

# Ultrafast Imaging of Strain Patterns in Crystals

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Solid Mechanics and 4th Generation  
Light Sources

Mathematical Institute

Oxford University

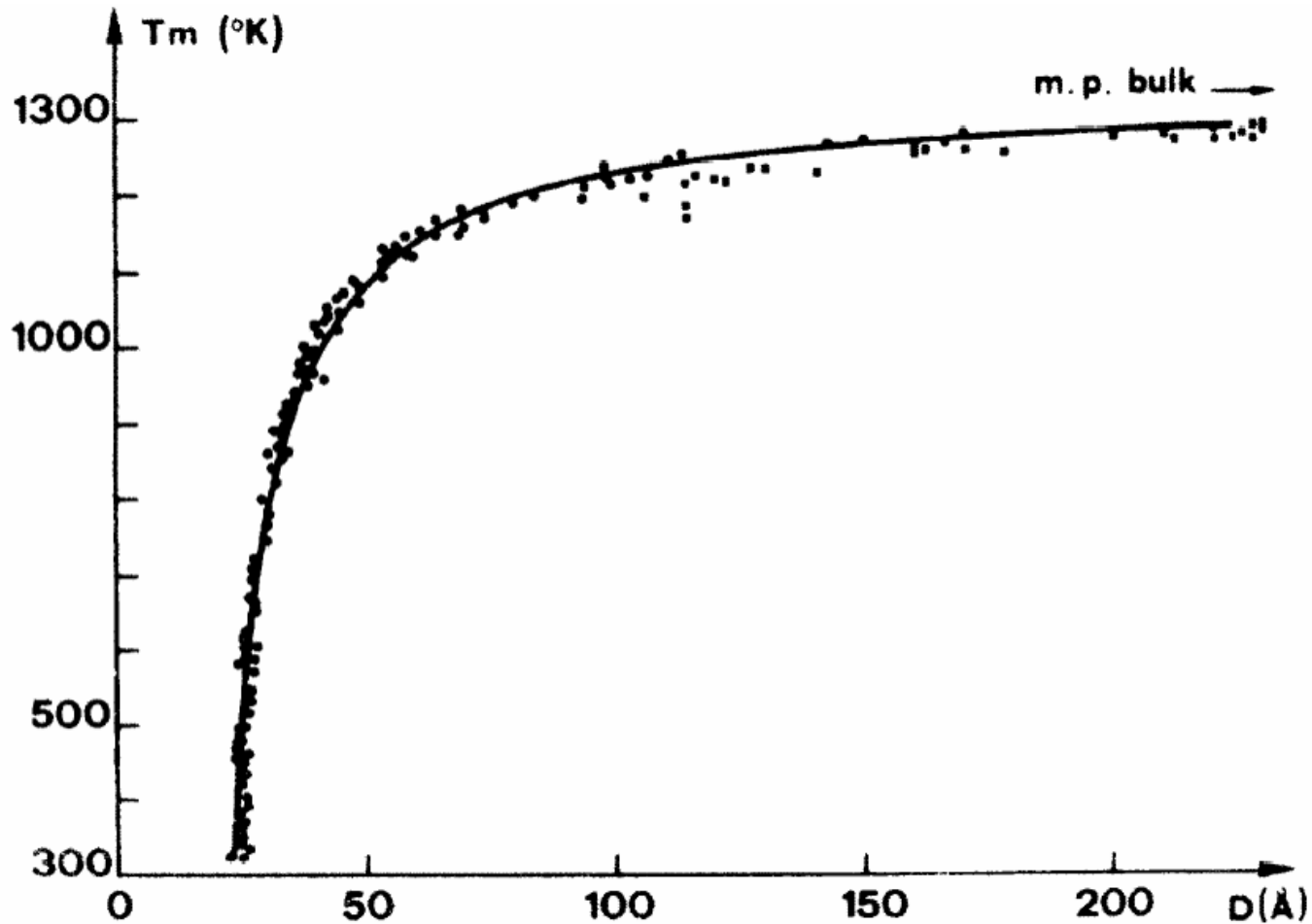
January 2013

# Outline

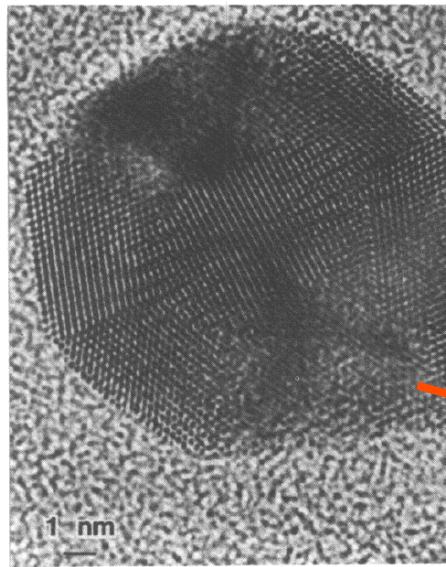
- Nanocrystal structures
- Coherent X-ray Diffraction Imaging
- Crystal strain as complex density
- SOI nanostructures
- Ultrafast CDI of nanocrystals
- Materials Science by XFEL?

# Size-dependent Melting of Au Particles

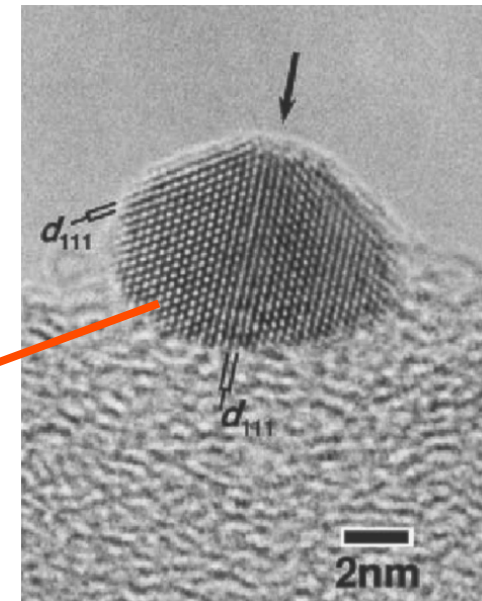
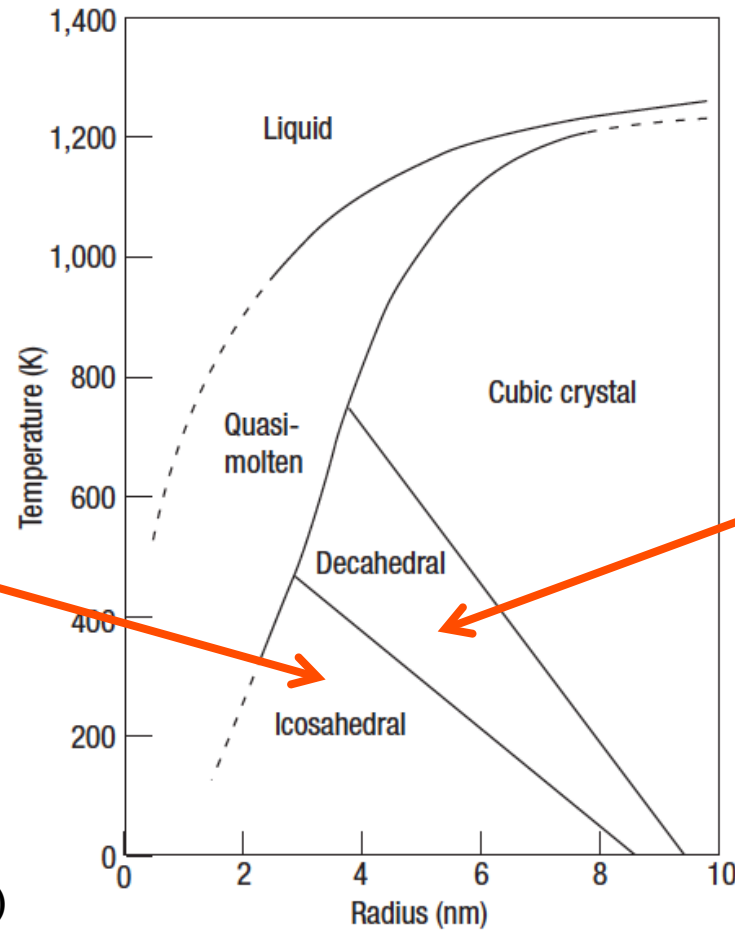
P. Buffat and J-P. Borel, Phys. Rev. A 2287-97 (1975)



# Structure of Gold vs Size



L. D. Marks, RPP (1994)

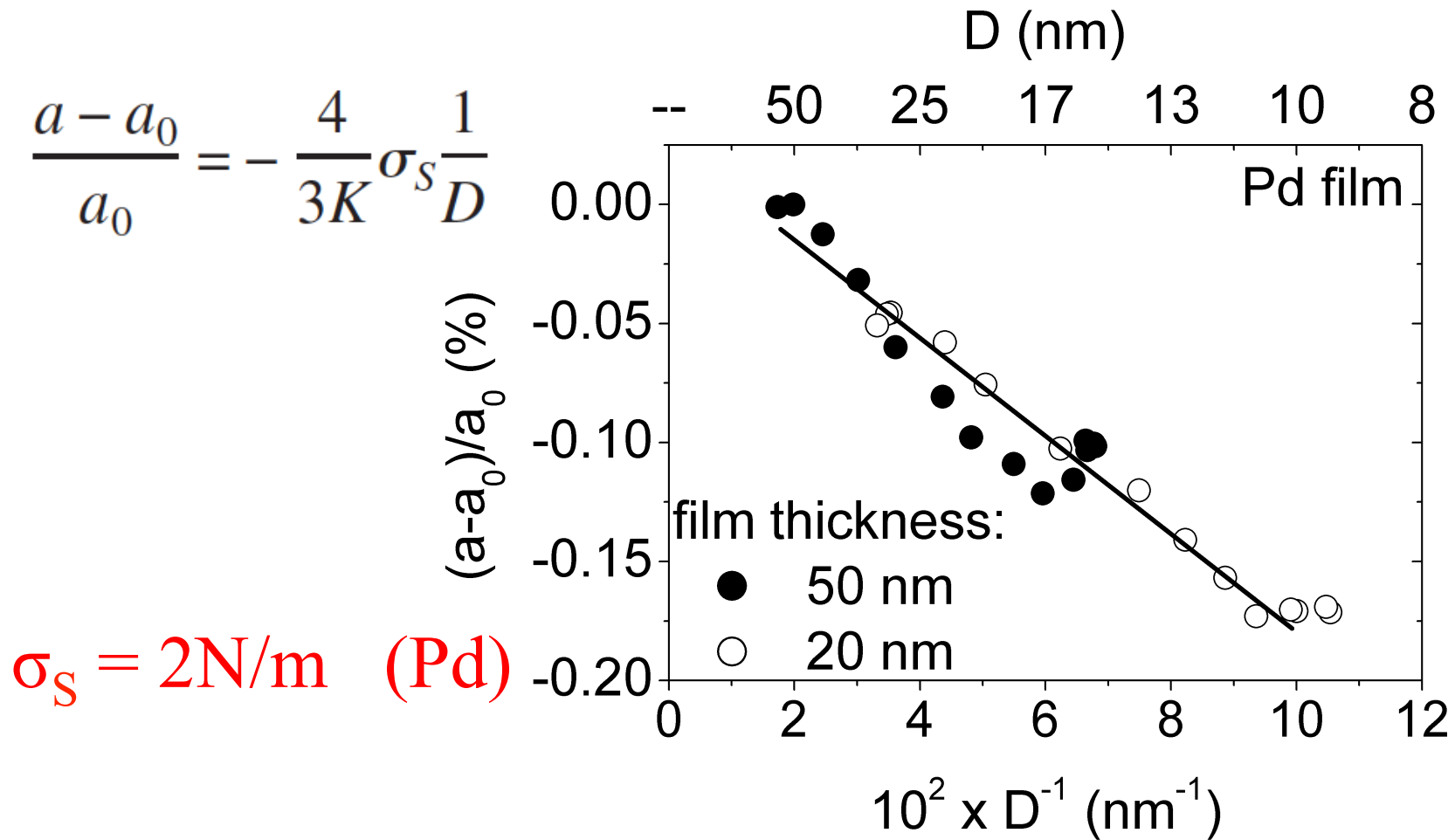


Koga and Sugawara (2003)

# Contraction of Small Particles

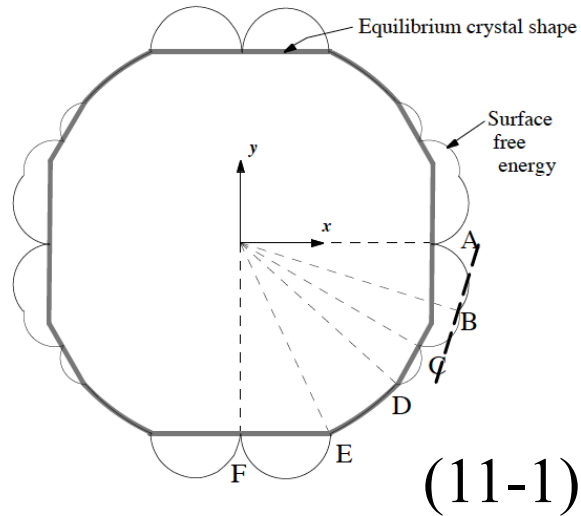
Gibbs Thomson pressure + Bulk modulus

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



# Equilibrium crystal shape

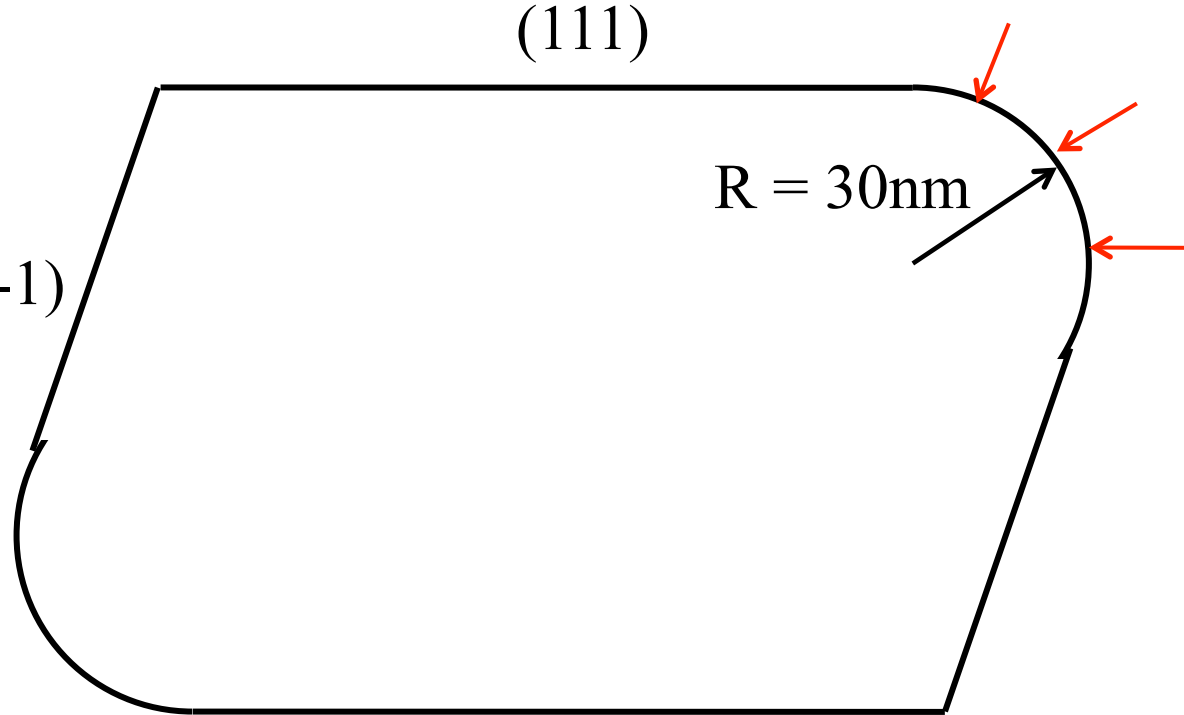
Wulff construction + Gibbs Thomson (Young-Laplace) pressure



