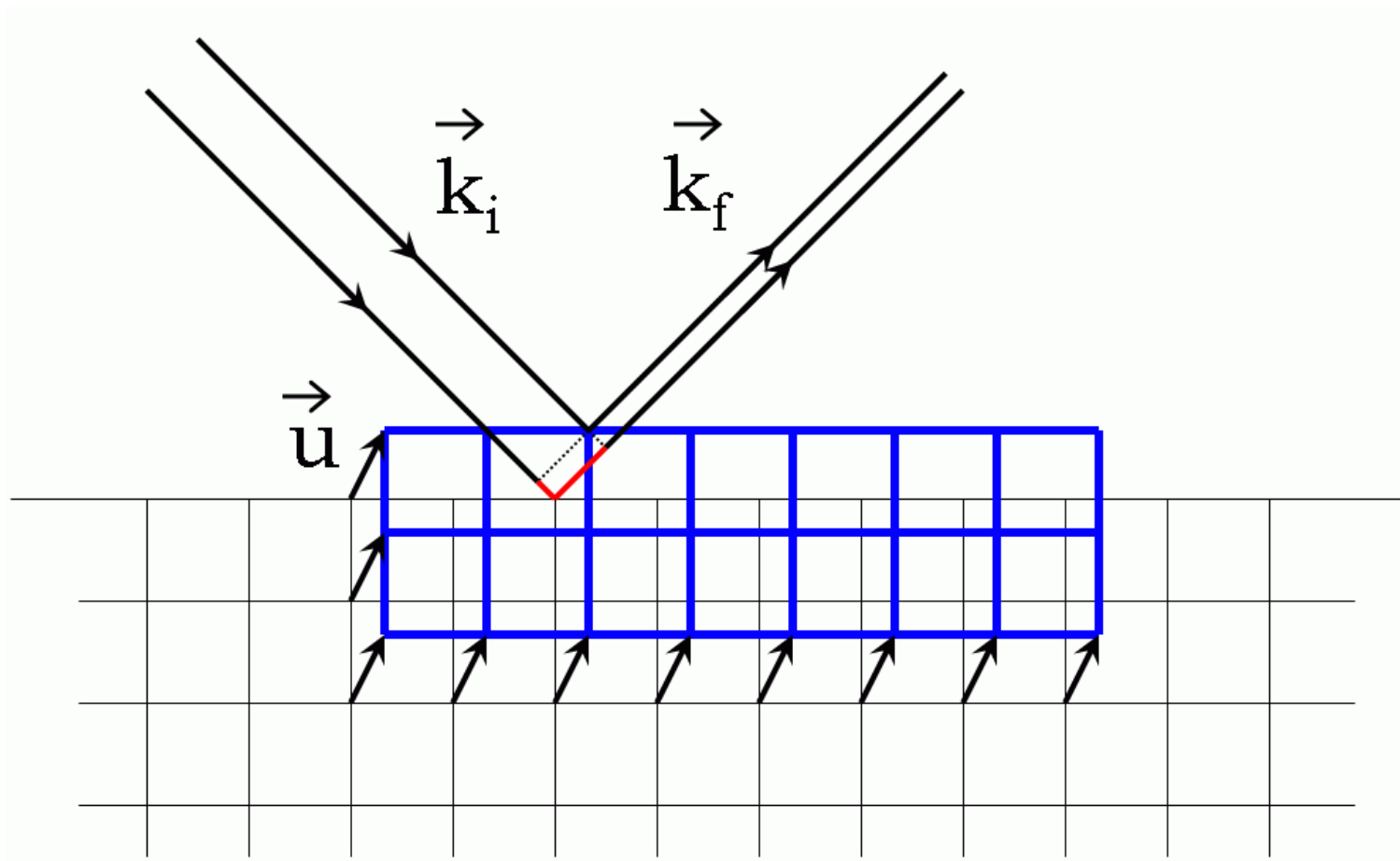


Phase isosurface of residual strain

I. K. Robinson, JPSJ 82 021012 (2013)

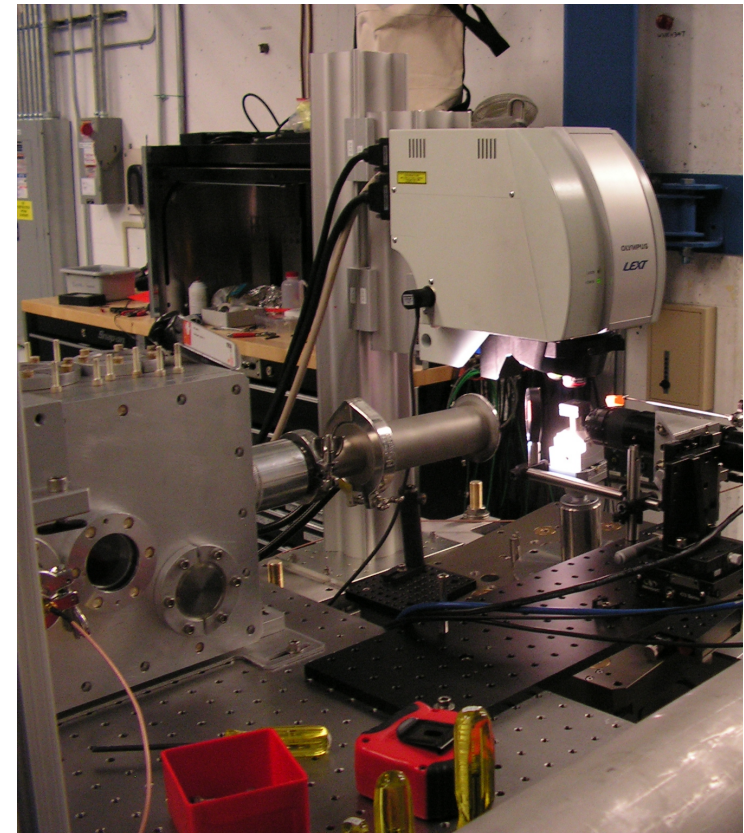
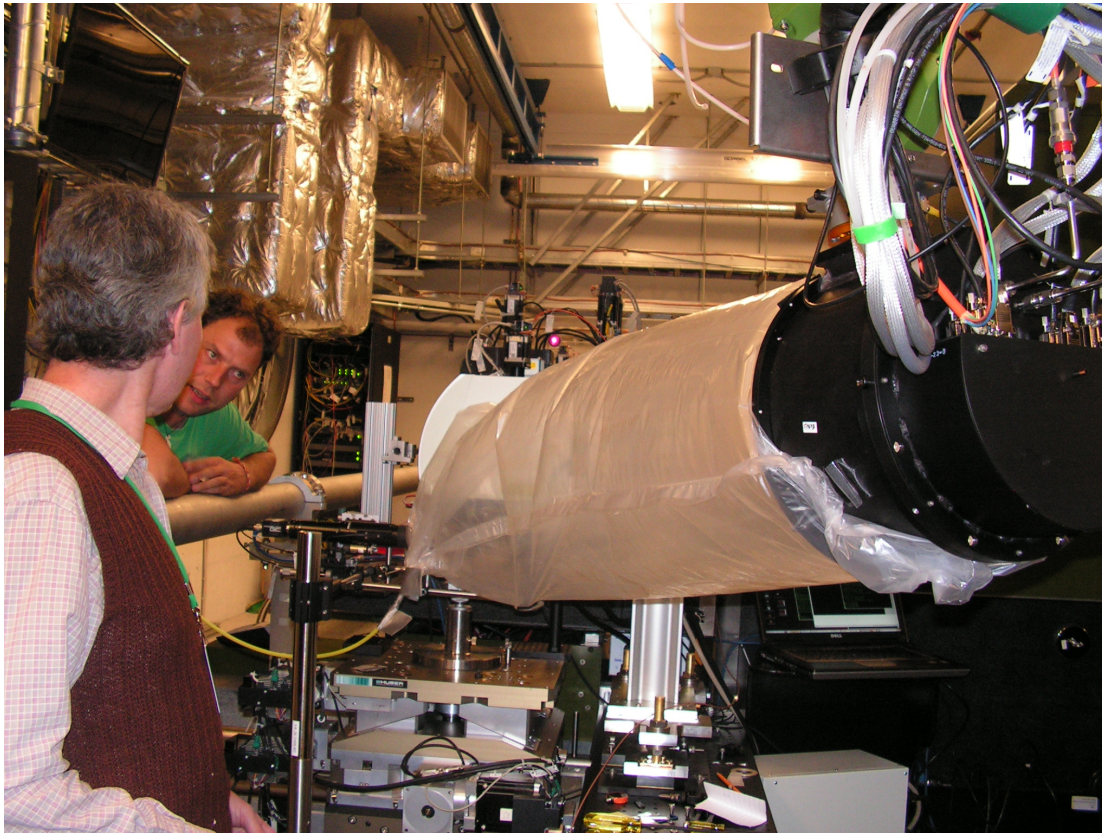