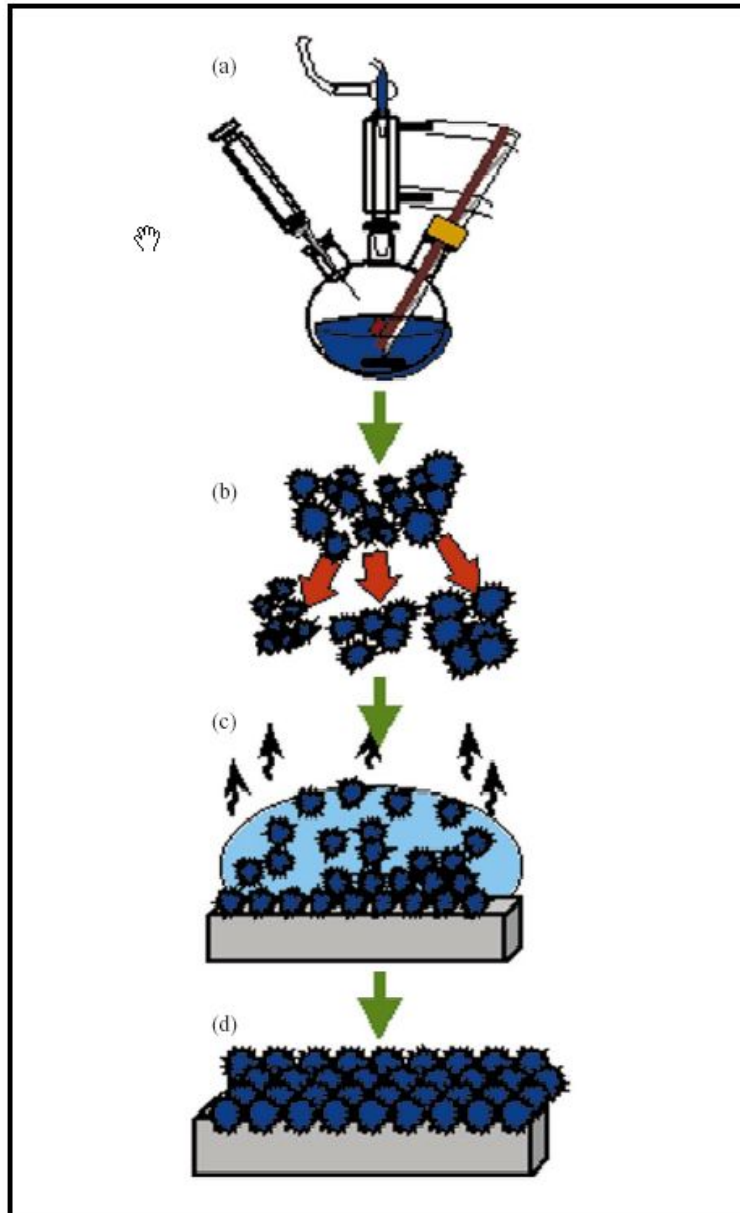
$$\gamma = 2\text{N/m}$$

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

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

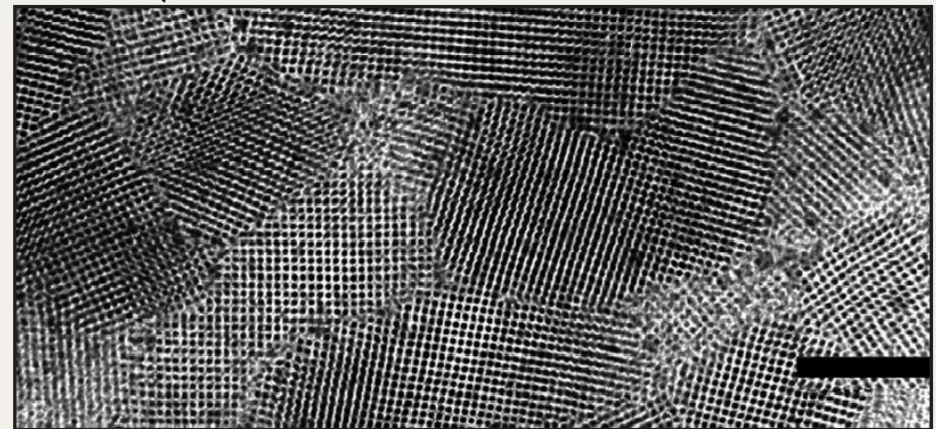


# Chemical Synthesis of Nanocrystals

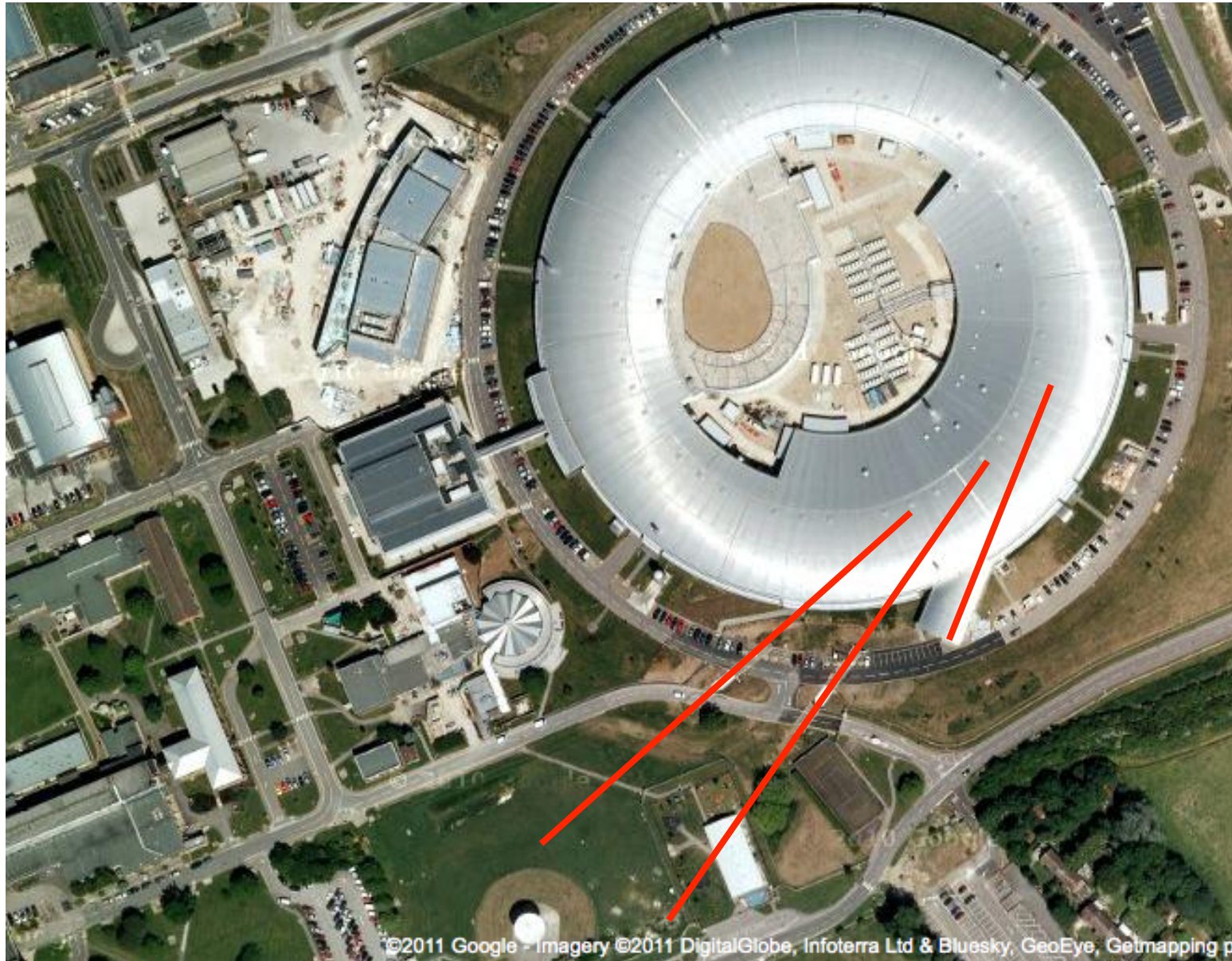


- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

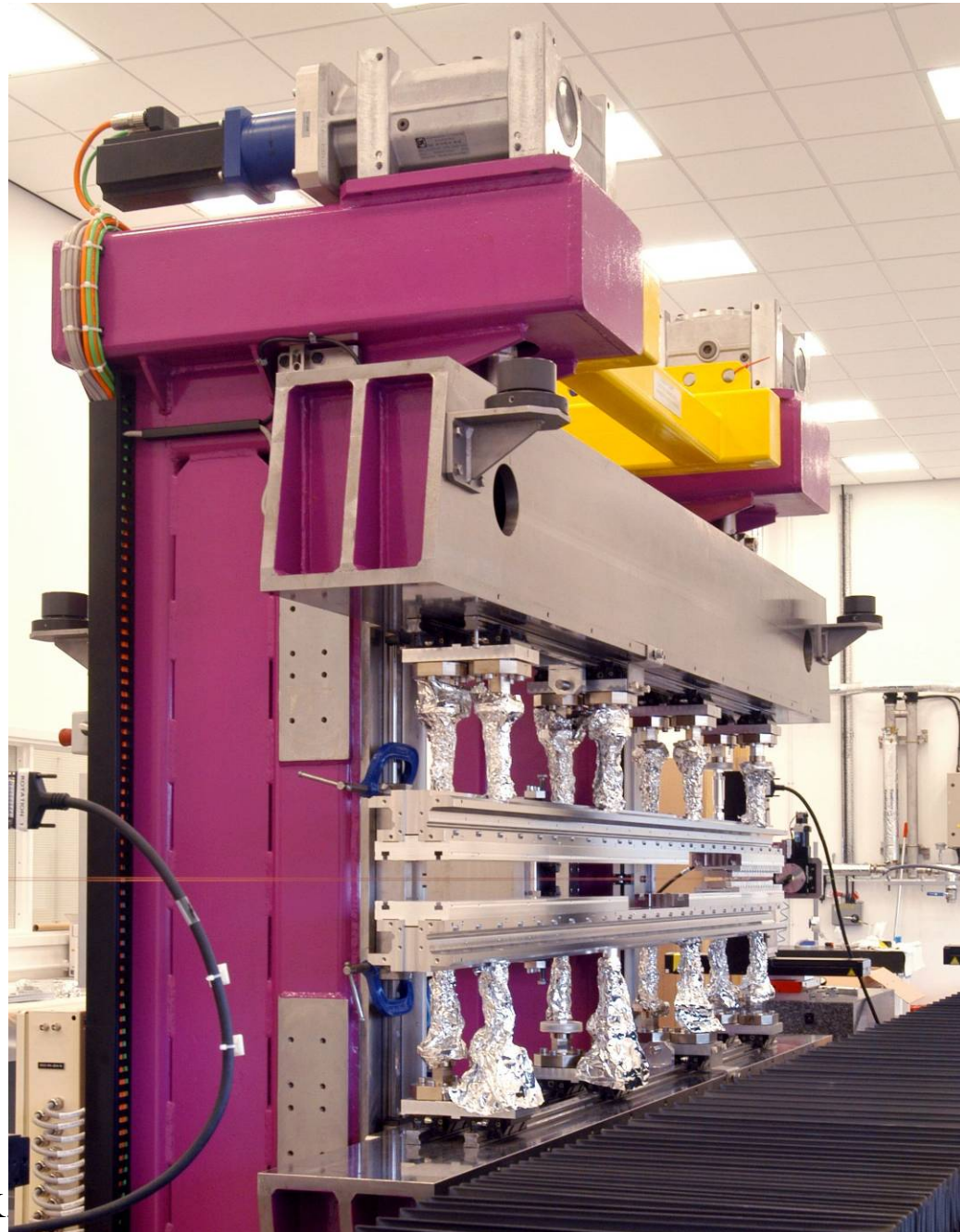
C. B. Murray, *IBM J. Res. & Dev.*  
**45** 47 (2001)



# Diamond Light Source, 2009

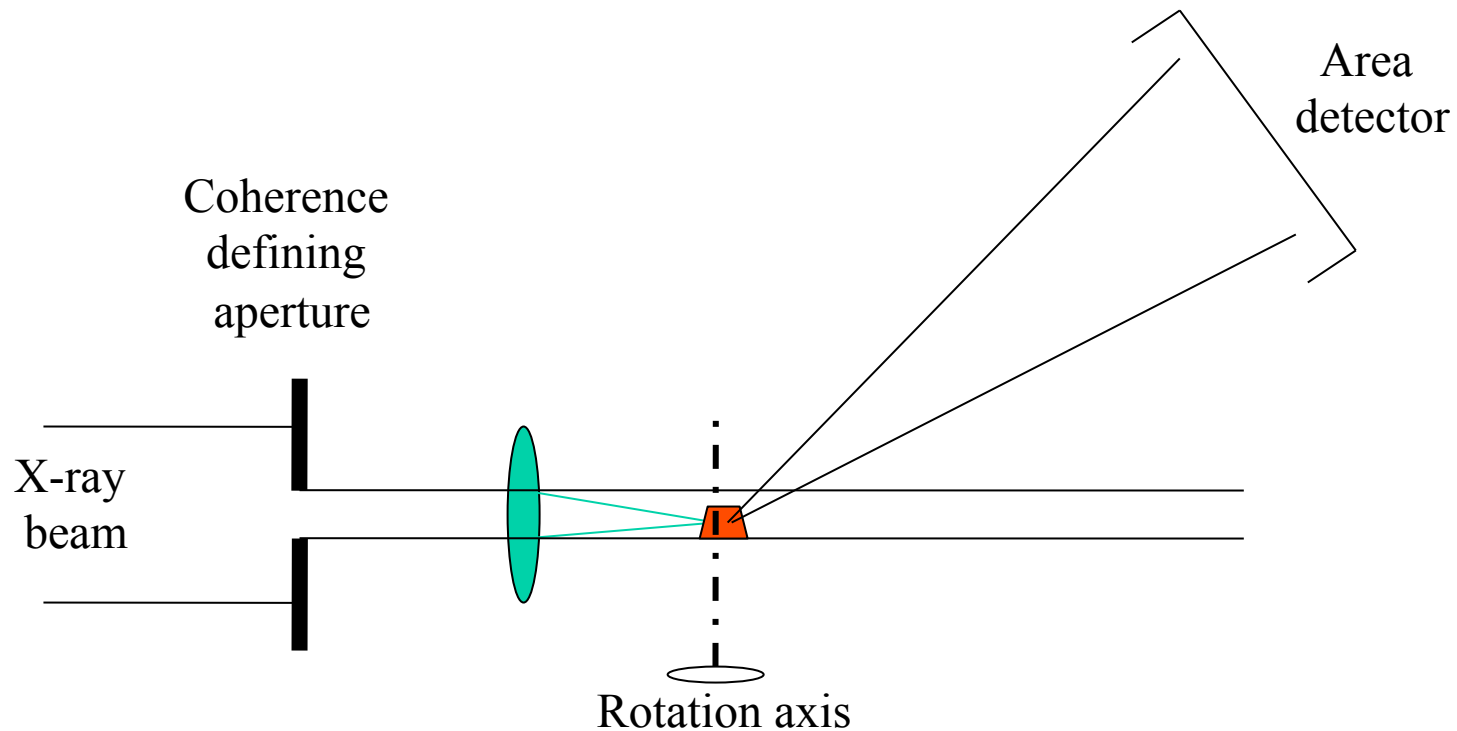


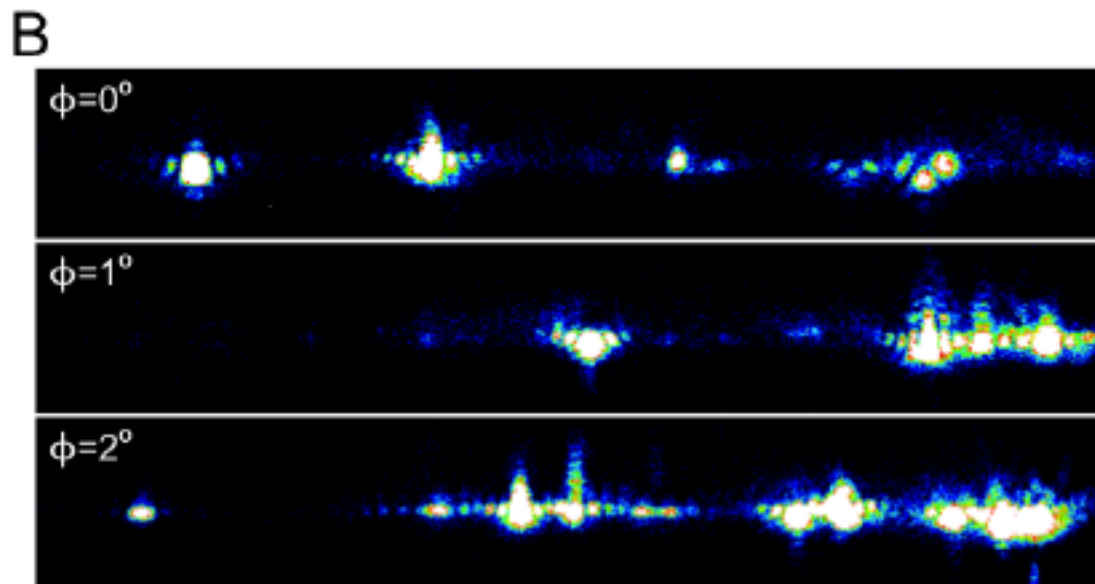
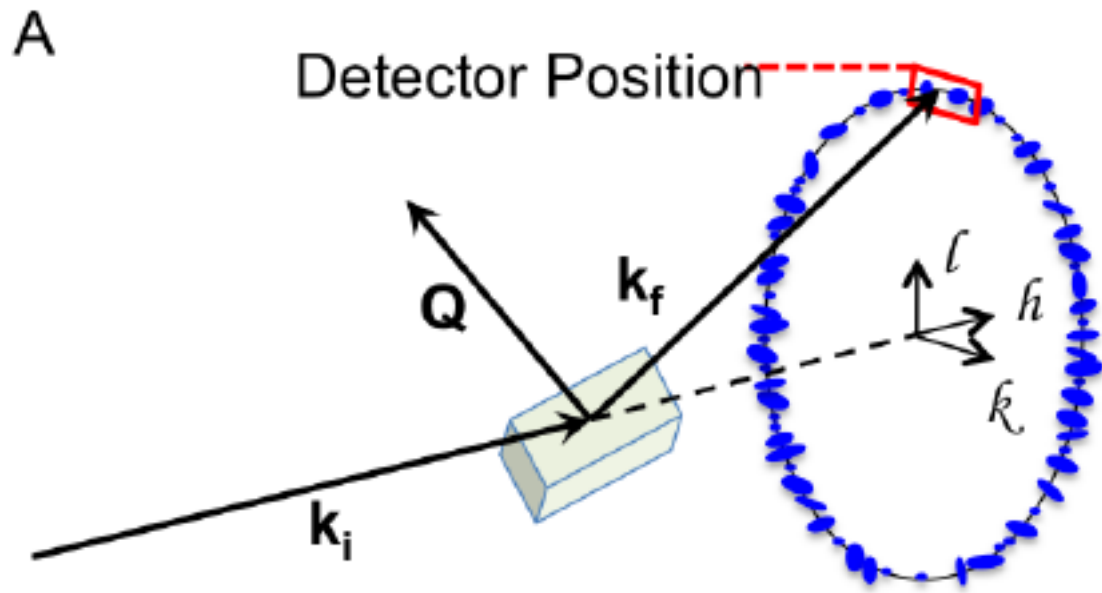
# Diamond in-vacuum X-ray Undulator