Sensitivity to strain

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


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

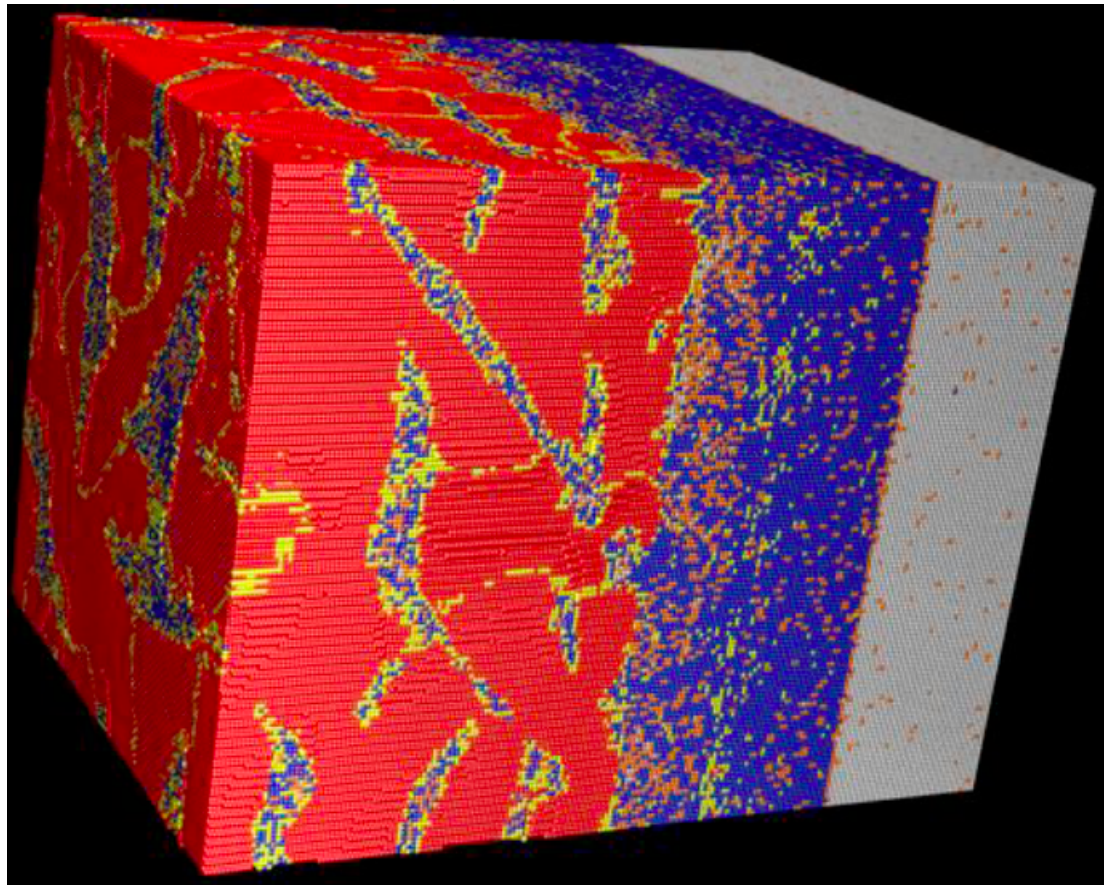


MD simulation of Shock Wave

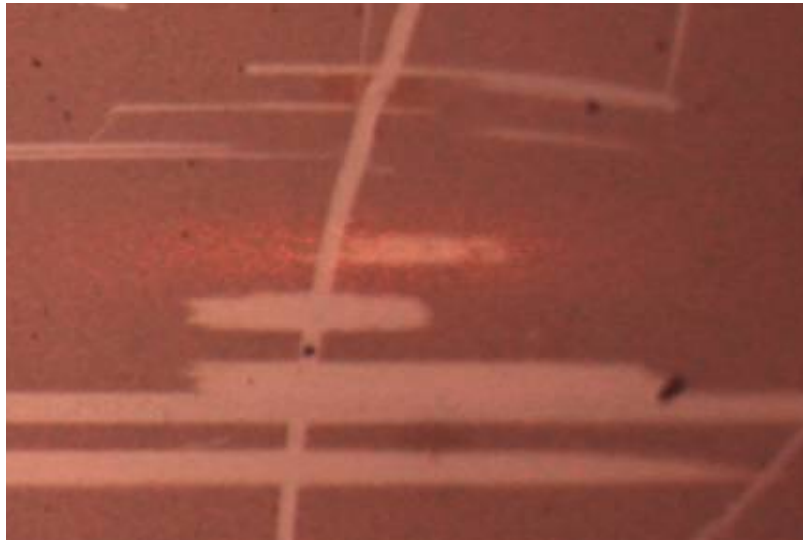
Damage in Fe along (001) direction

K Kadau, TC Germann, PS Lomdahl, and BL Holian.