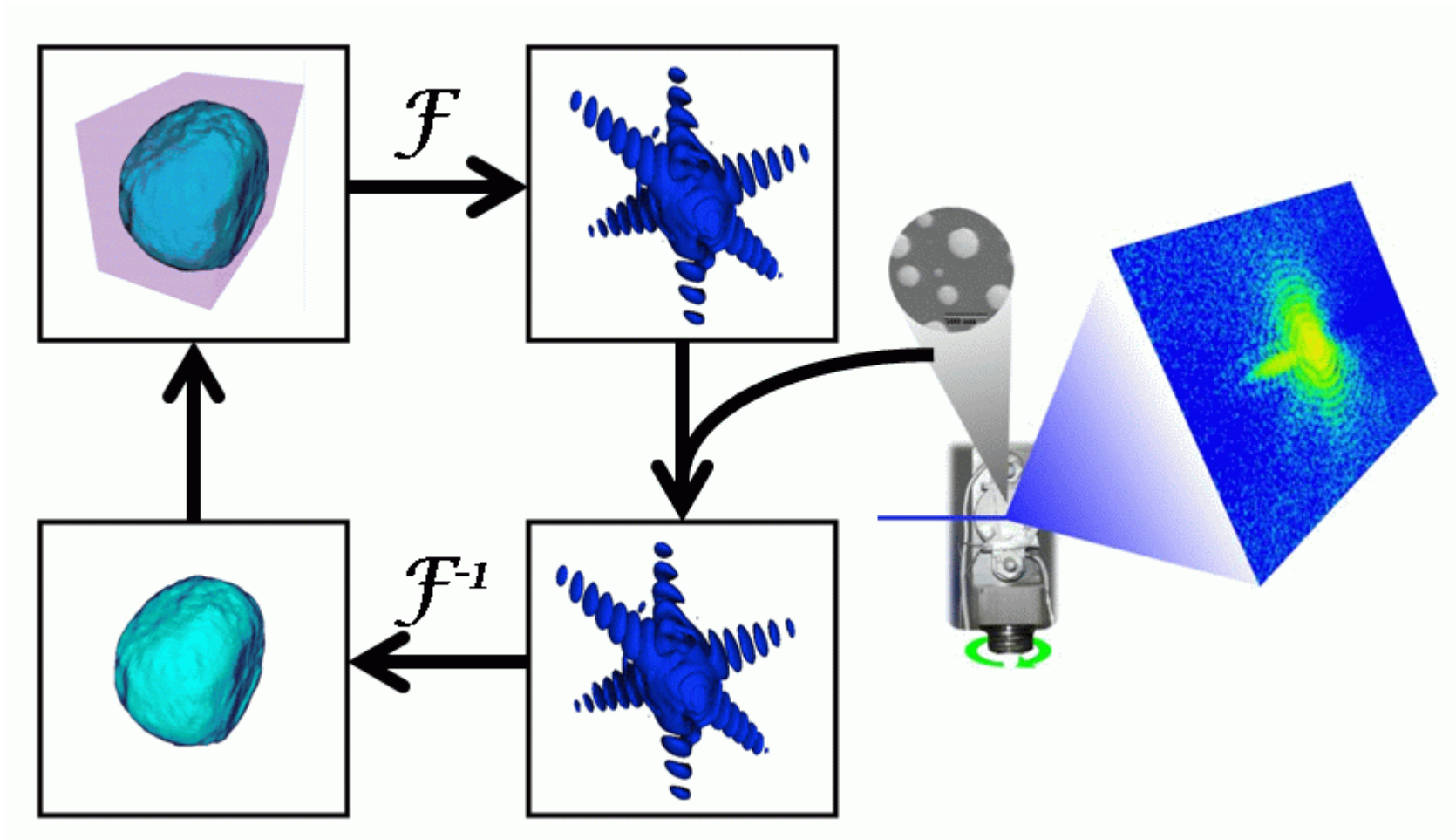
I. K

# Lensless X-ray Microscope, 2003



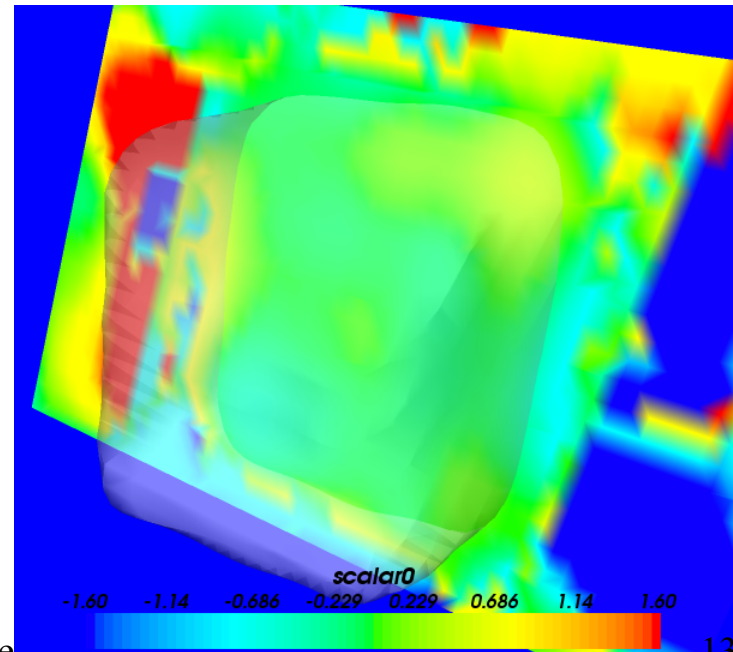
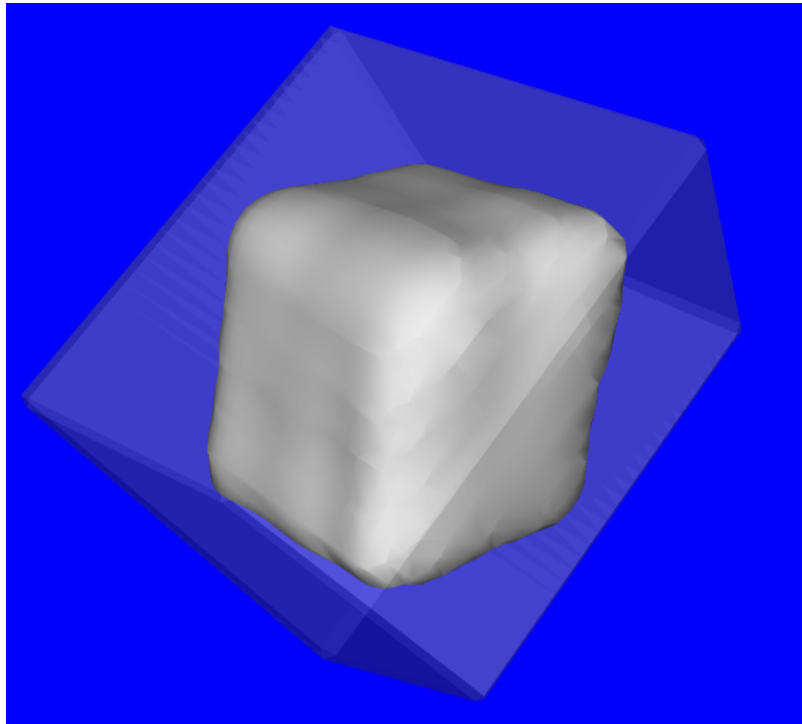
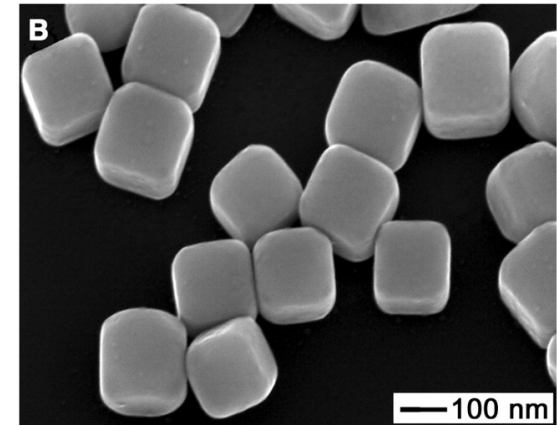
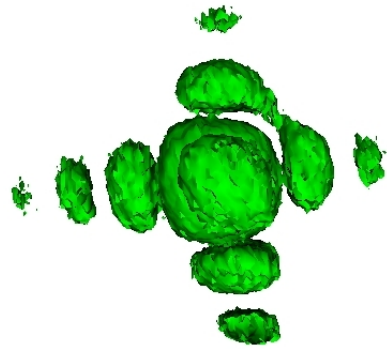
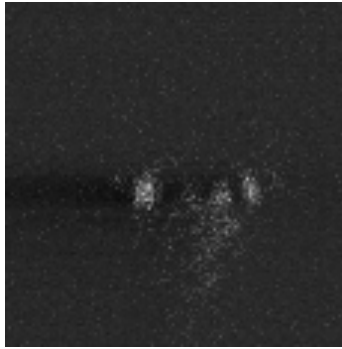


# Generic “Error Reduction” method



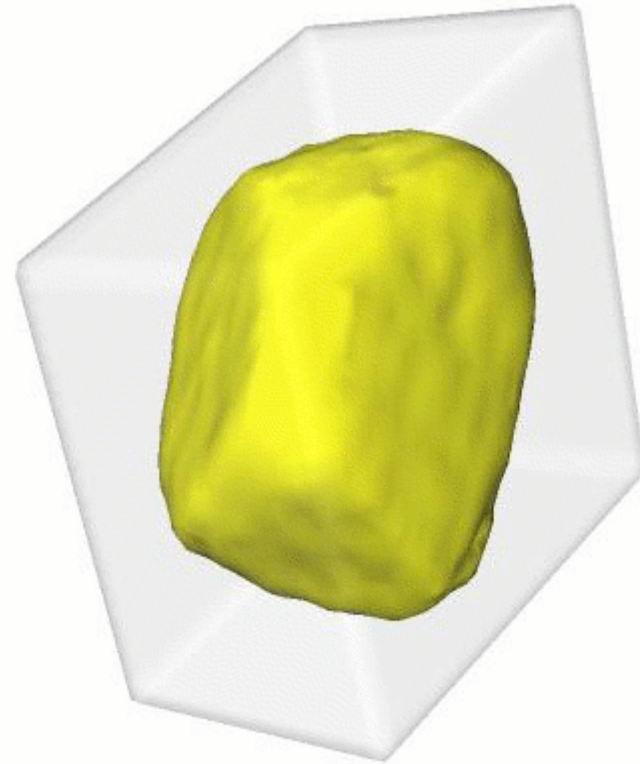
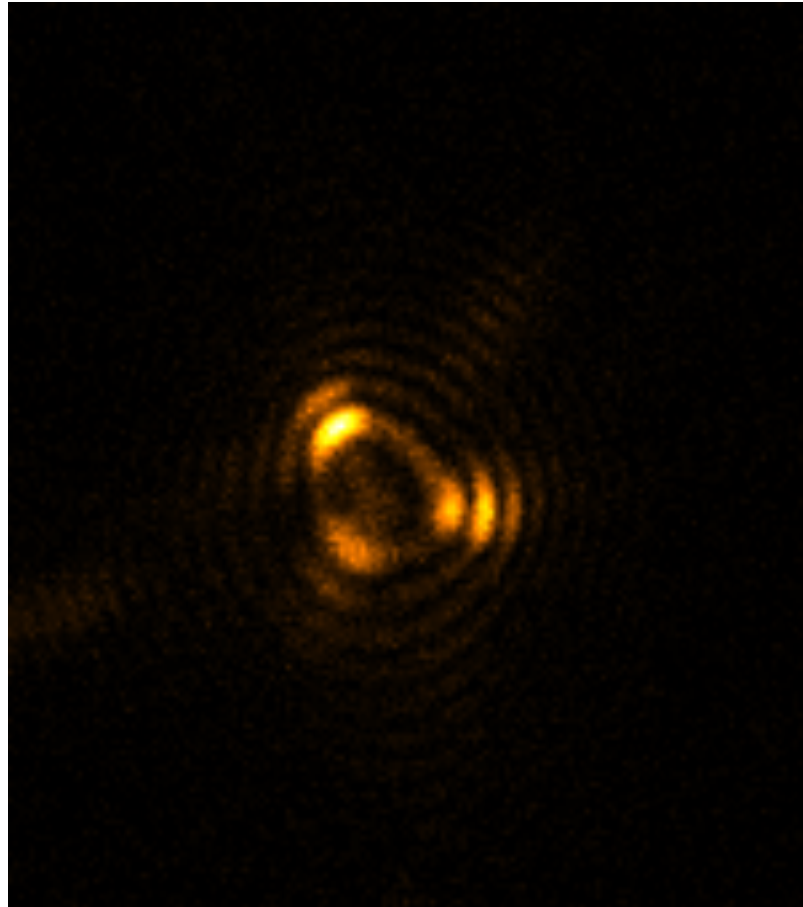
J. R. Fienup *Appl. Opt.* 21 2758 (1982)

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

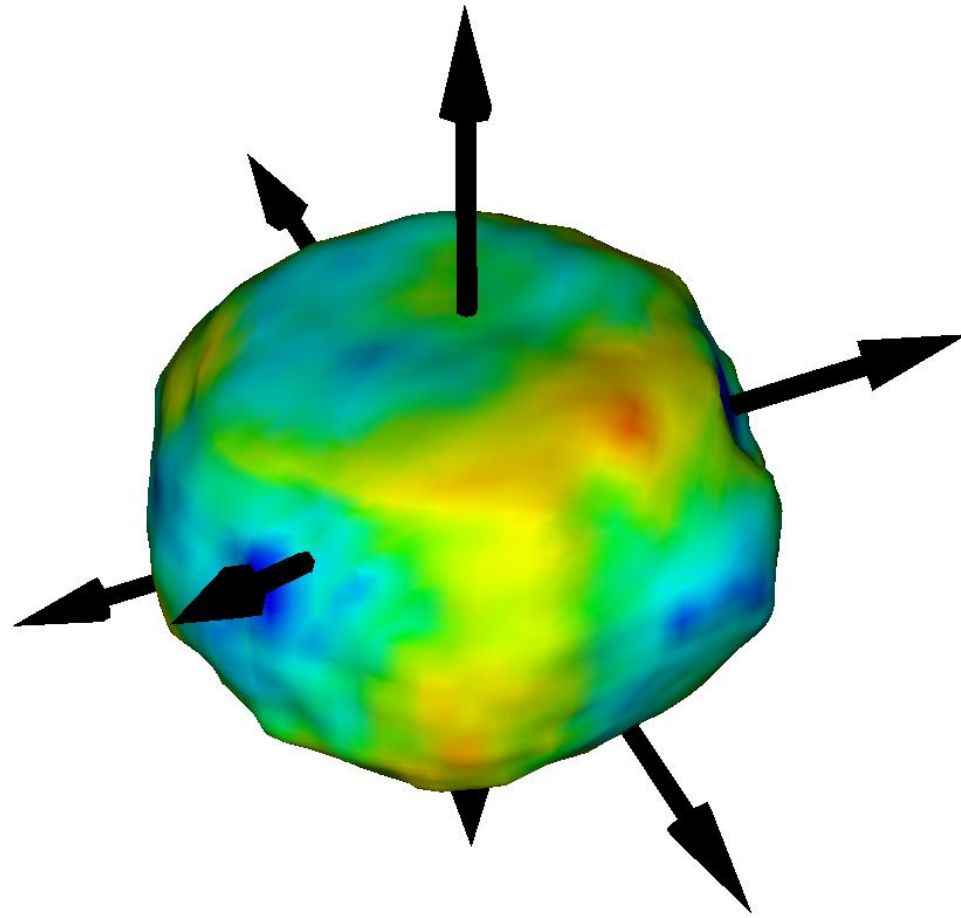


# Gold nanocrystal reconstruction

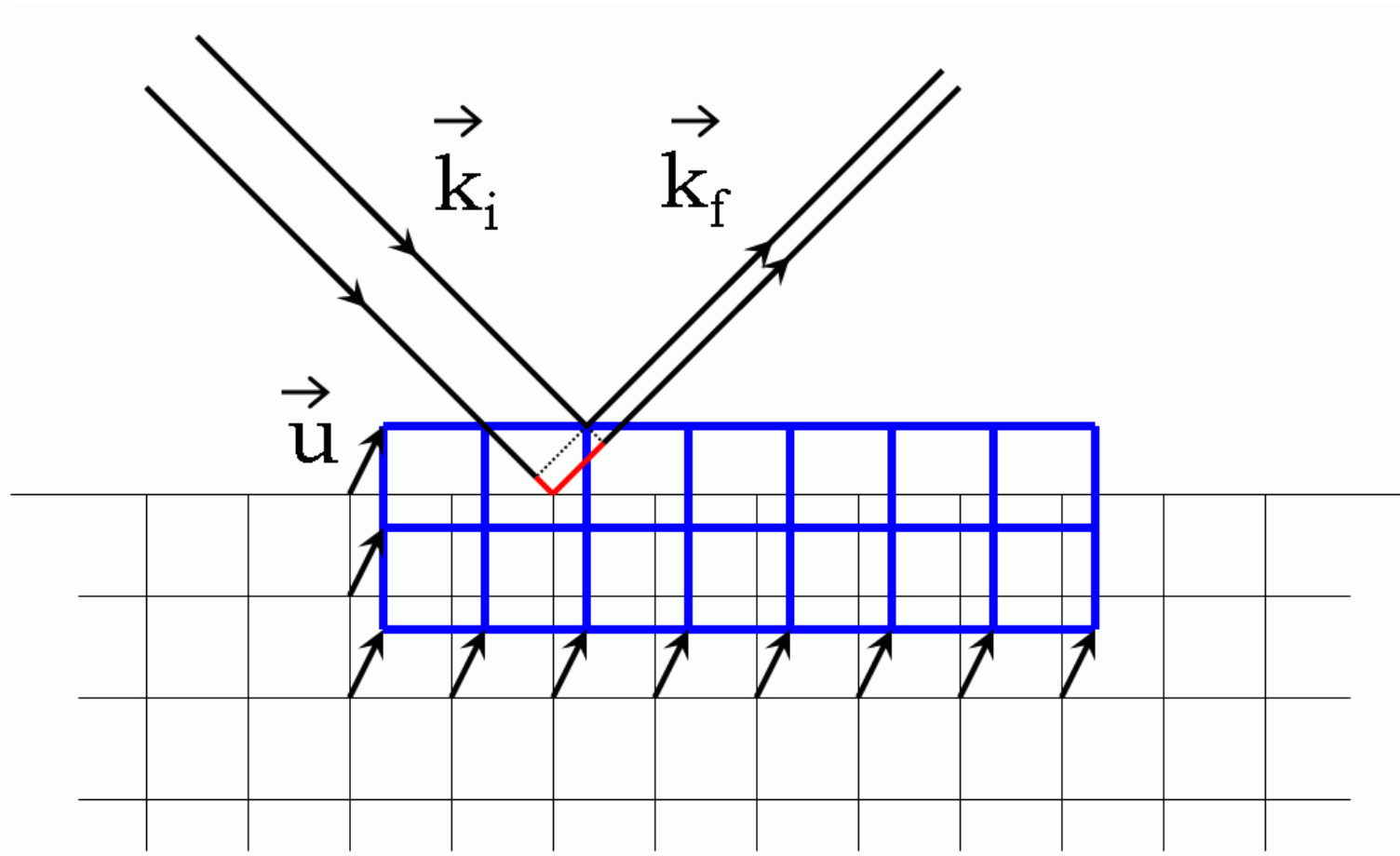
showing support used for 20 HIO followed by 10 ER



# Phase isosurface of residual strain

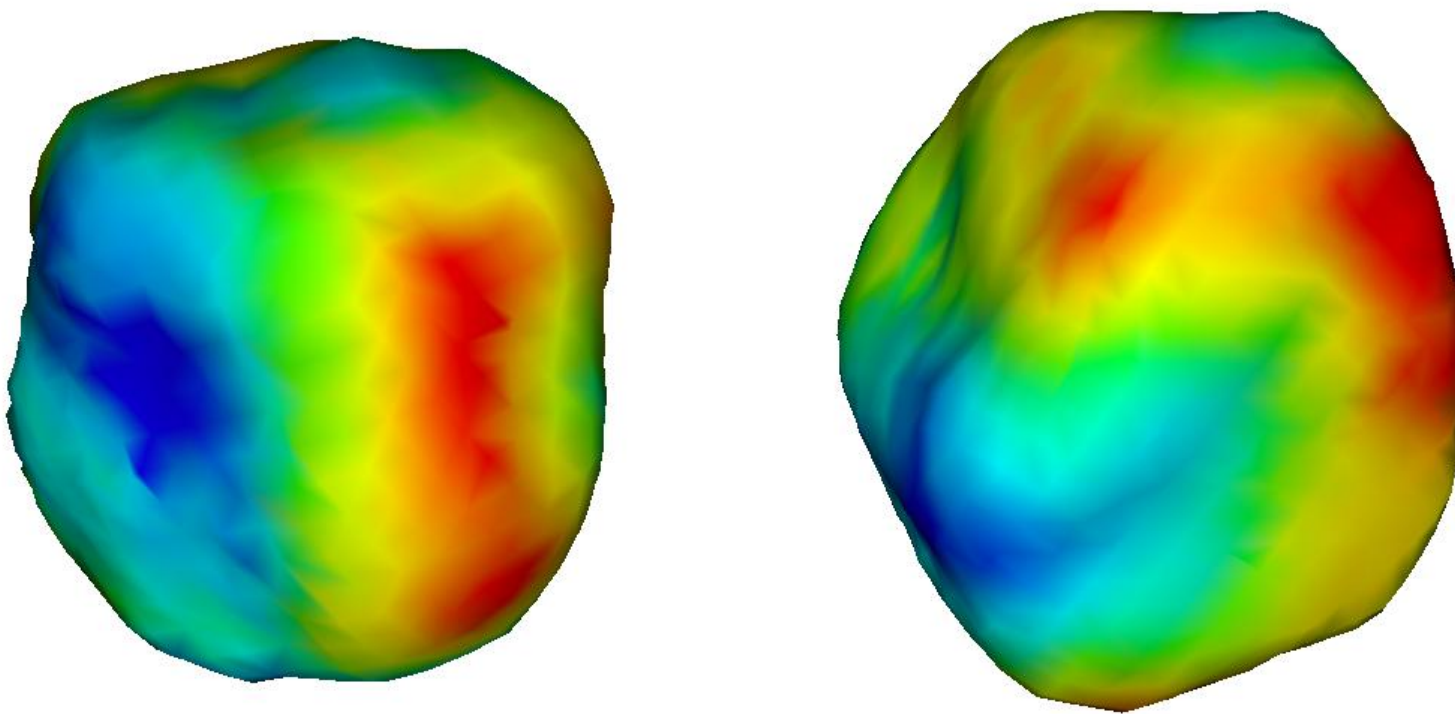


# Sensitivity to strain

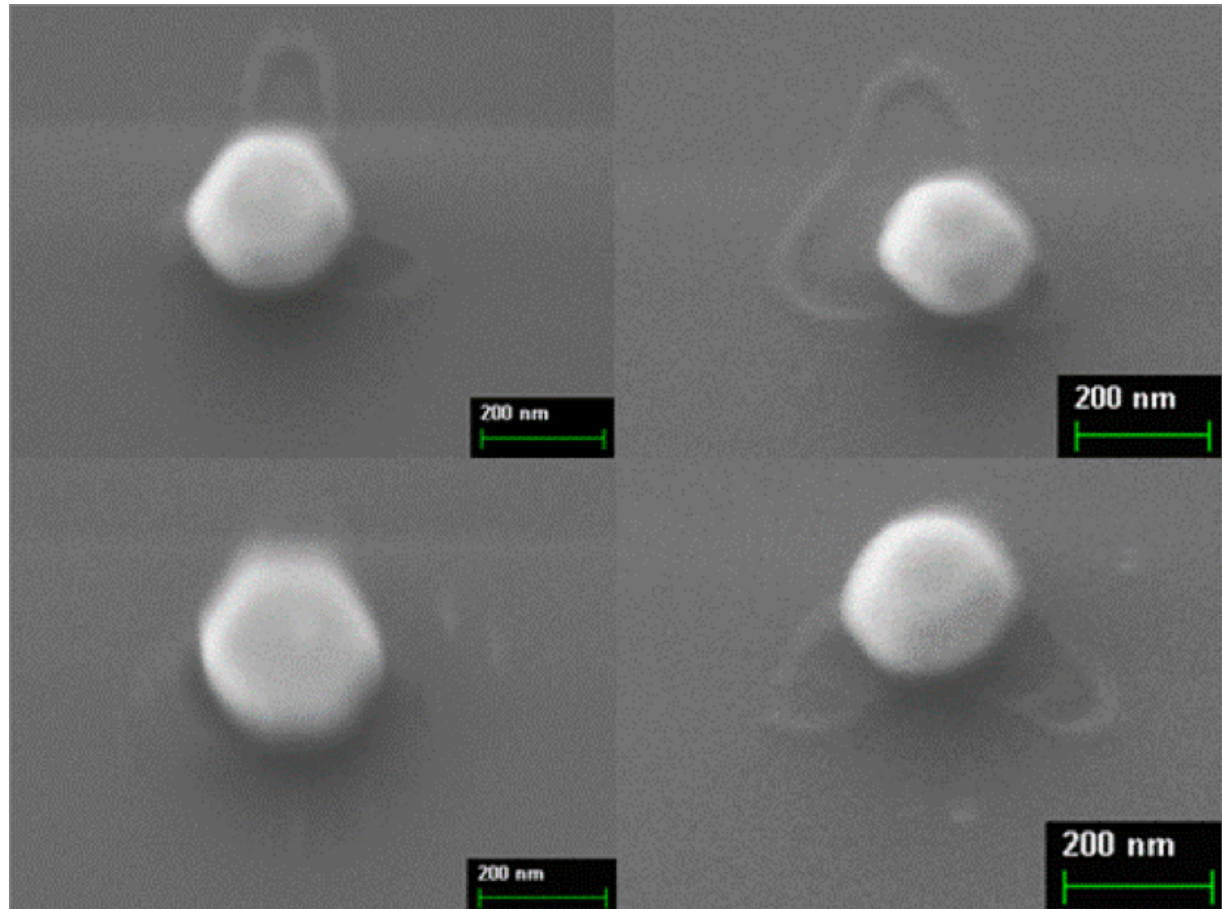
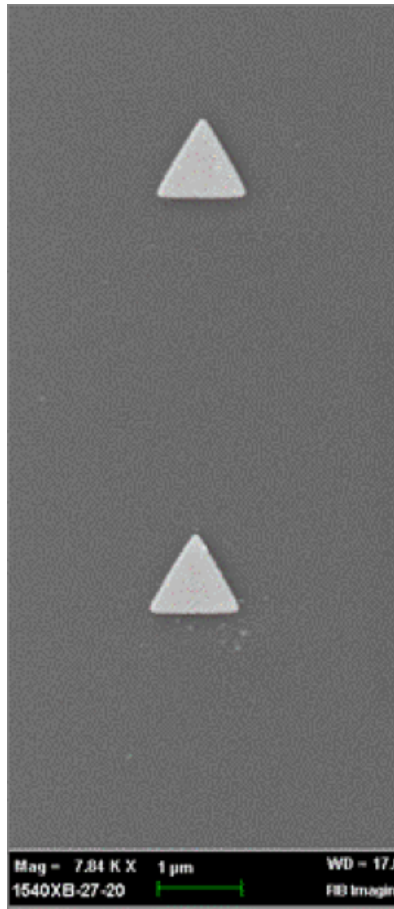
$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$