Science, 296 1681 2002

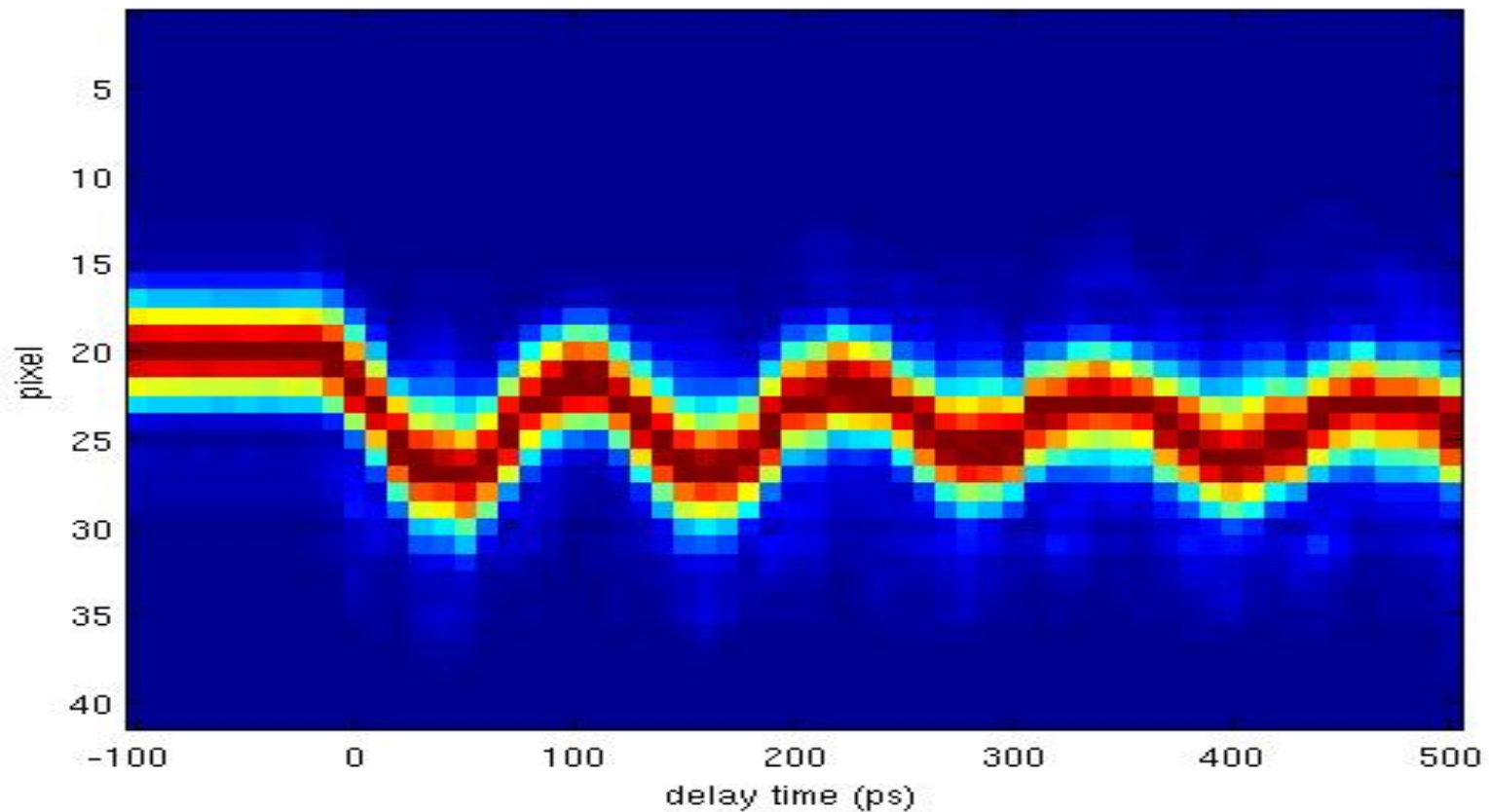


Visible and Confocal microscopy



Pump-probe at LCLS (XPP)

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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)

(a) Two-temperature model

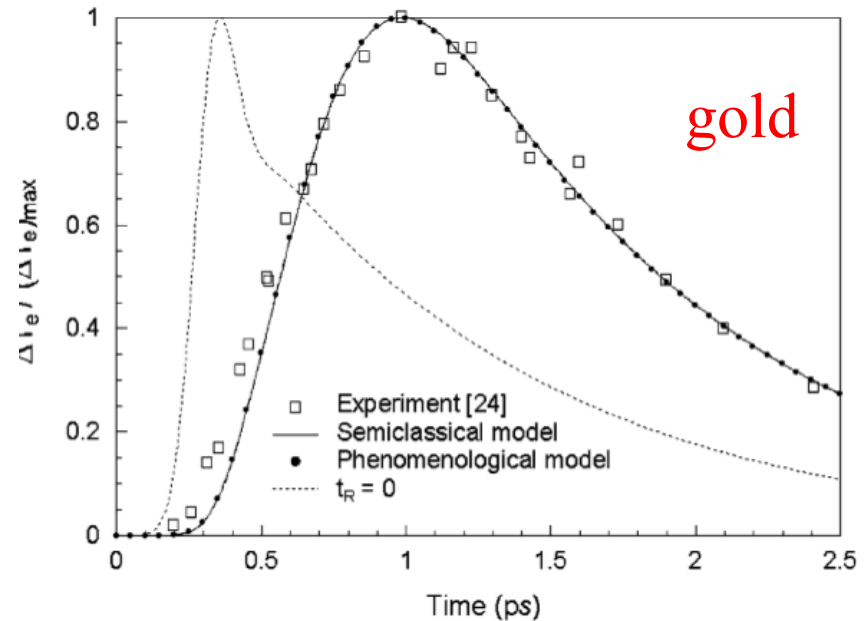
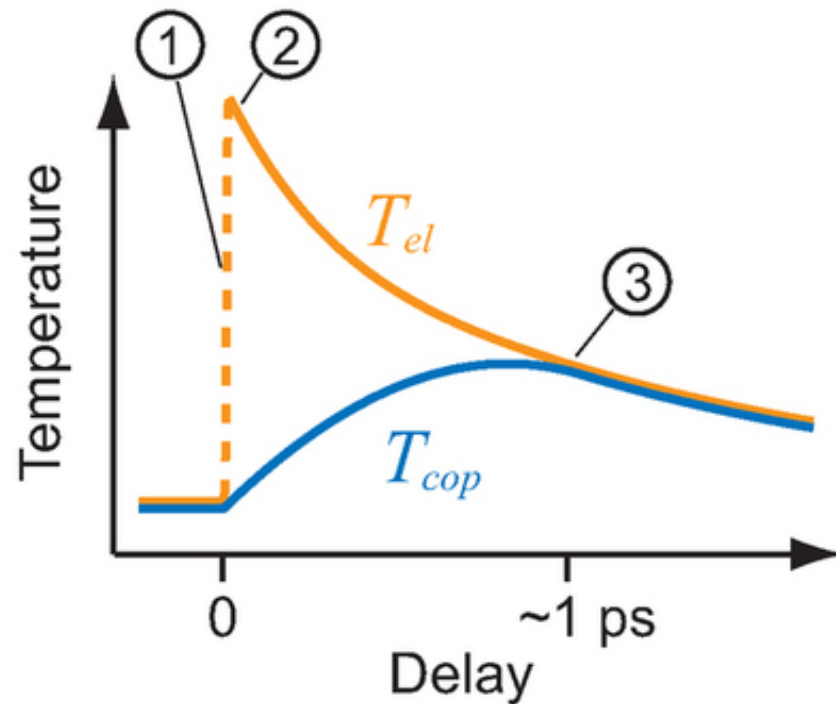
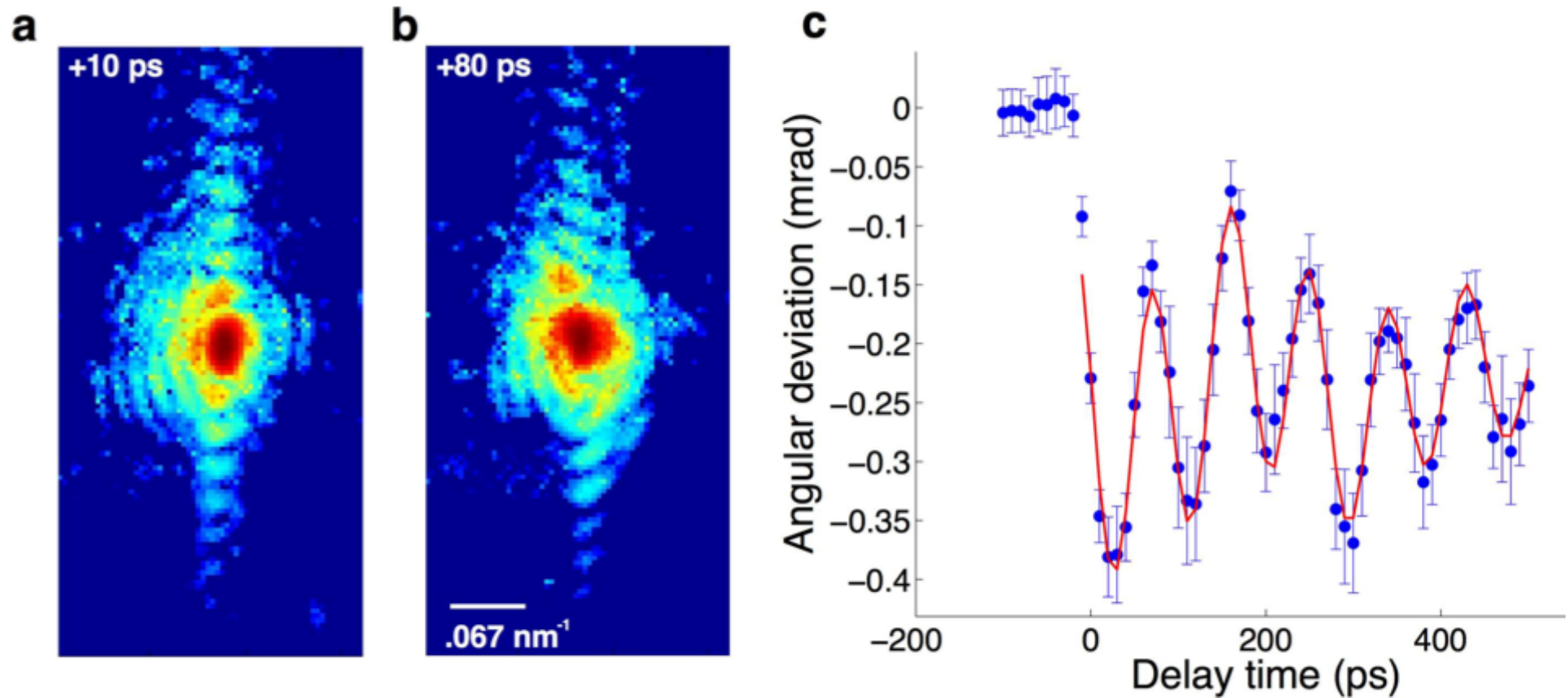