# Phase isosurface of residual strain

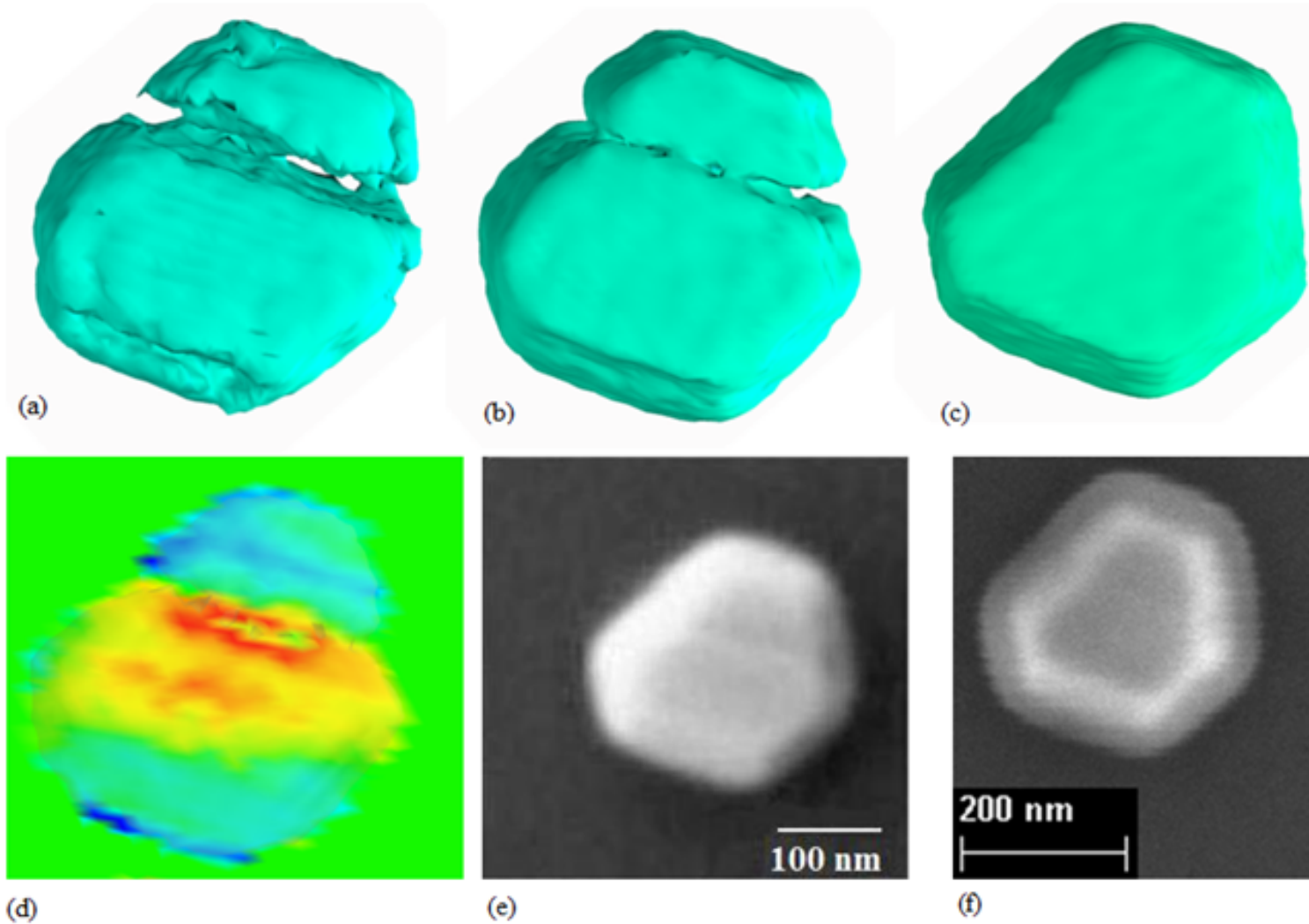
## 200nm Barium Titanate (BTO) crystals



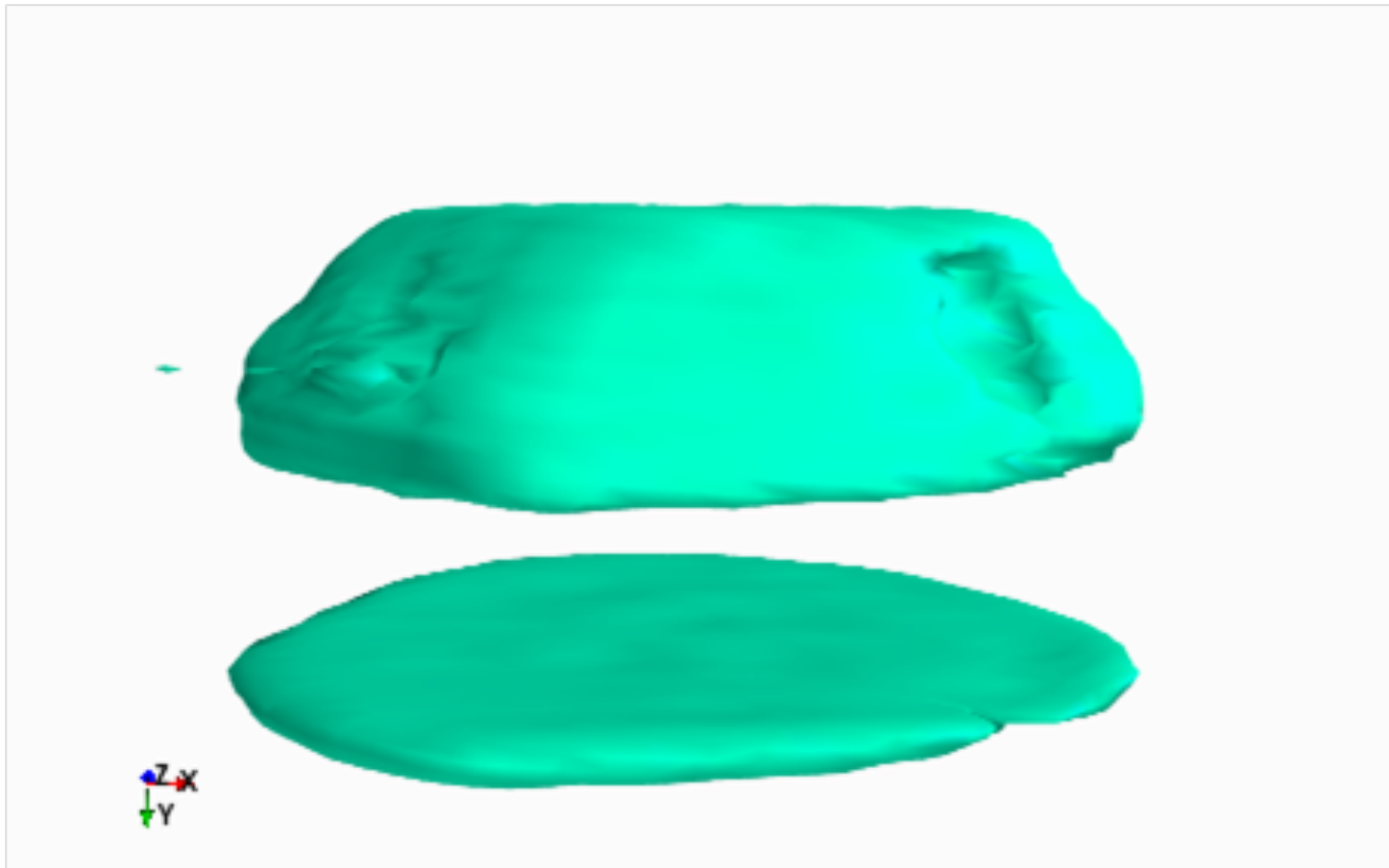
# Single Au nanocrystal synthesis



# Different Bragg Peaks

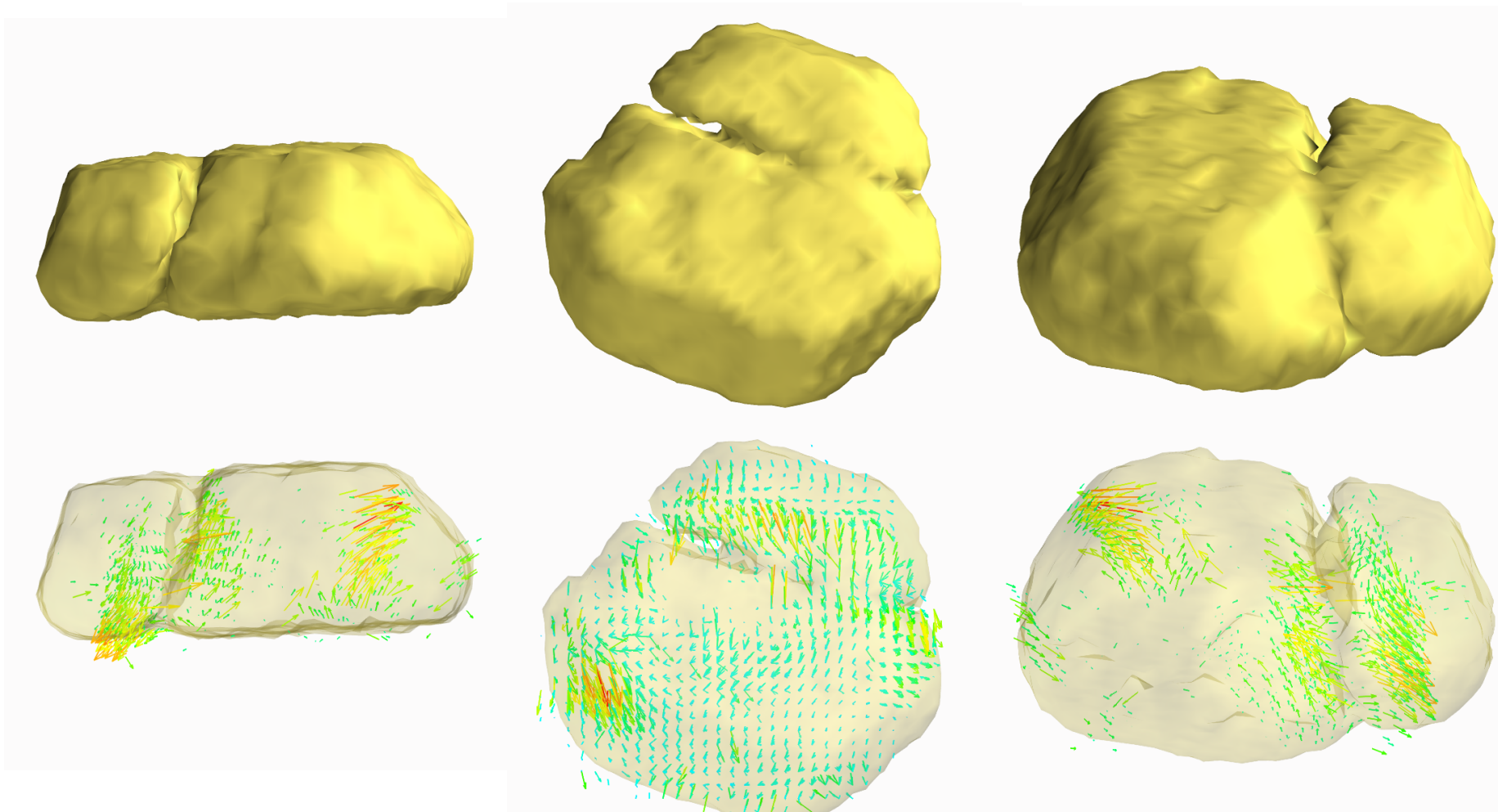


# Horizontally Faulted Slab



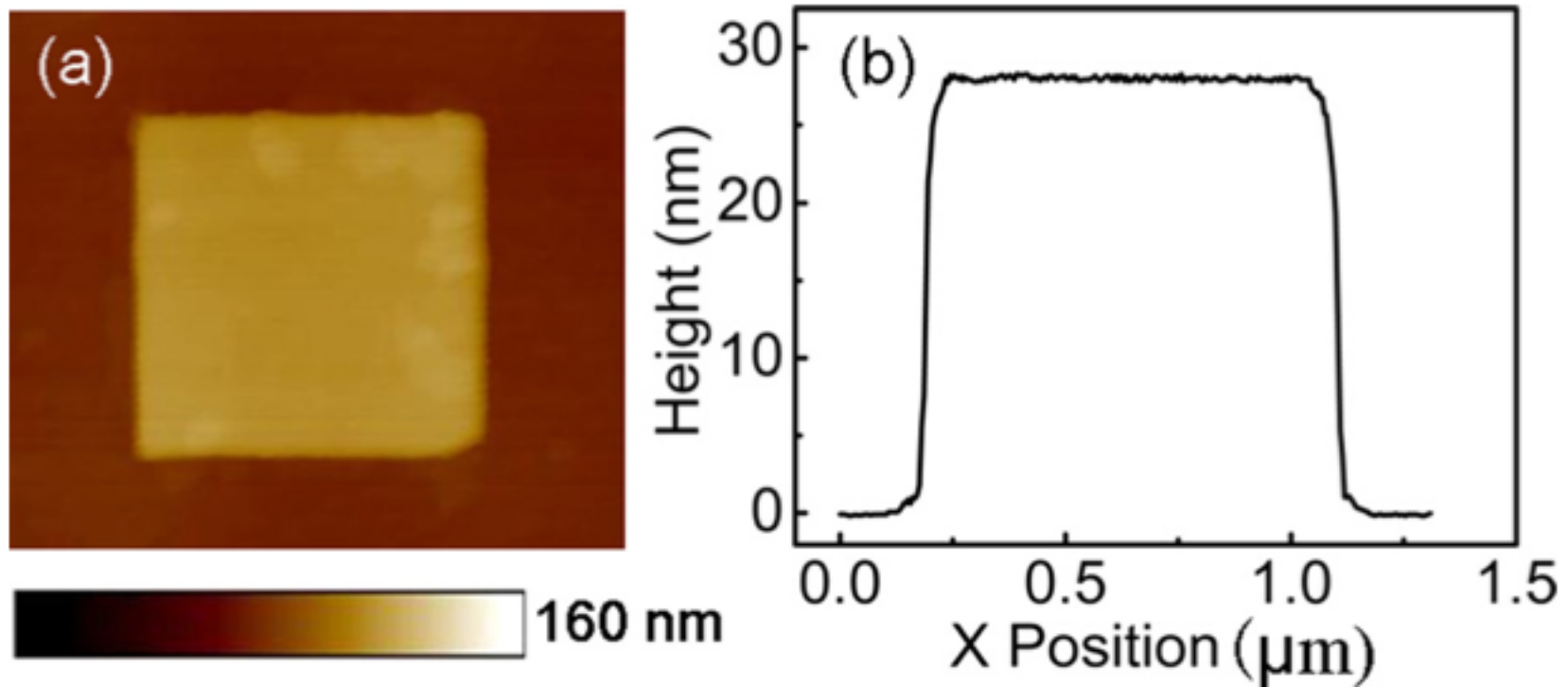
# Vector displacement field

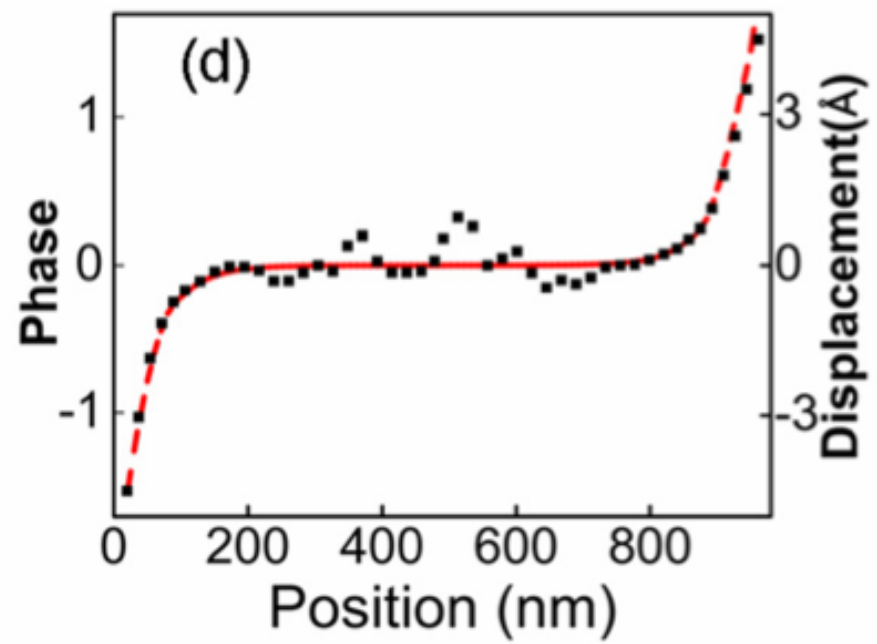
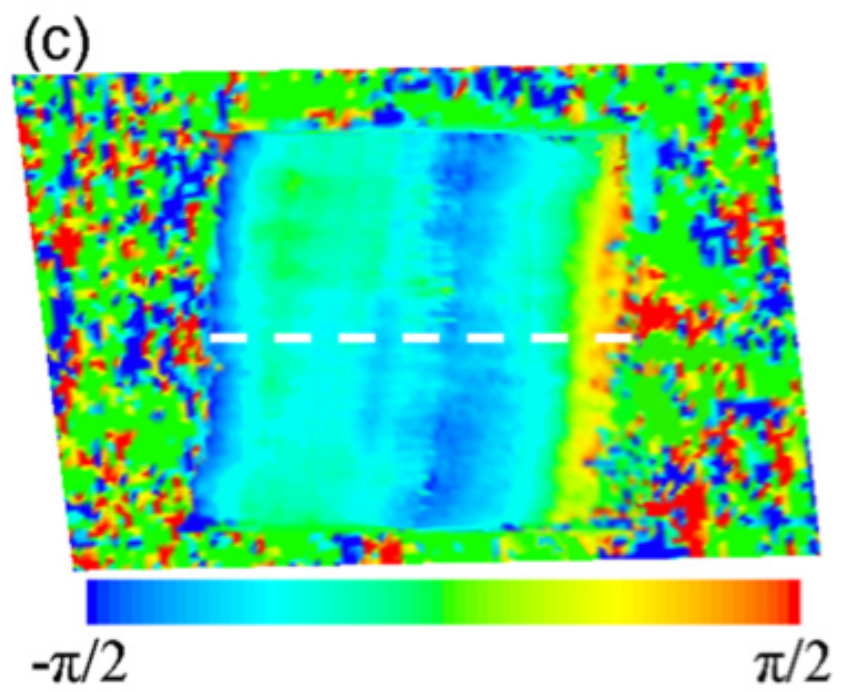
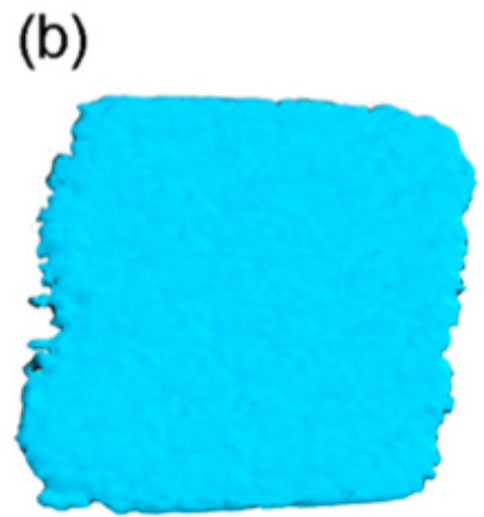
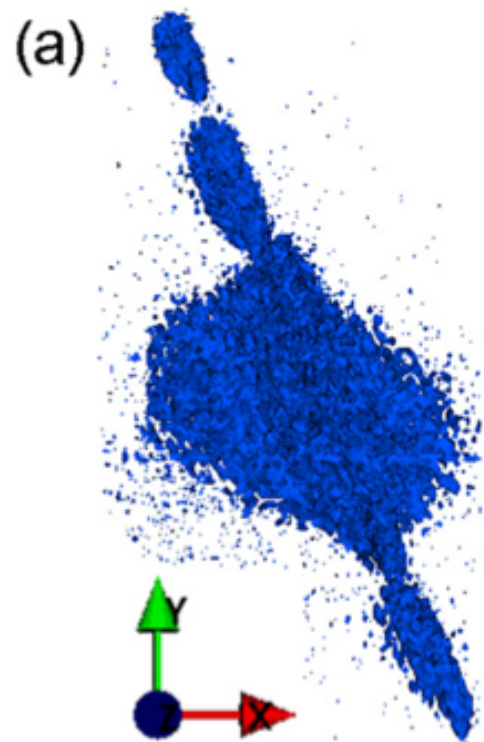
Merged reconstructions from (11-1) (020) and (-111)



# In-plane elastic relaxation in single ultrathin strained silicon-on-insulator structure

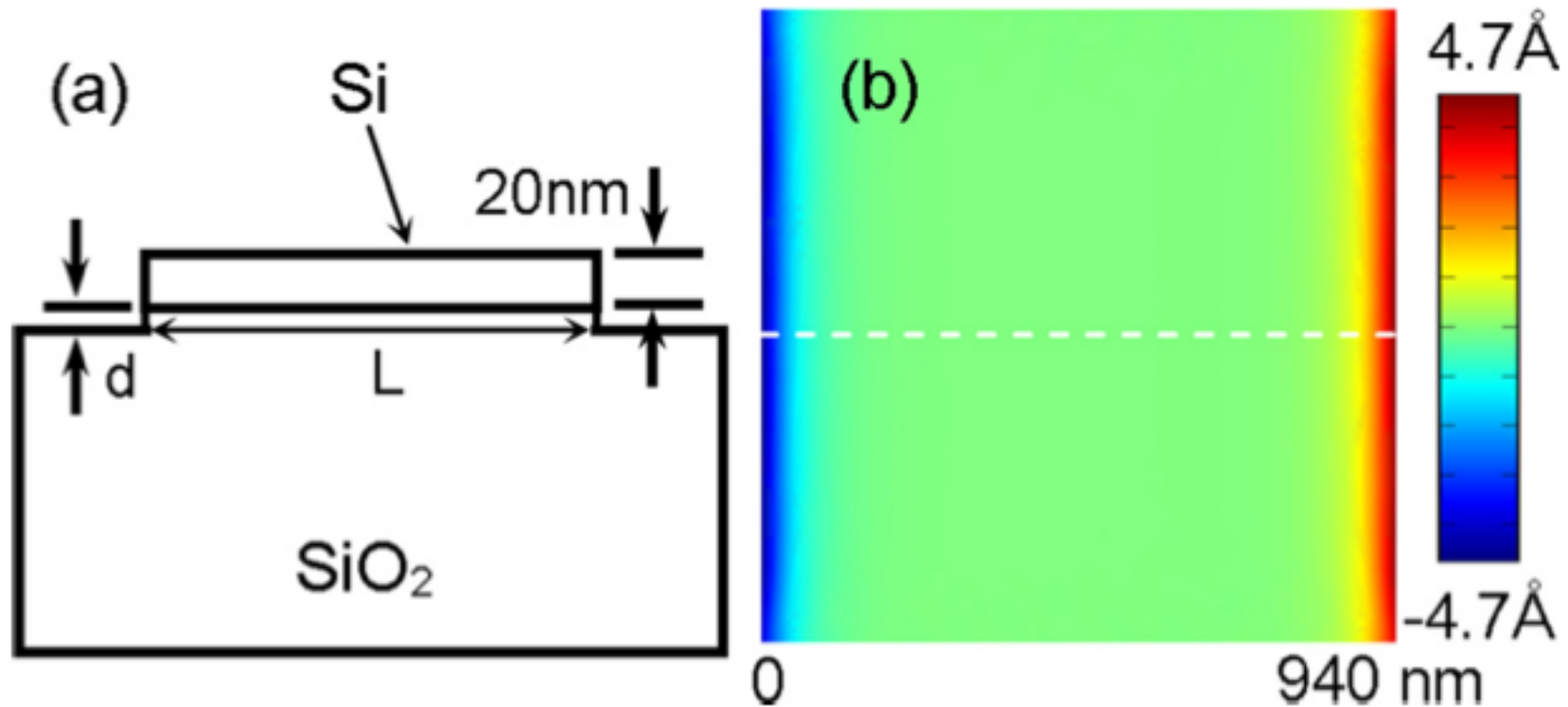