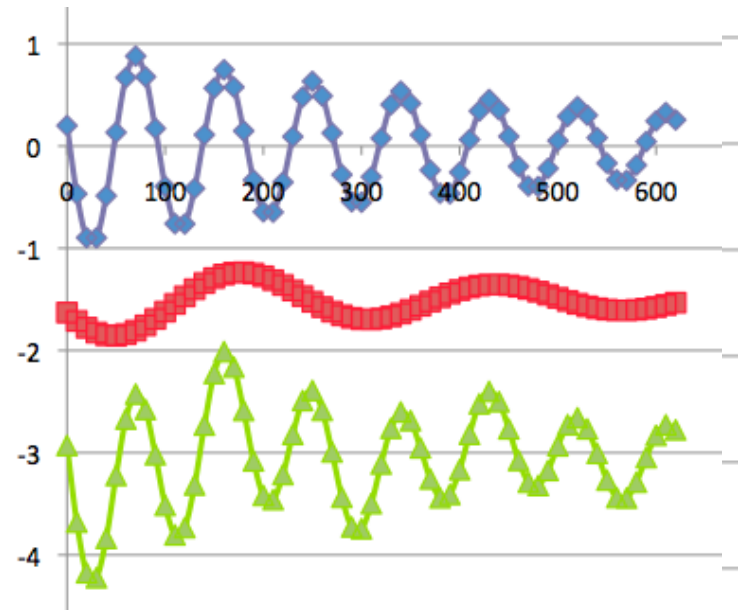
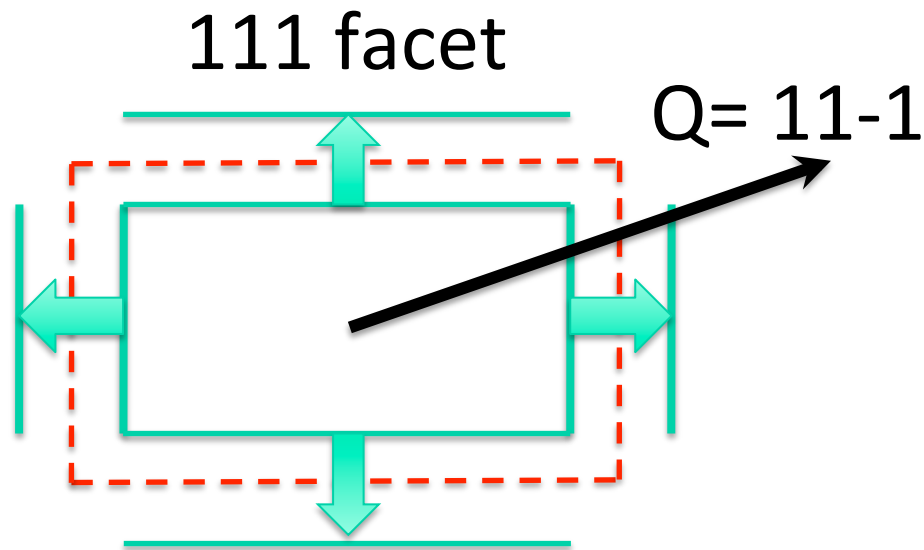
fig. 2. Comparison of the change in electron temperature at the front surface of an 80-nm gold film irradiated by a 2.8 mJ/n², 800 nm, 150-fs laser pulse.

Time resolved Bragg peak position



Two Normal Modes of Vibration

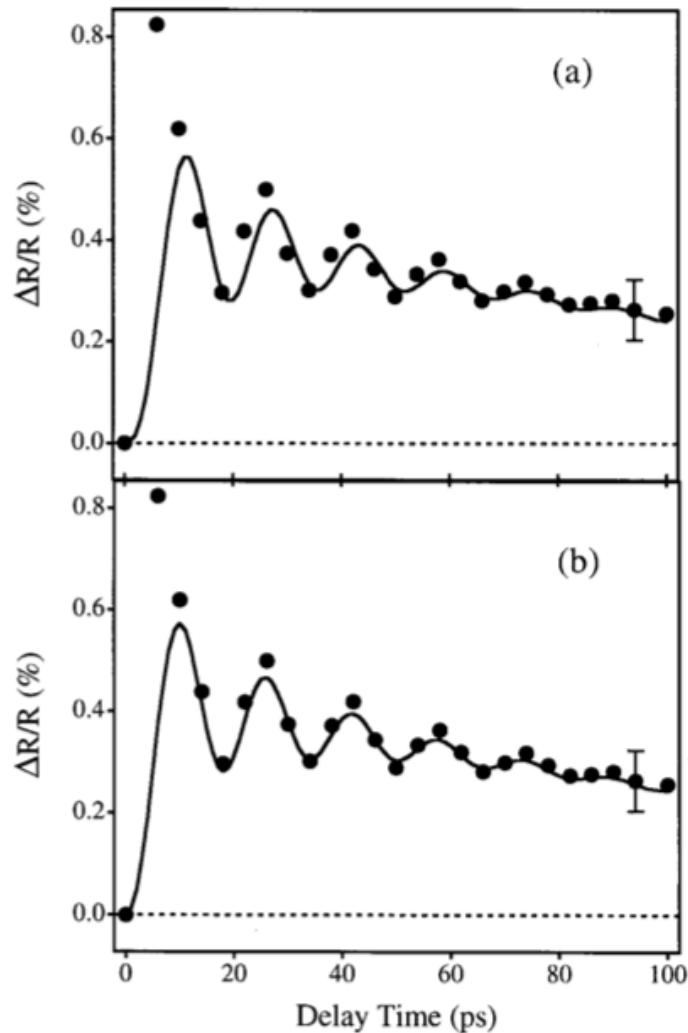
$$S(\tau) = \sum_{n=1}^N A_n \exp[-(\tau/\tau_{d,n})^2] \cos(\omega_n \tau + \varphi_{0,n})$$



$$T_1 = 90\text{ps} \quad h_1 = 145\text{nm} \quad c_S = 3240\text{ m/s}$$
$$T_2 = 259\text{ps} \quad h_2 = 420\text{nm}$$

Ultrafast Absorption Spectroscopy

24nm Au nanoparticles in H₂O, converted to radius
G. V. Hartland, J. Chem. Phys. 116, 8048 (2002)

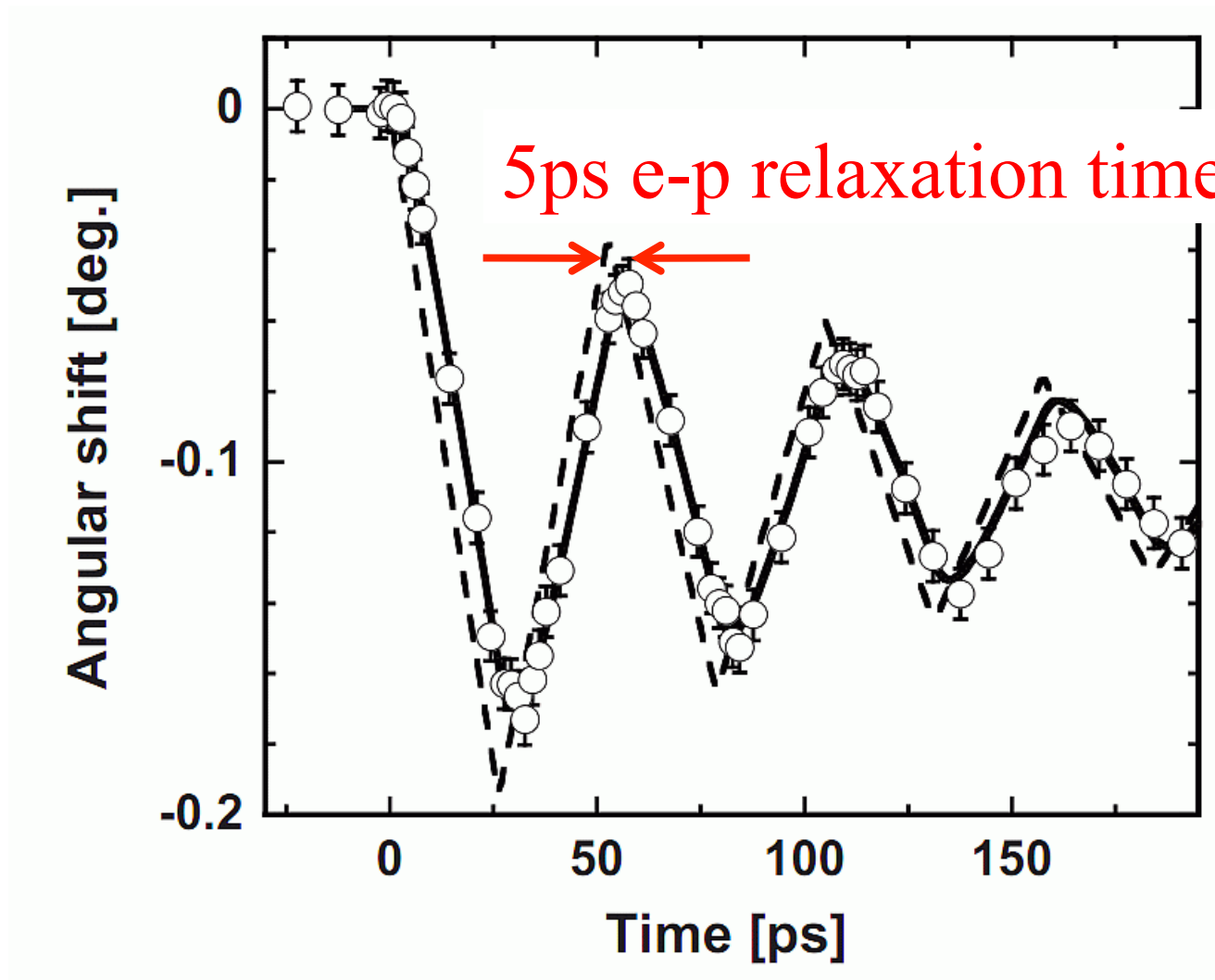


(a) Simple normal mode analysis with impulse heating.

(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)

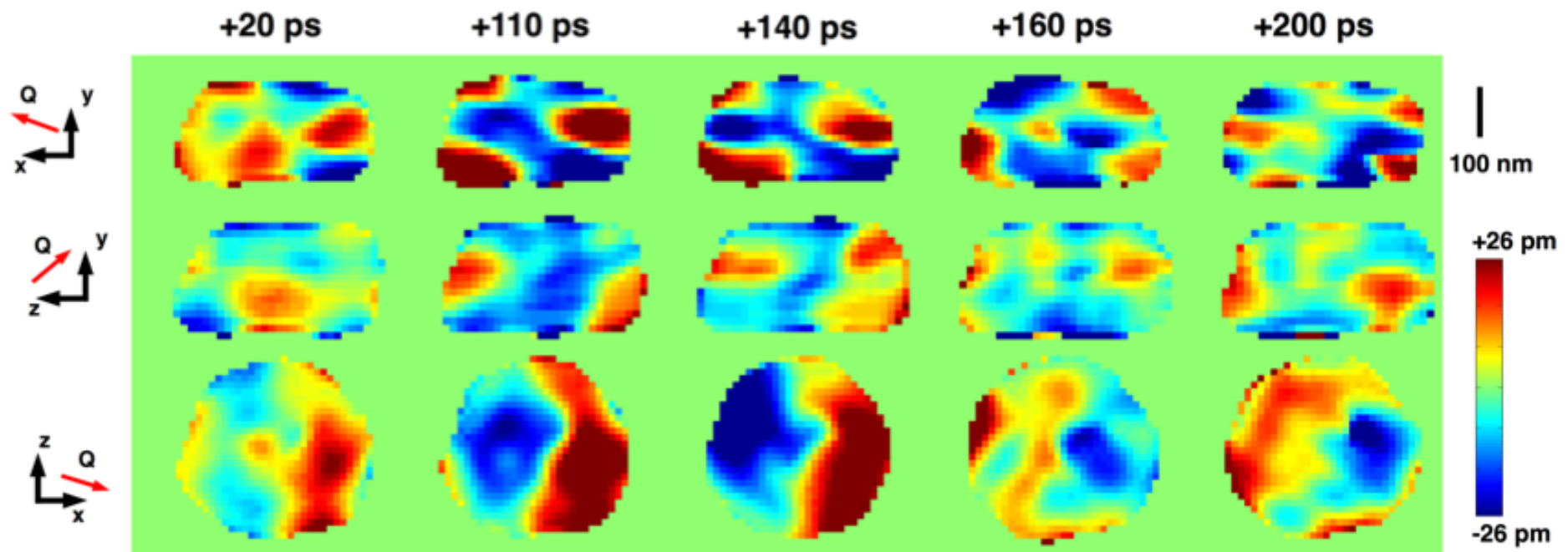


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

1000 frames averaged at each point of rocking curve

Jesse Clark et al Science 341 56 (2013)