G. Xiong, O. Moutanabbir, X. Huang, S.A. Paknejad, X. Shi, R. Harder, M. Reiche and I.K. Robinson, APL 99 114103 (2011)





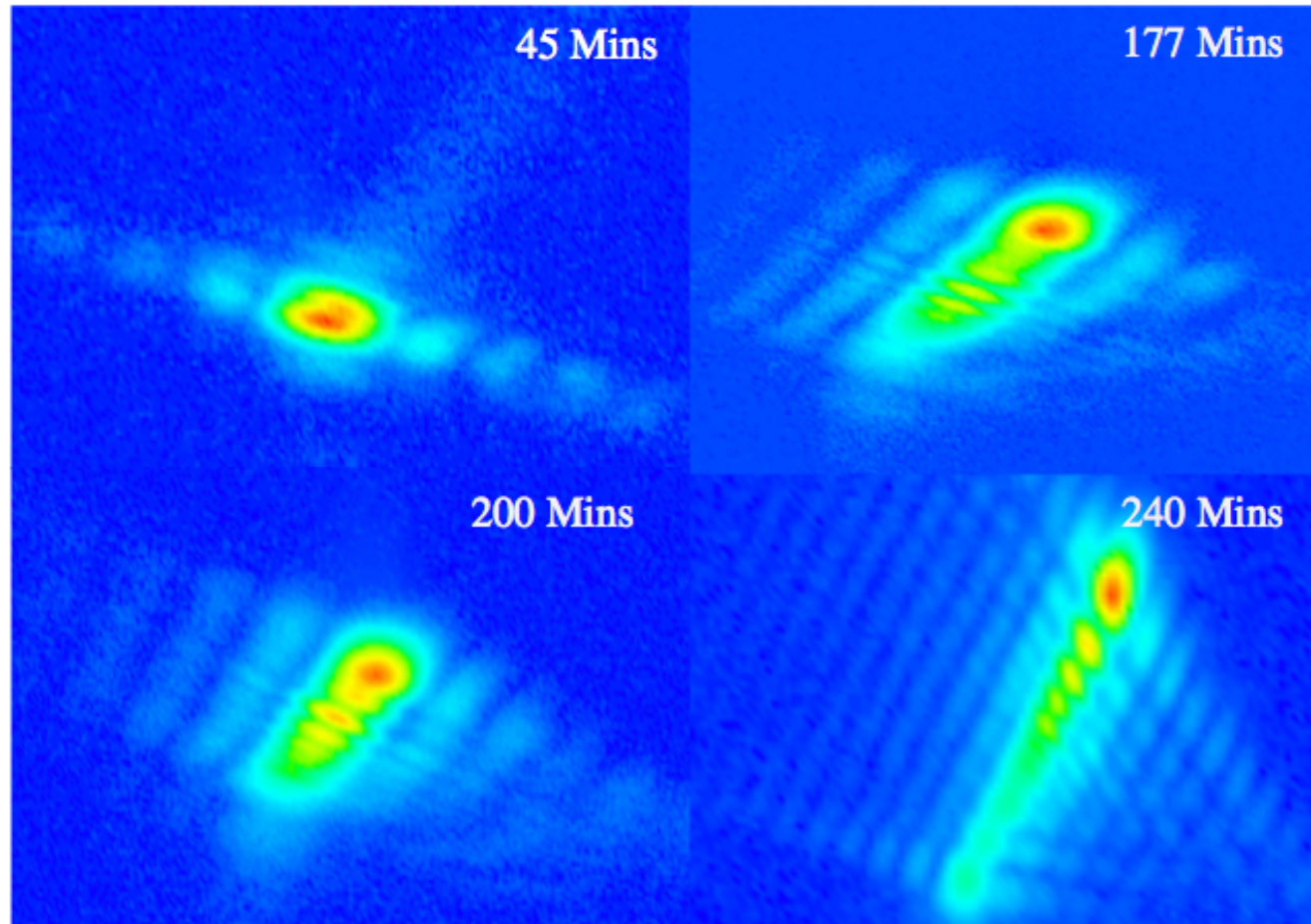
# In-plane elastic relaxation in single ultrathin strained silicon-on-insulator structure

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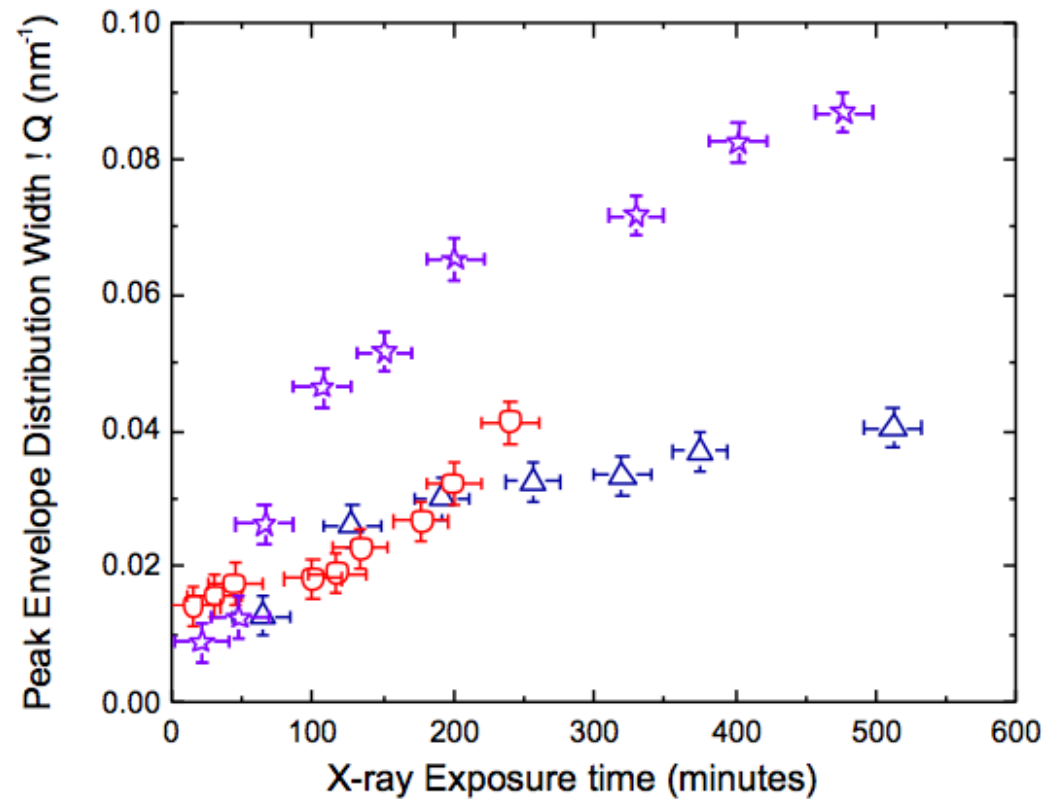
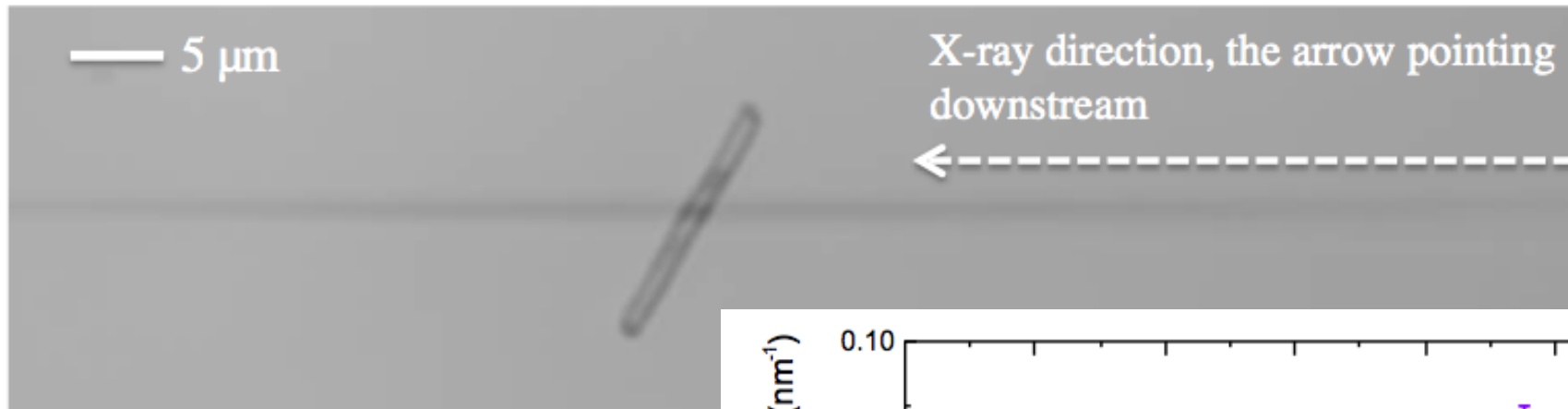


# Radiation Induced Bending of Si Nanowires

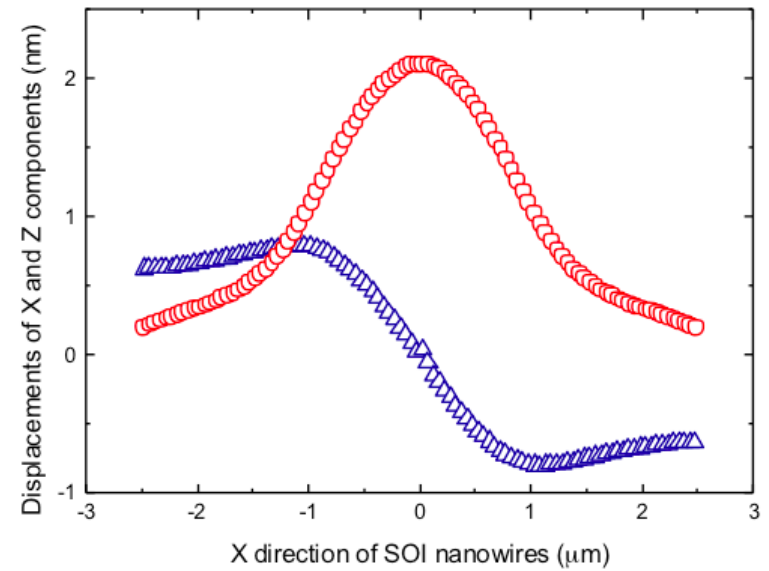
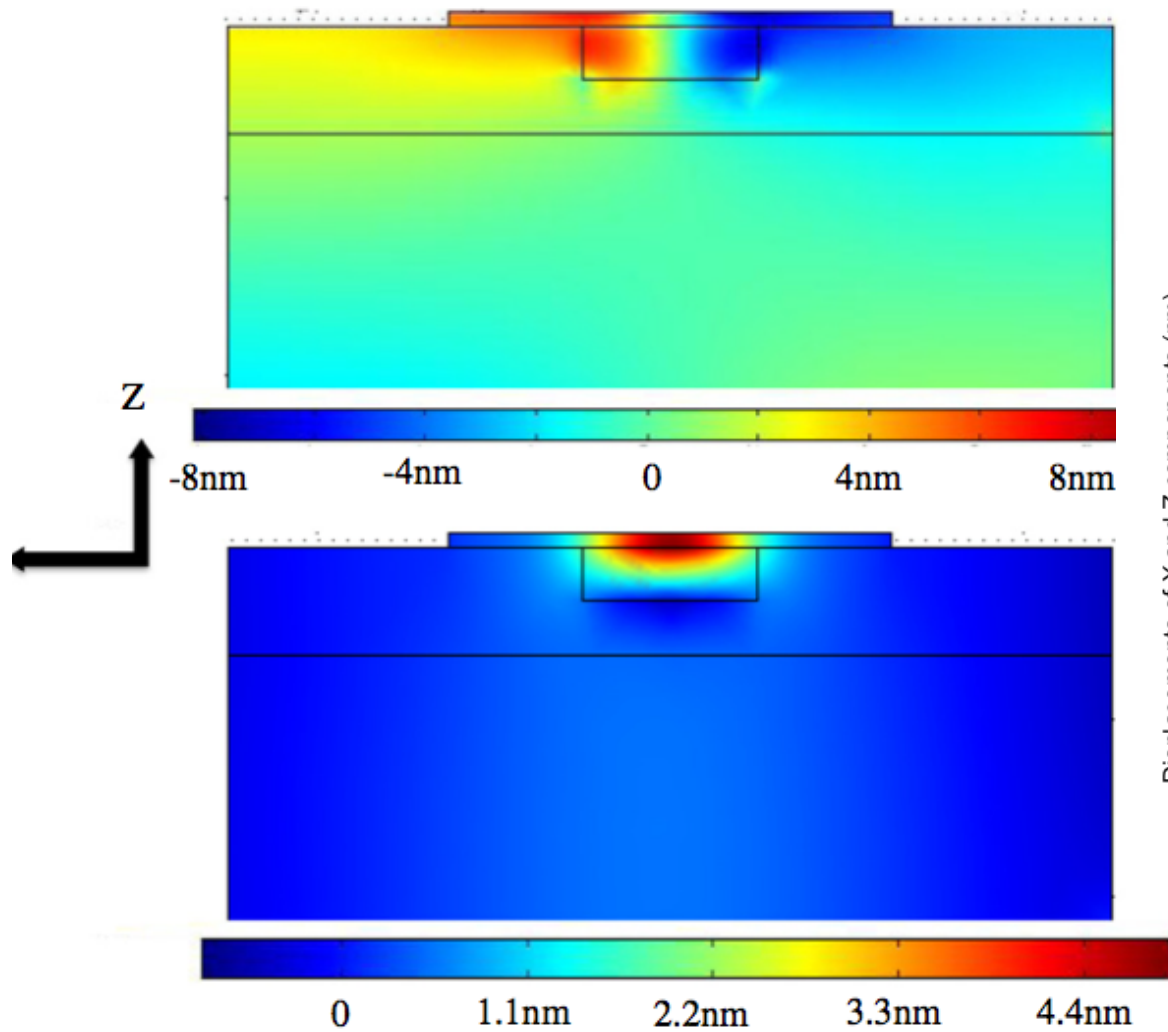
Xiaowen Shi, Gang Xiong, Xiaojing Huang, Ross Harder and Ian Robinson, New Journal of Physics 14 063029 (2012)



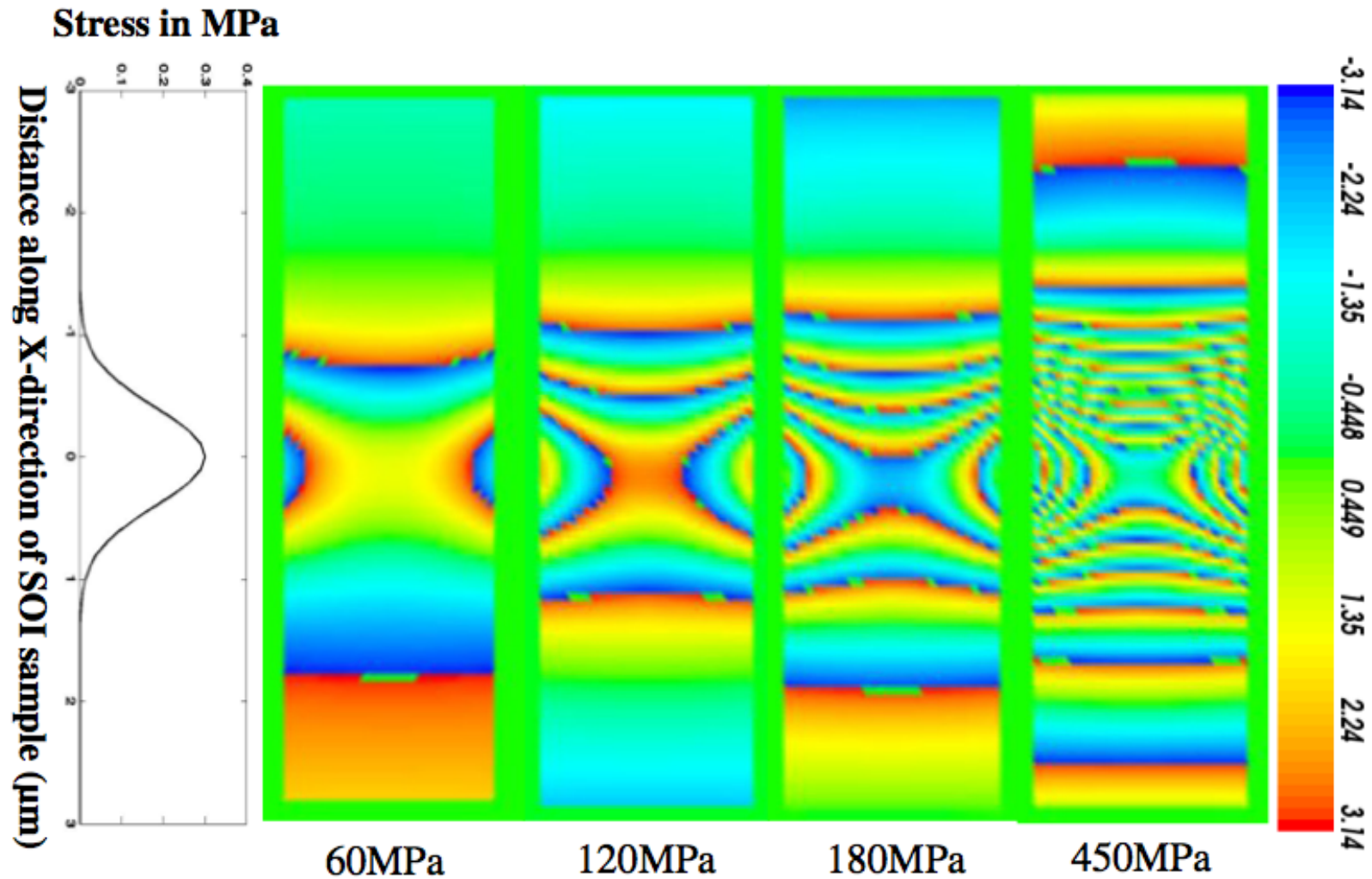
# Confocal Image of Si Nanowire



# FEA Model of Bending of Si Nanowires

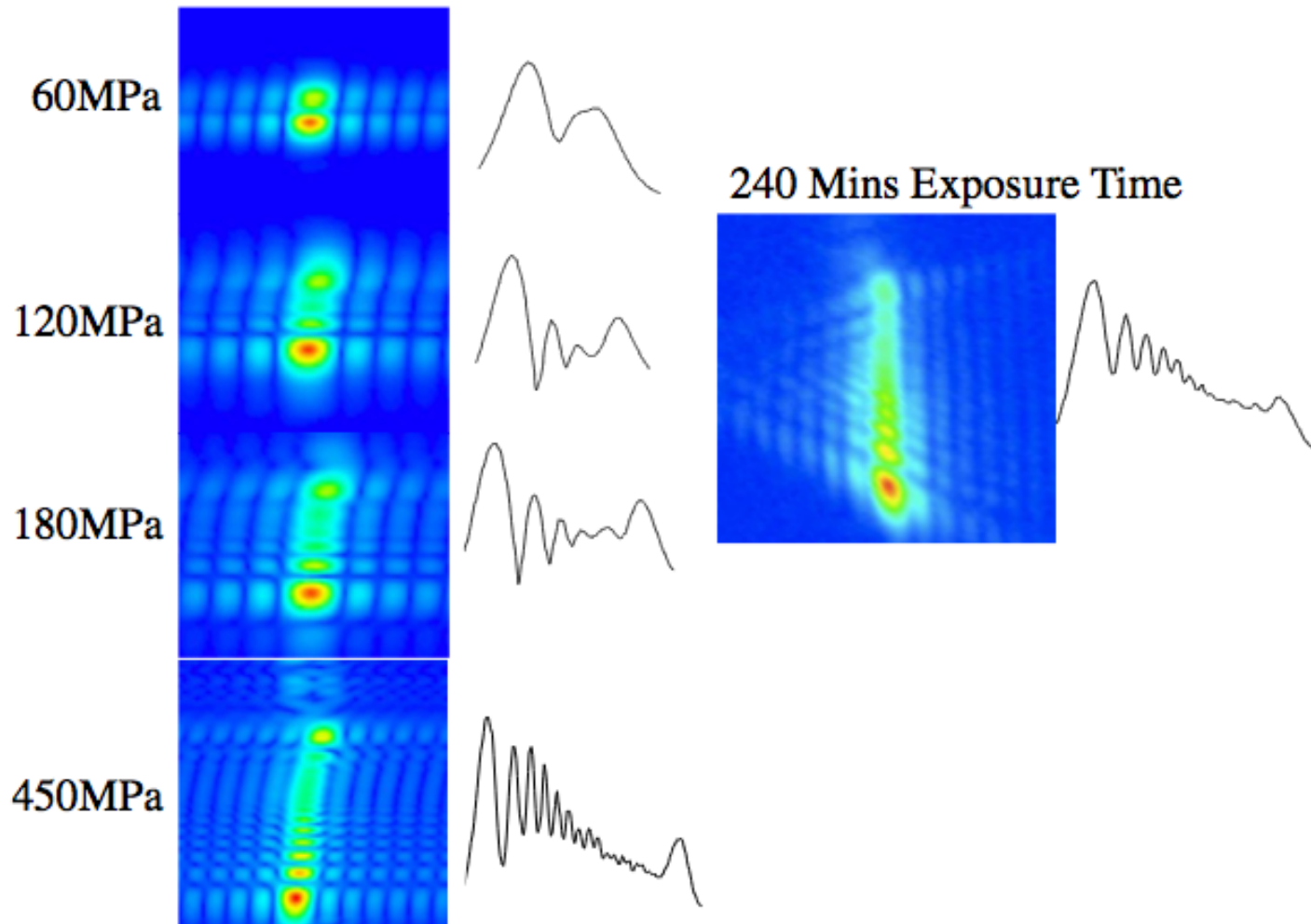


# Calculated Phase in Si Nanowires

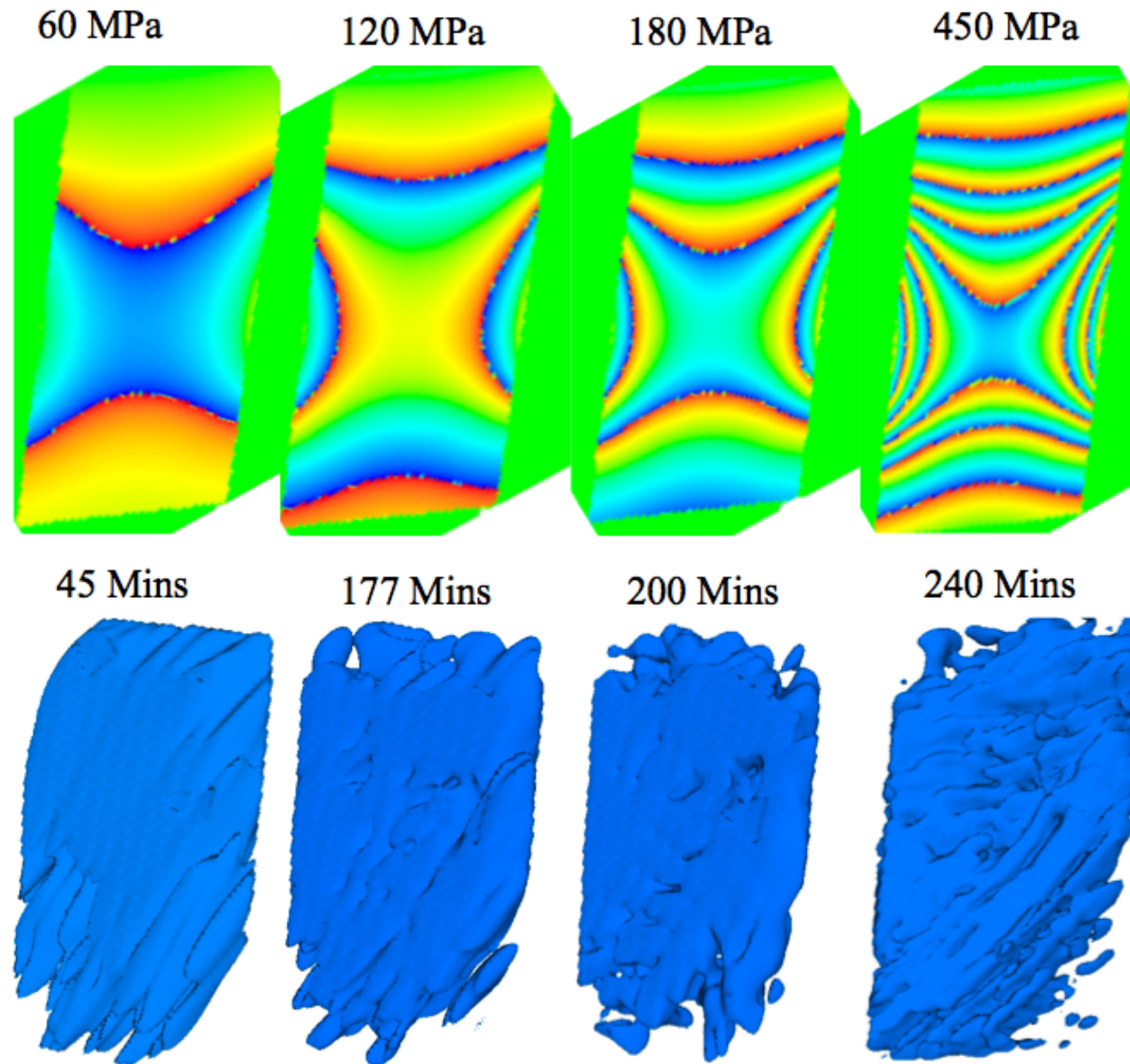


# Radiation Induced Bending of Si Nanowires

Xiaowen Shi, Gang Xiong, Xiaojing Huang, Ross Harder and Ian Robinson, New Journal of Physics 14 063029 (2012)

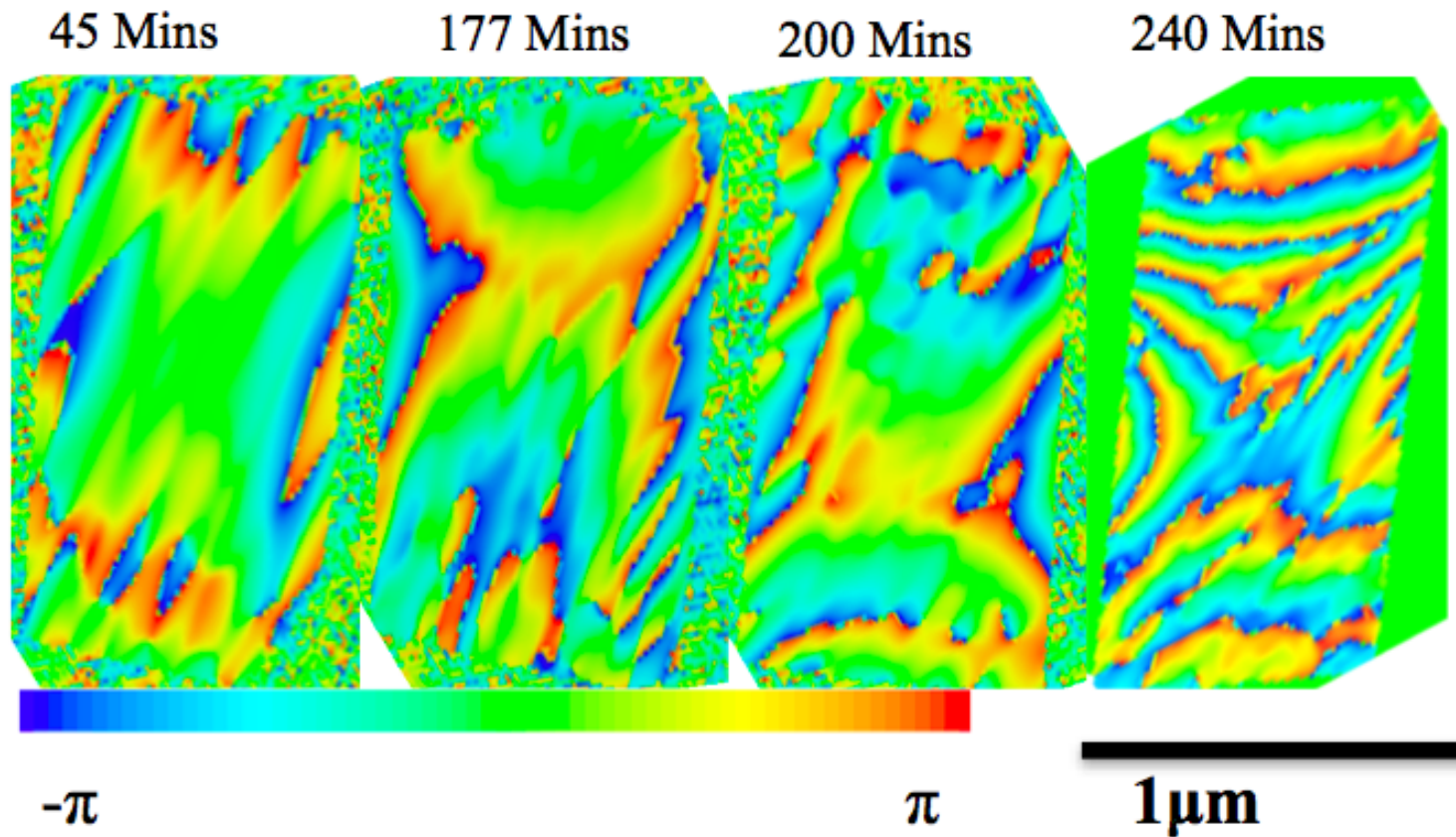


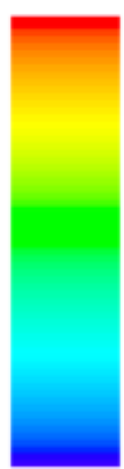
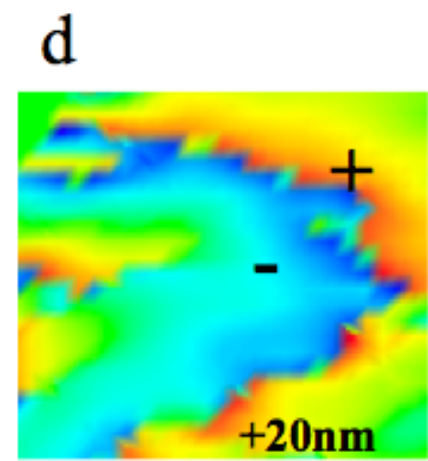
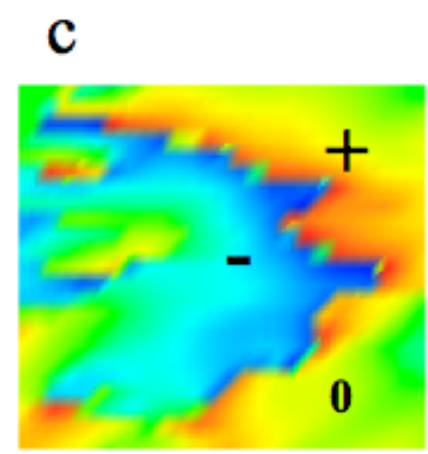
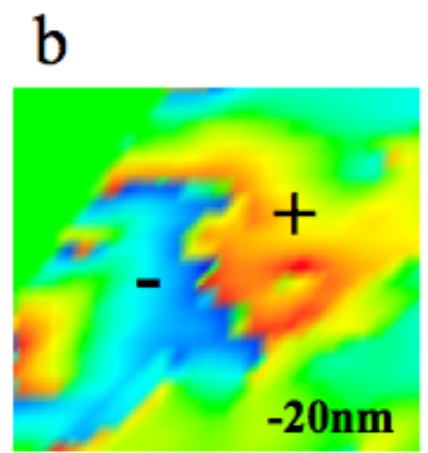
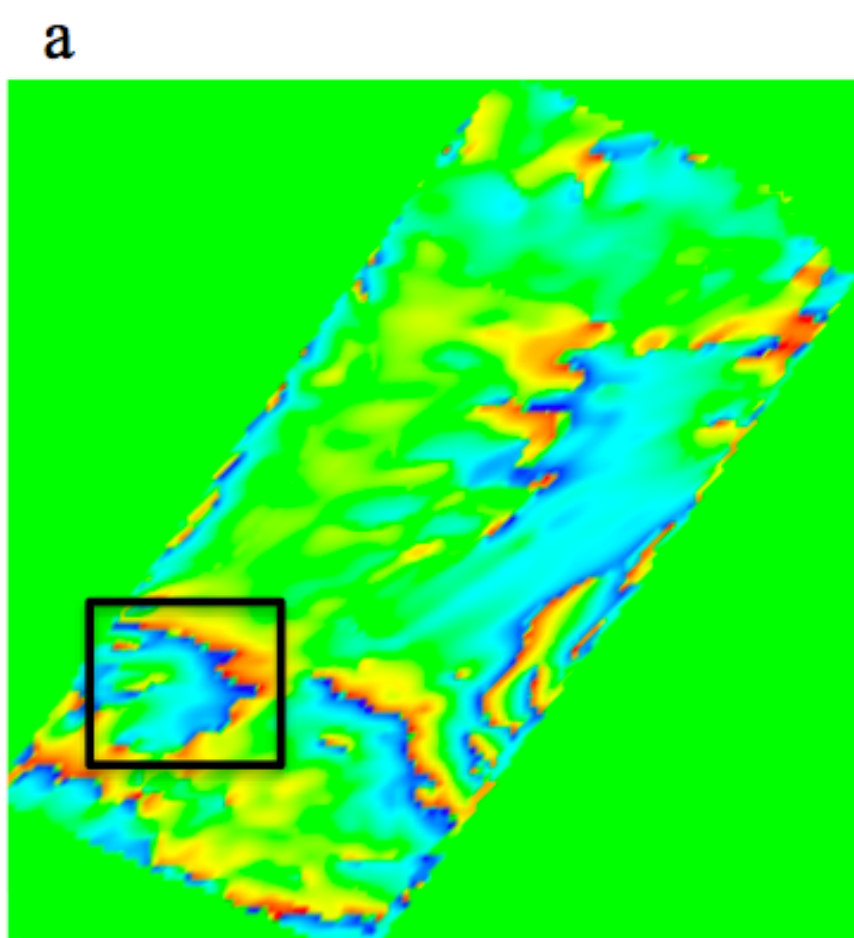
# Guided-phase coherent diffraction imaging