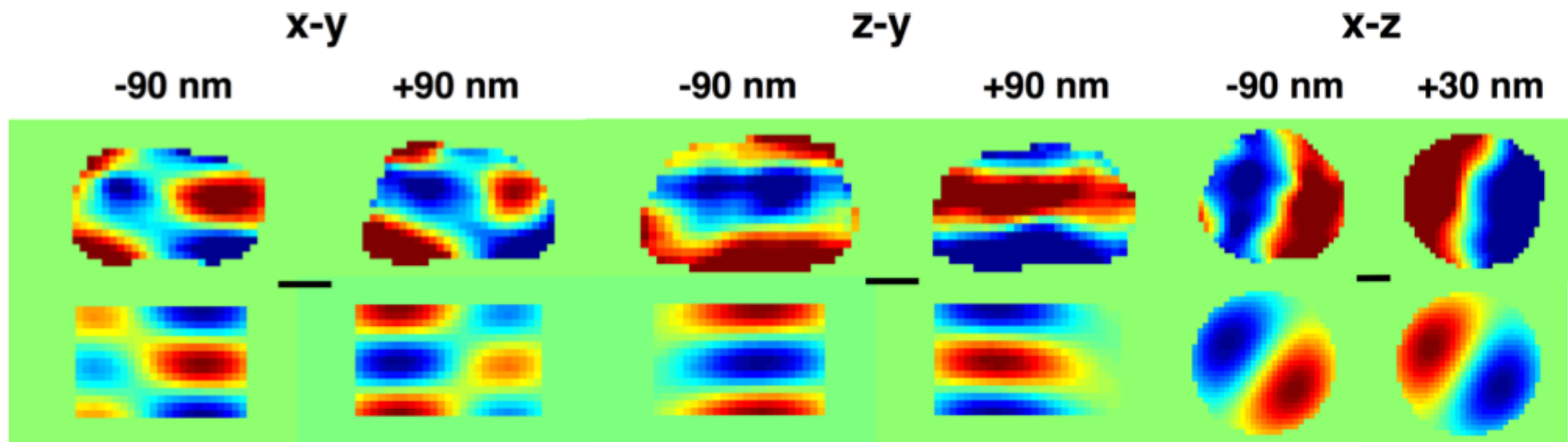


Dynamic imaging of displacements

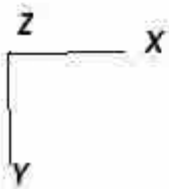
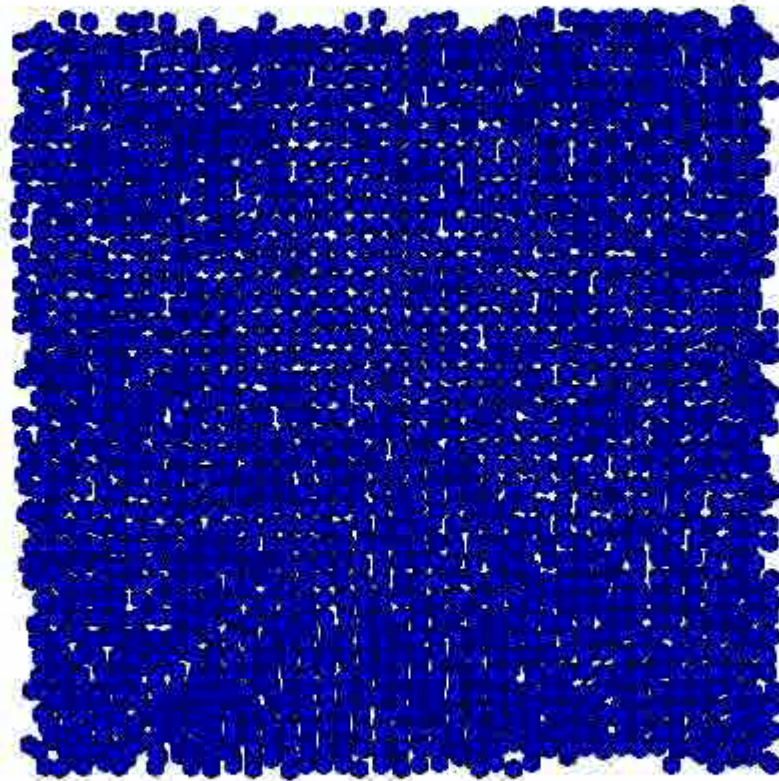
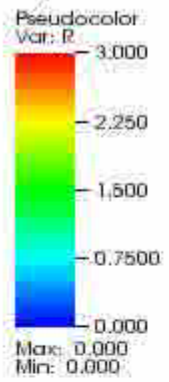
CDI inversion of 3D diffraction patterns

Comparison with (1,1) normal mode of cylinder

Jesse Clark et al Science 341 56 (2013)