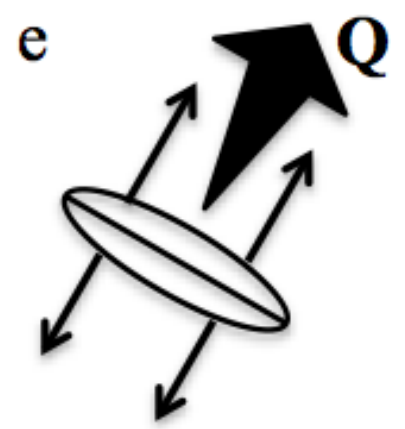
# Guided-phase coherent diffraction imaging of strongly bent Silicon nanowires

Xiaowen Shi, Gang Xiong, Xiaojing Huang, Jesse Clark, Ross Harder and Ian Robinson, submitted to Physical Review Letters (2013)



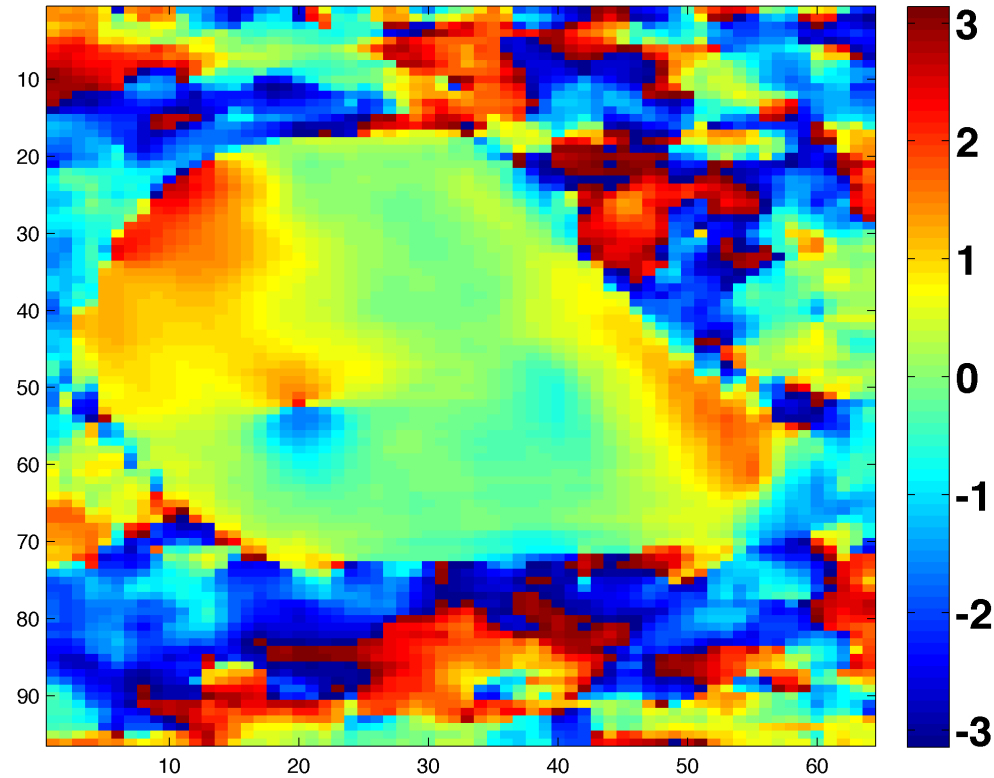


$\pi$   
 $-\pi$



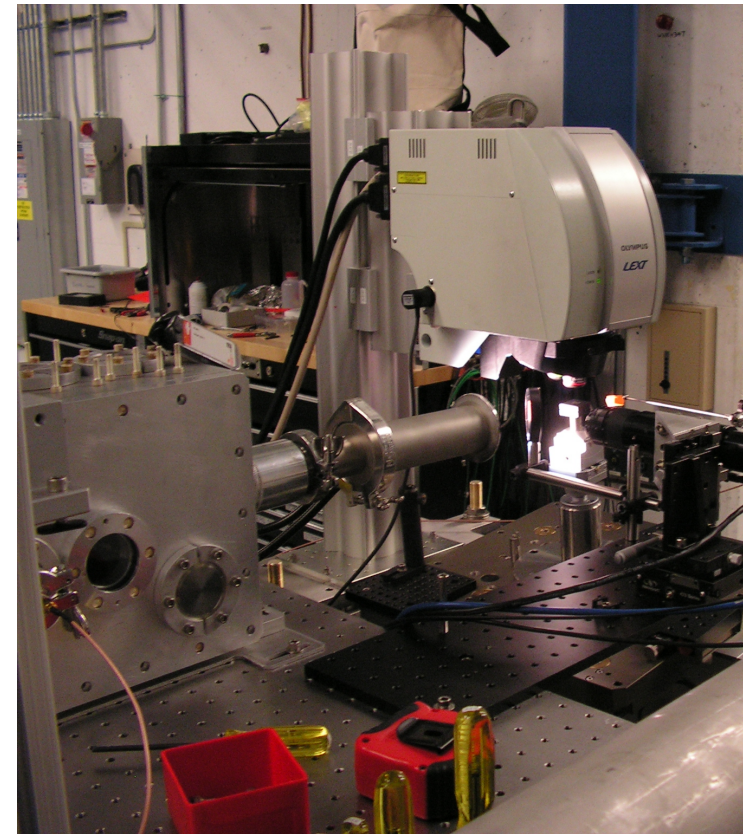
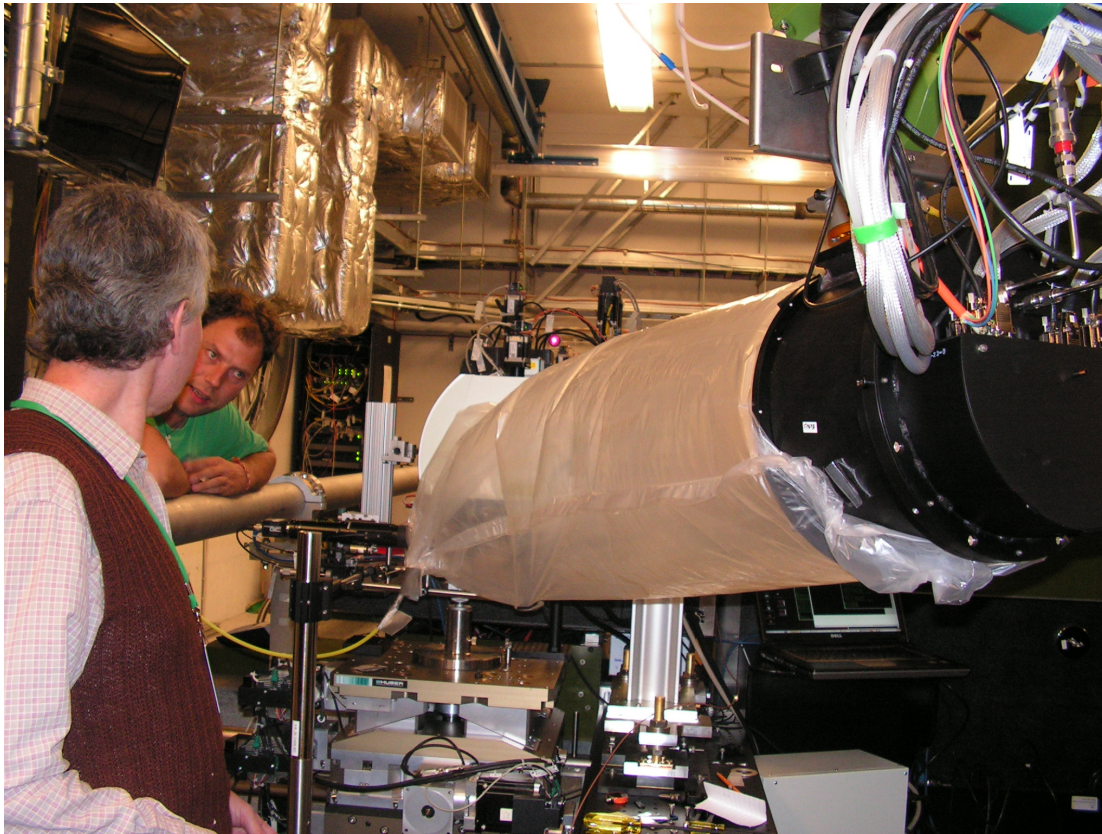
# Strain around Dislocation in Au

Jesse Clark, August 2012



# 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

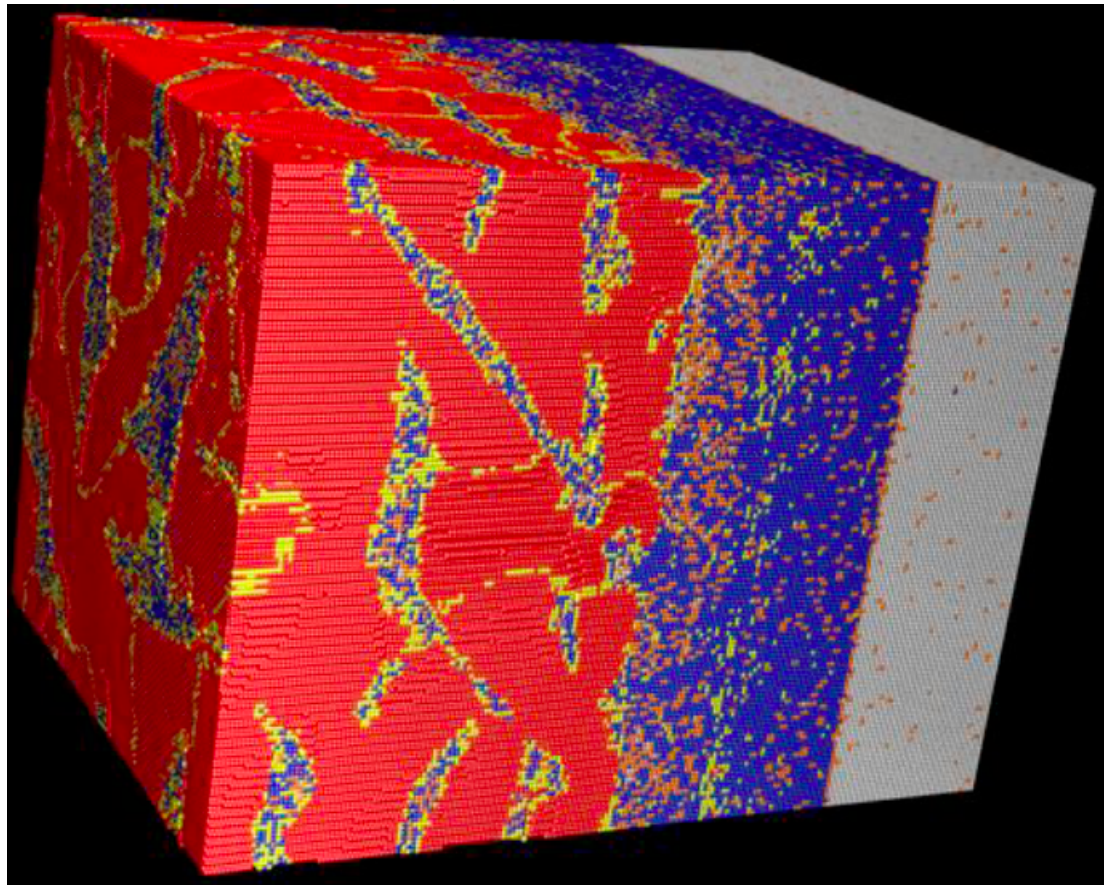


# MD simulation of Shock Wave

Damage in Fe along (001) direction

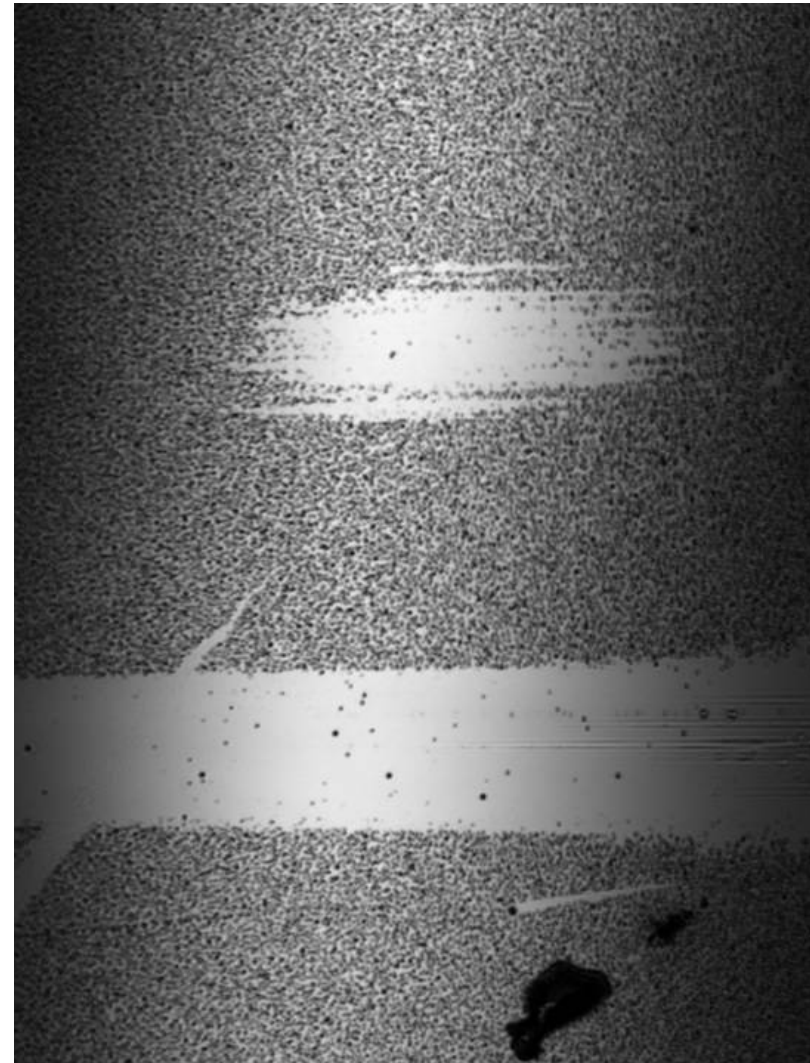
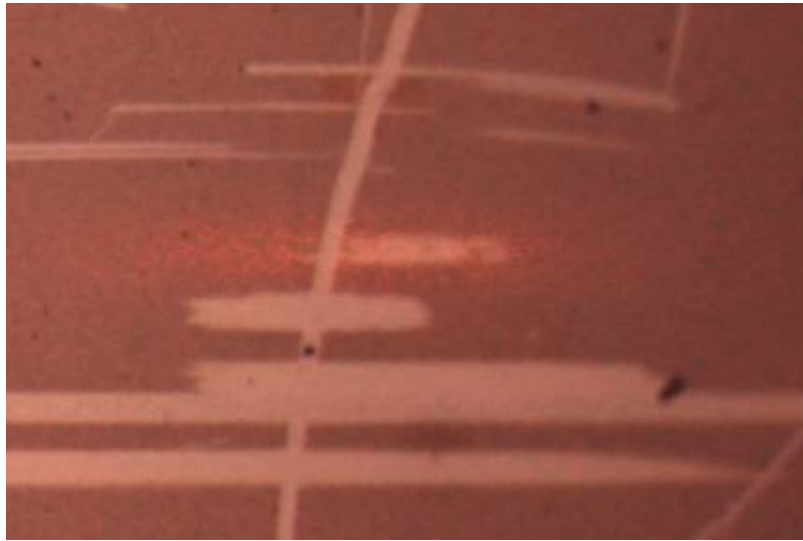
K Kadau, TC Germann, PS Lomdahl, and BL Holian.

Science, 296 1681 2002



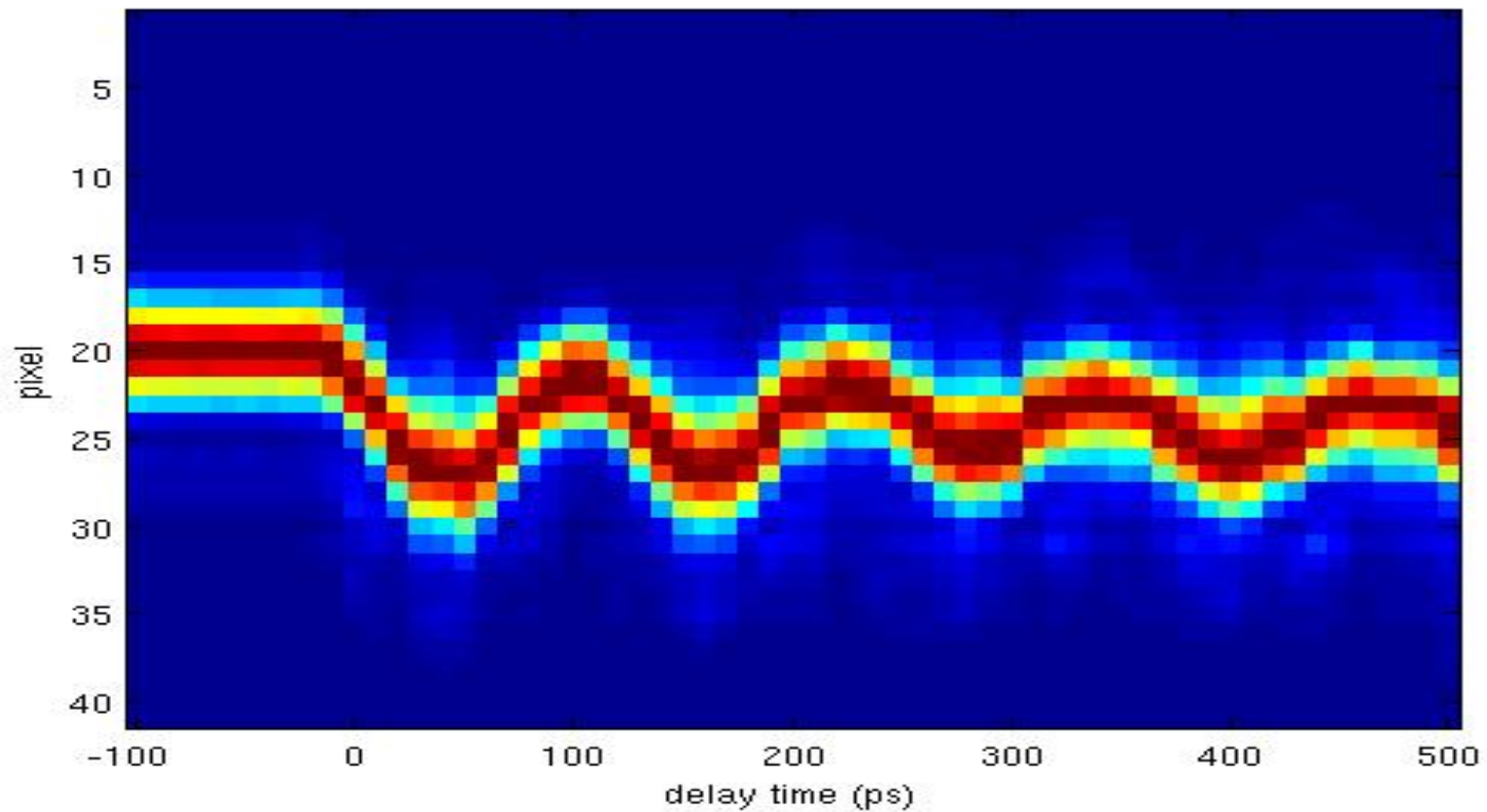
I. K. Robinson, Solid Mechanics 2013

# Visible and Confocal microscopy



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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