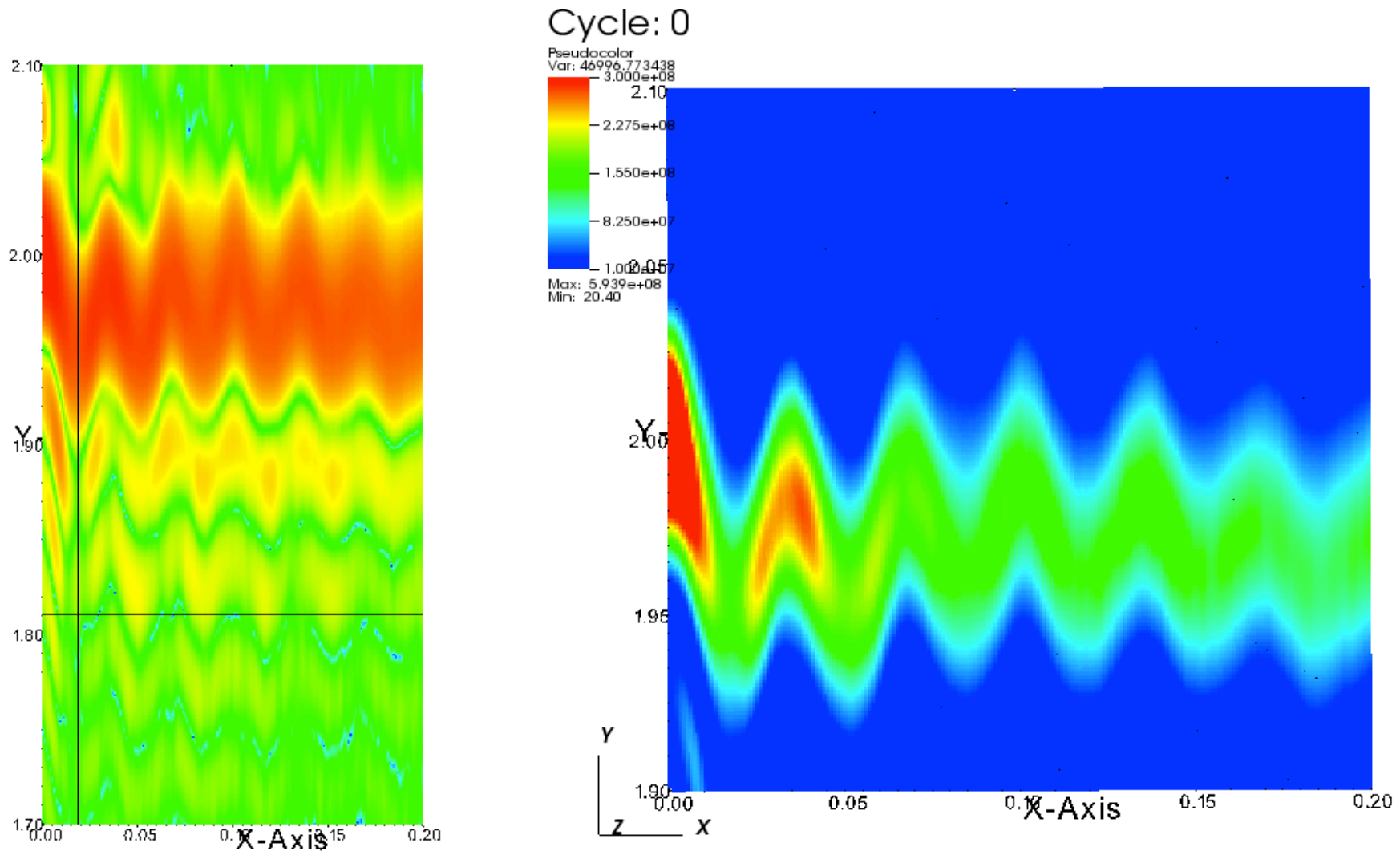


DB: dump.0
Cycle: 0 Time: 0



MD Simulation (LAMMPS)

Andy Higginbotham and Loren Beitra

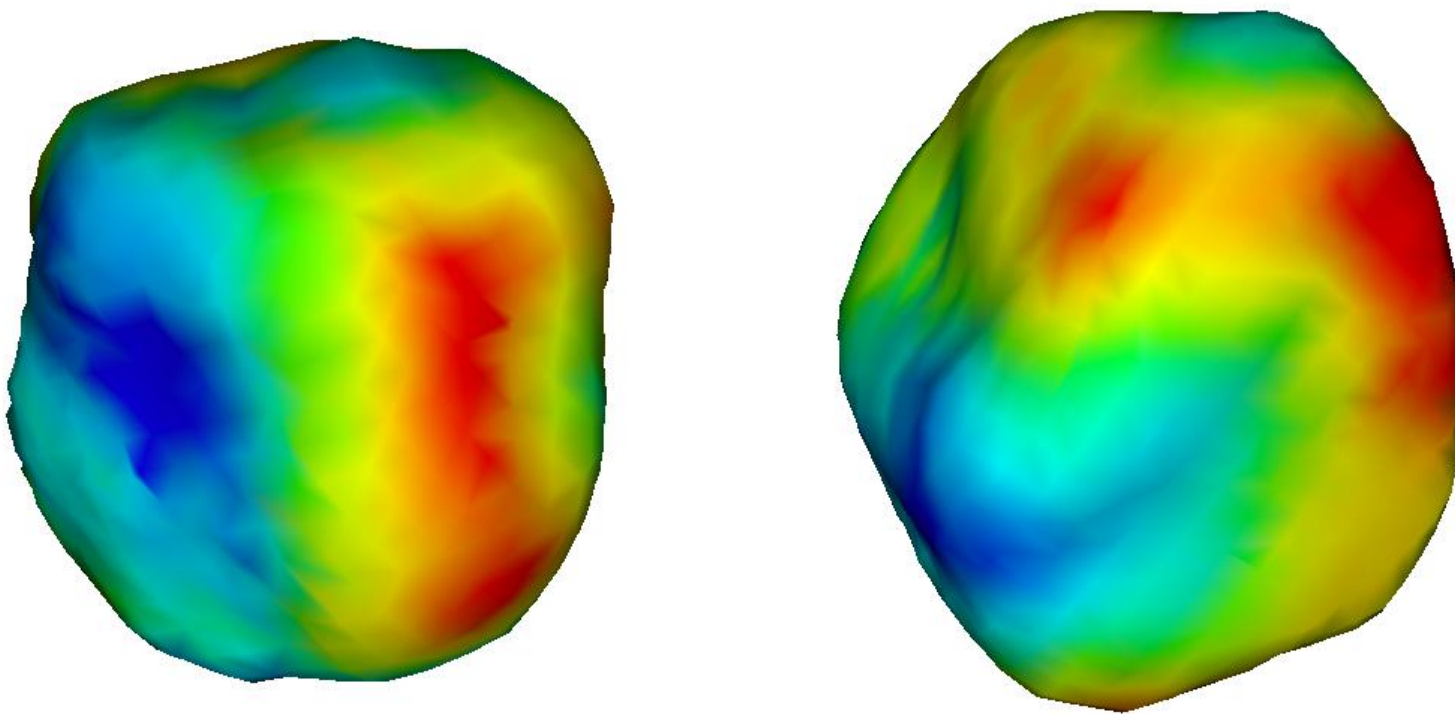


Materials Science using XFELs

- Ground rule #1: €13,000 per **hour**
- 27,000 pulses/sec at XFEL.EU, 2700x10
- 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

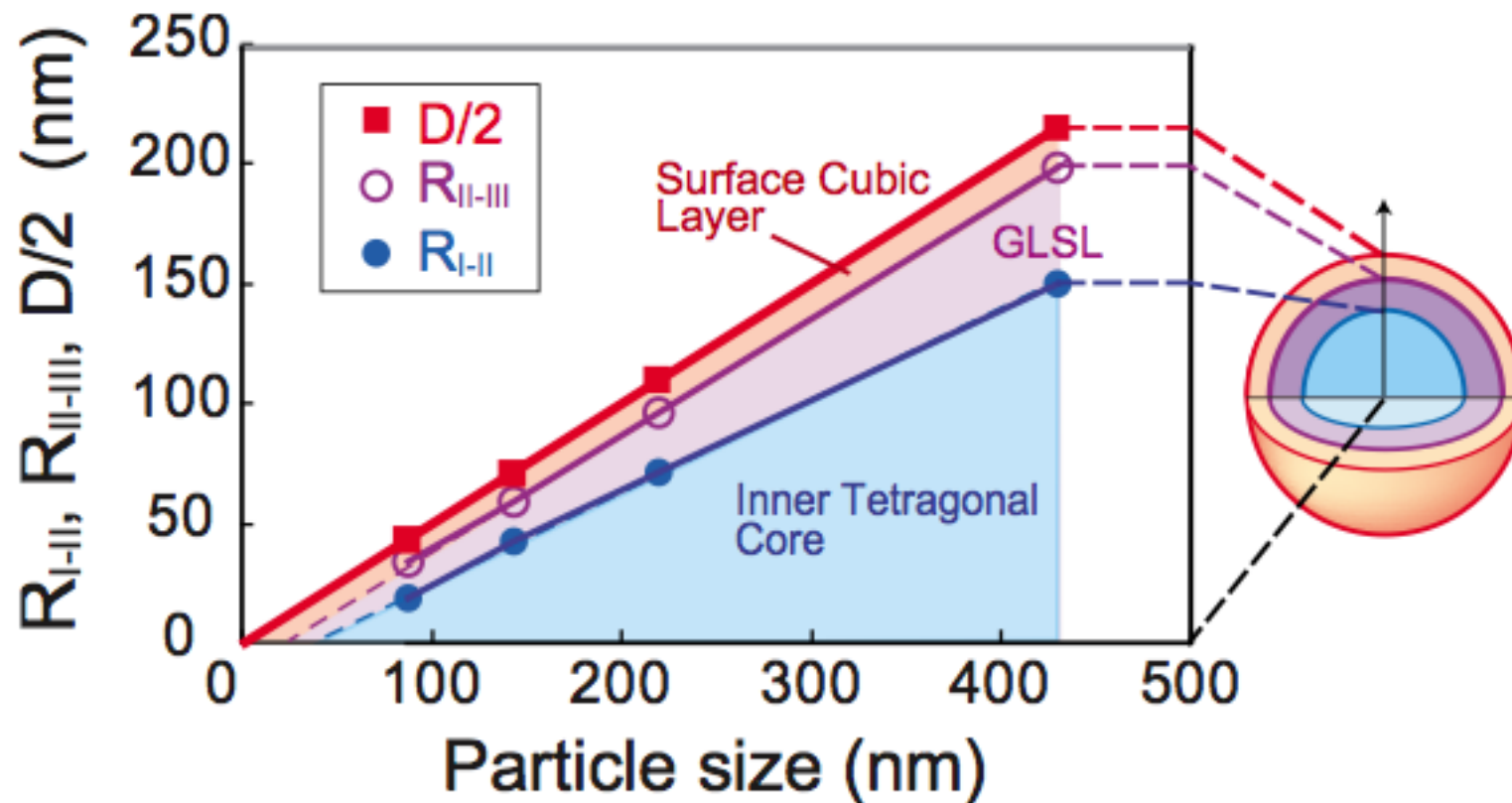
Phase isosurface of residual strain

200nm Barium Titanate (BTO) crystals



Core-shell structure of BTO

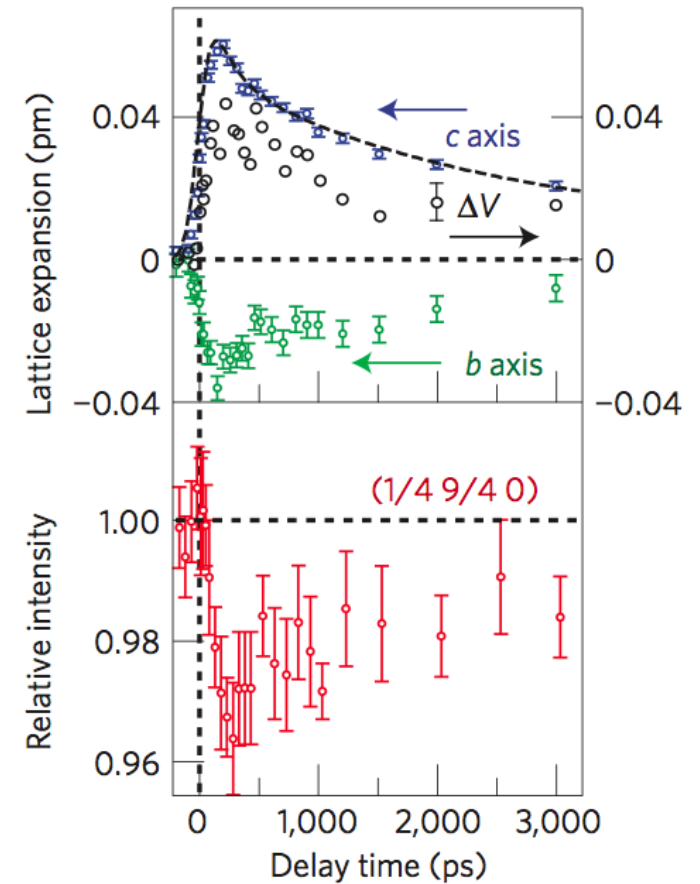
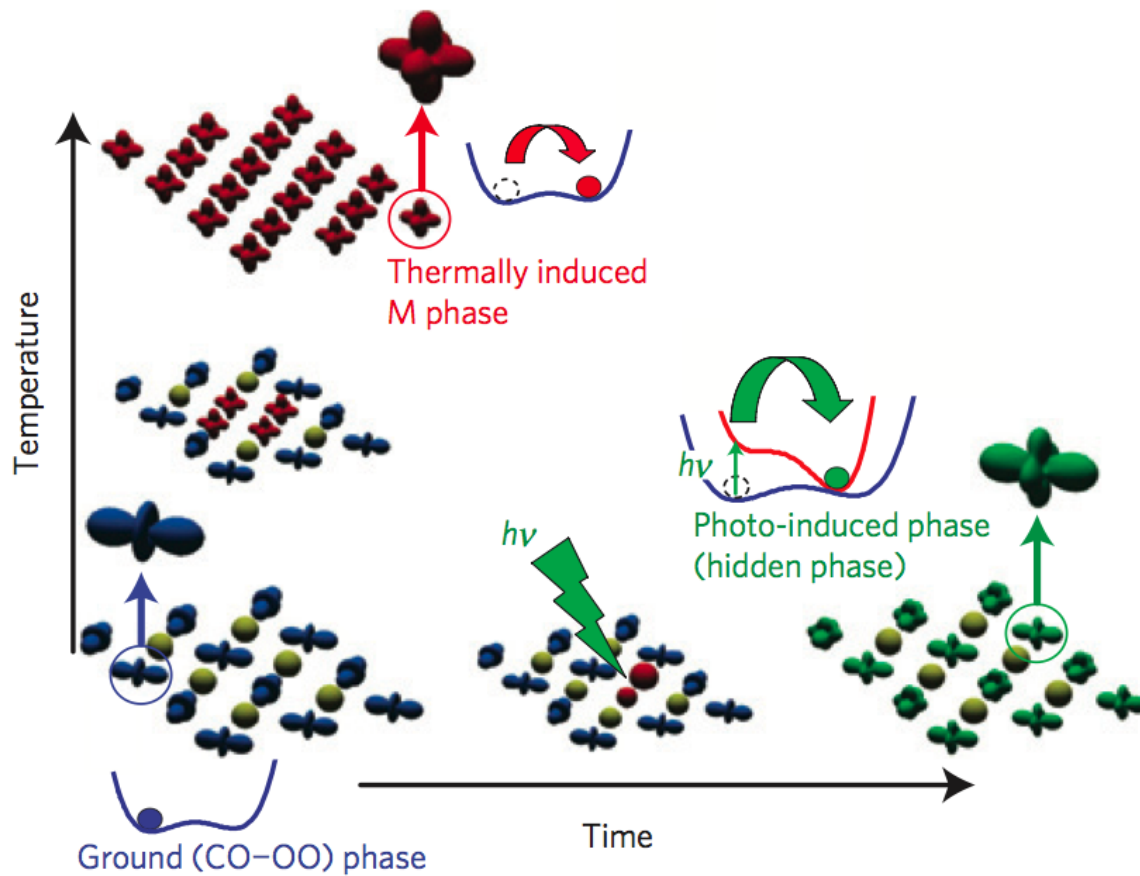
Takuya Hoshina, et al Appl. Phys. Lett. 93, 192914 (2008)



Transient “Hidden” Phase in Manganite

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

$\text{Nd}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$ (NSMO) film on STO



Coherent x-ray diffraction (CXD)

- Complex density can image strain
- Strain associated with nano-shape
- Time resolved strain patterns
- New vibration mode imaged
- New transient materials using lasers?