# “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

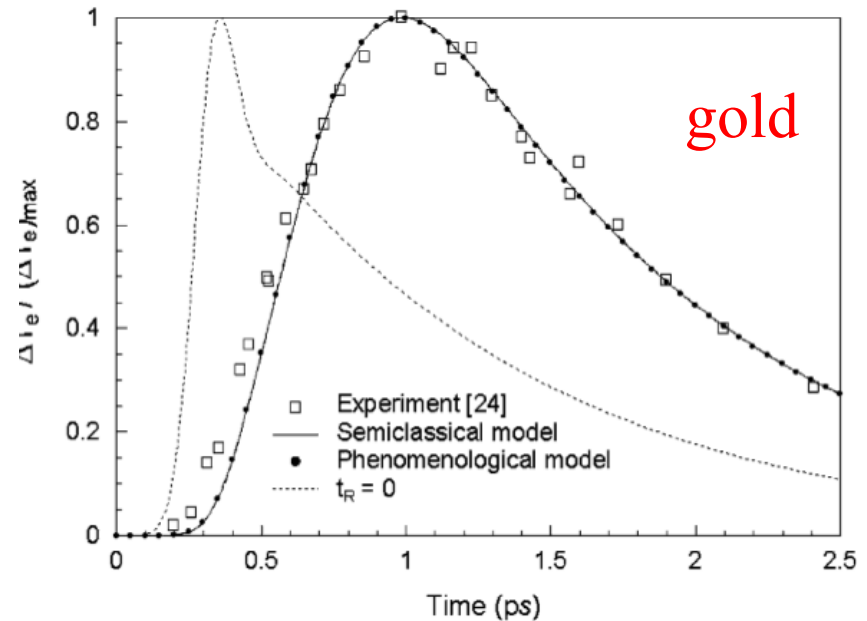
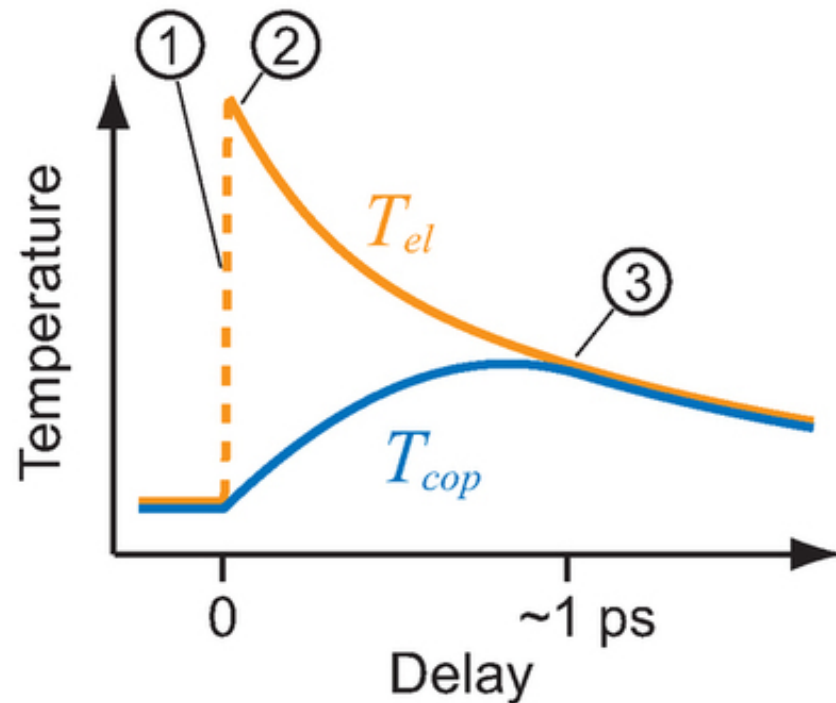
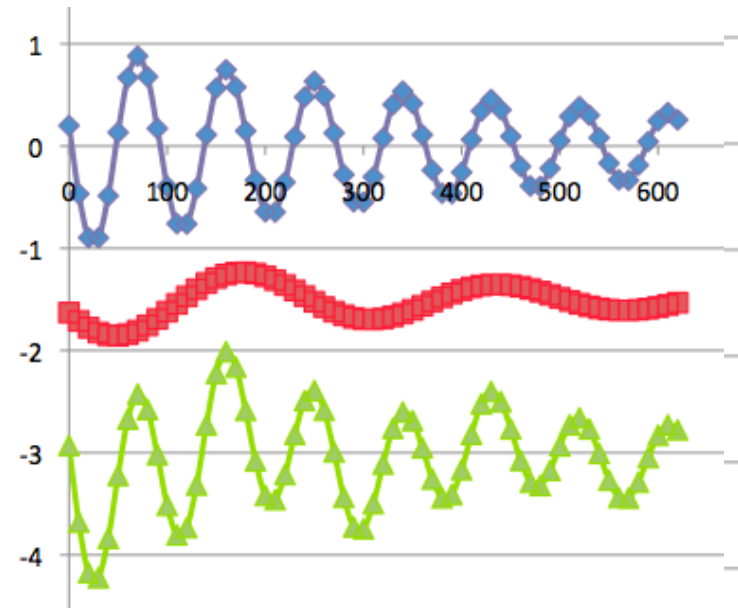
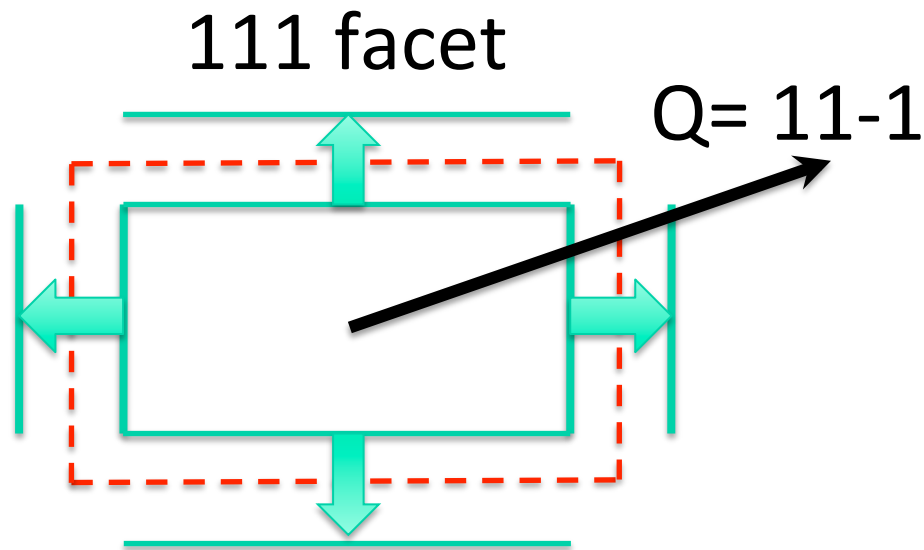


fig. 2. Comparison of the change in electron temperature at the front surface of an 80-nm gold film irradiated by a 2.8 mJ/n<sup>2</sup>, 800 nm, 150-fs laser pulse.

# Two Normal Modes of Vibration

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



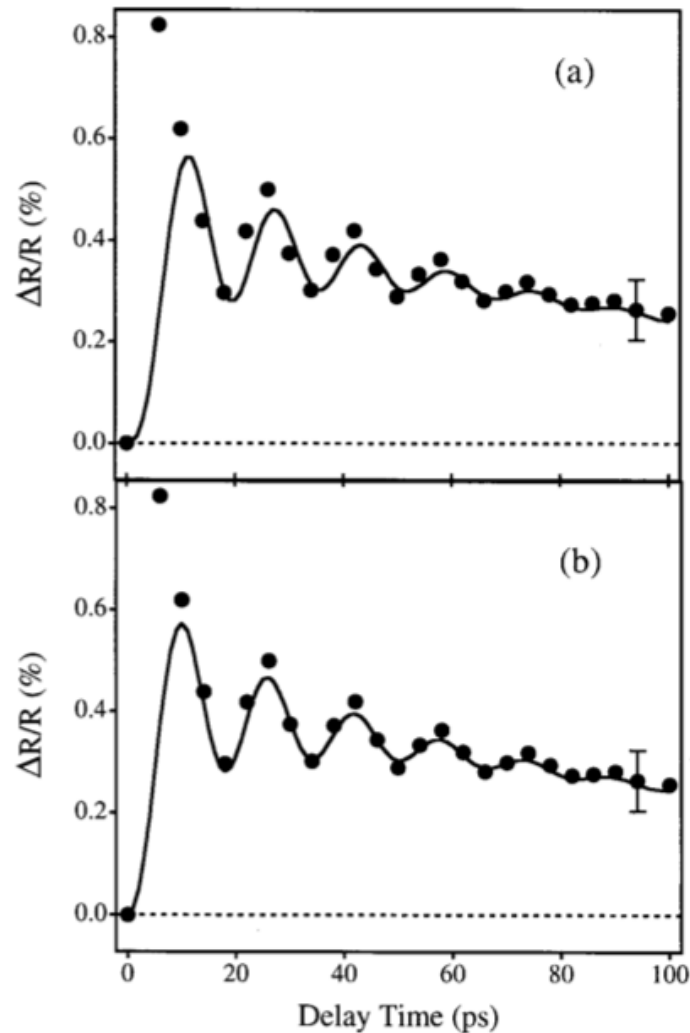
$$T_1 = 90\text{ps} \quad h_1 = 145\text{nm} \quad c_s = 3240\text{ m/s}$$

$$T_2 = 259\text{ps} \quad h_2 = 420\text{nm}$$

# Ultrafast Absorption Spectroscopy

24nm Au nanoparticles in H<sub>2</sub>O, converted to radius

G. V. Hartland, J. Chem. Phys. 116, 8048 (2002)

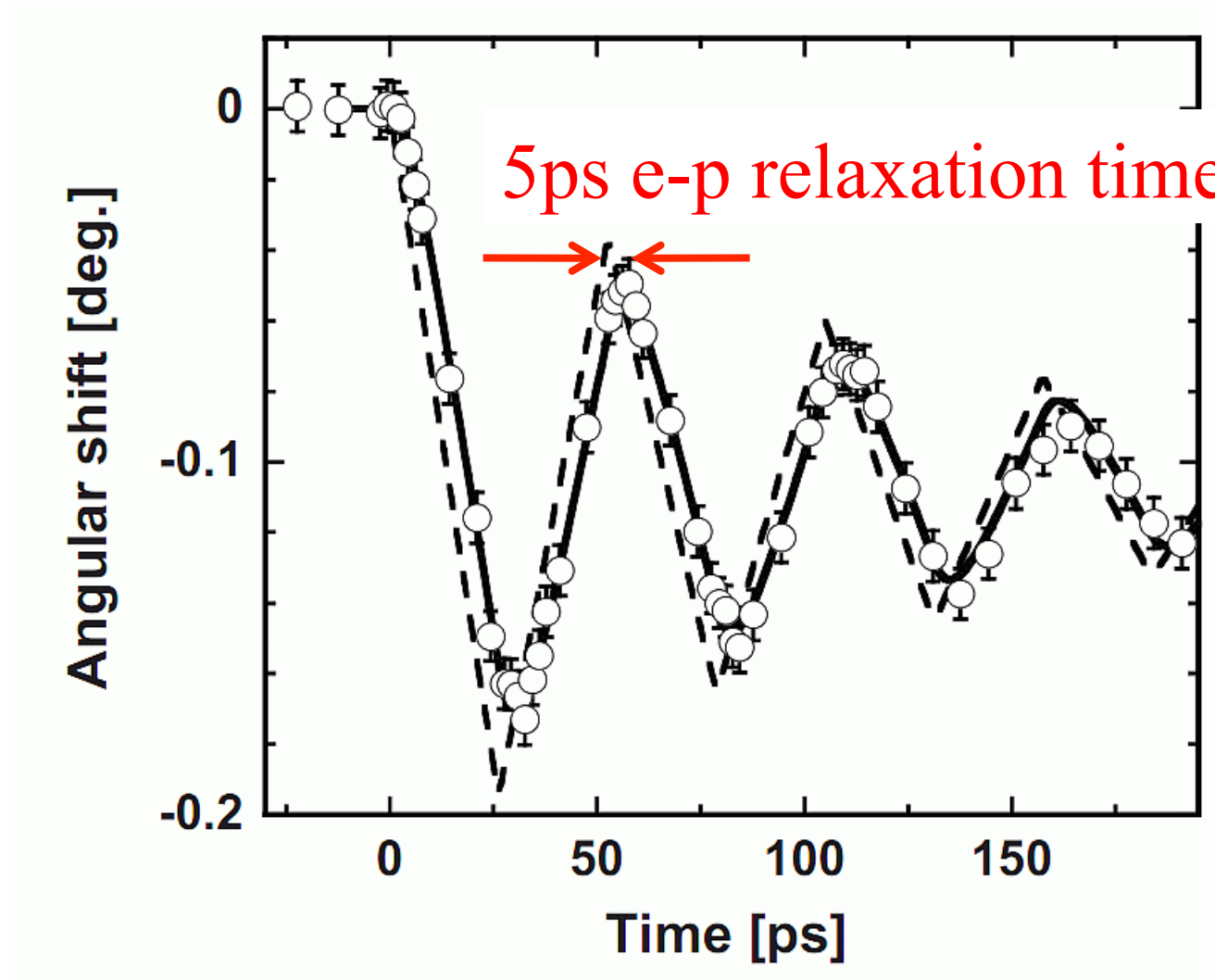


(a) Simple normal mode analysis with impulse heating.

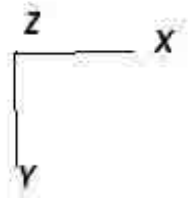
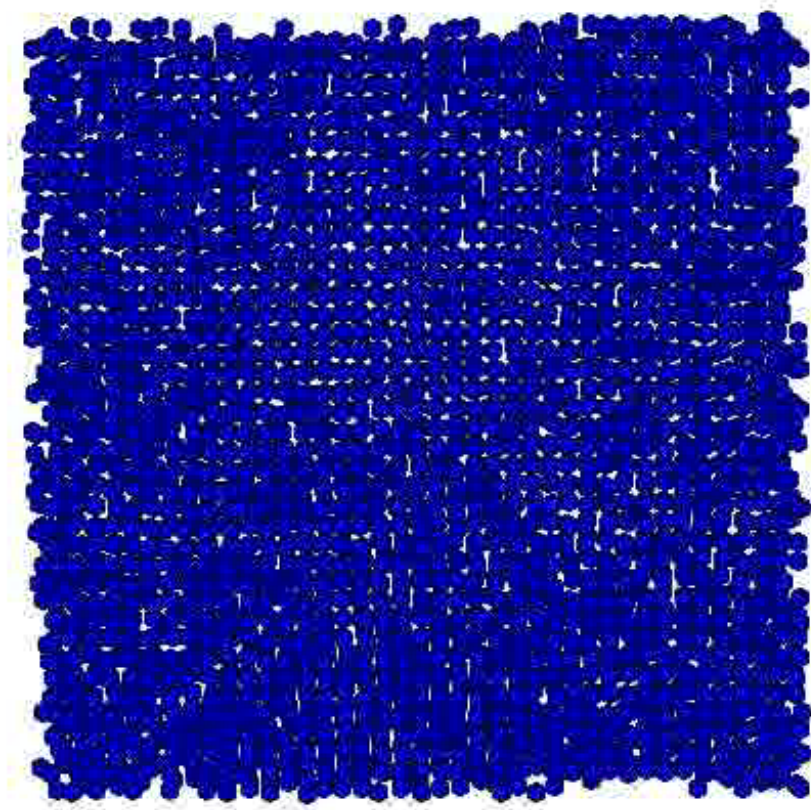
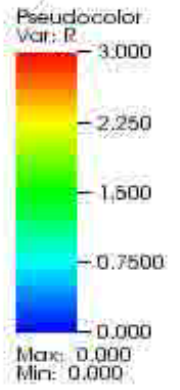
(b) Corrected by adding 2T model and electronic contribution to thermal expansion coefficient.

# Plasma Source on 90nm Au film

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

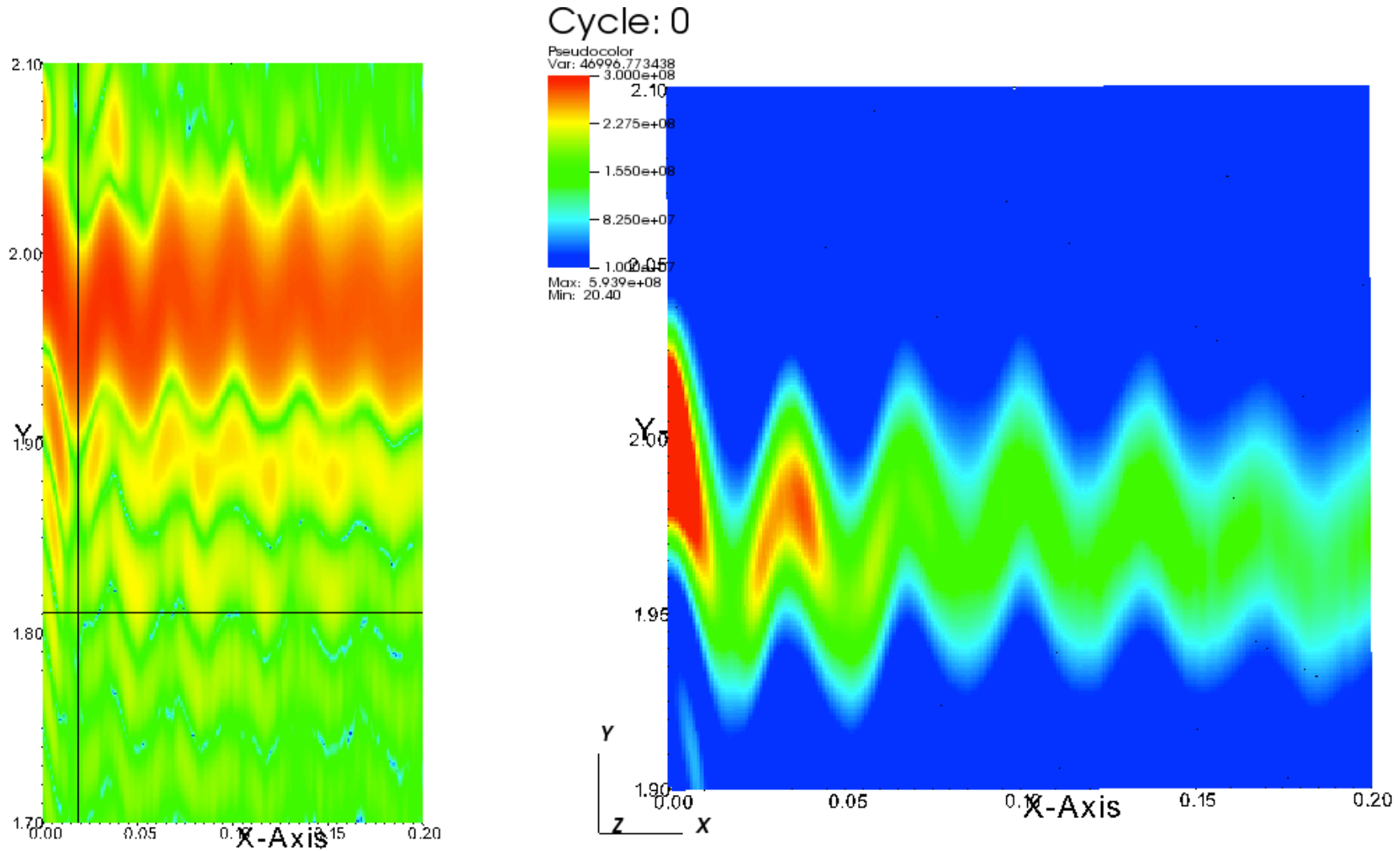


DB: dump.0  
Cycle: 0 Time: 0



# MD Simulation (LAMMPS)

Andy Higginbotham and Loren Beitra

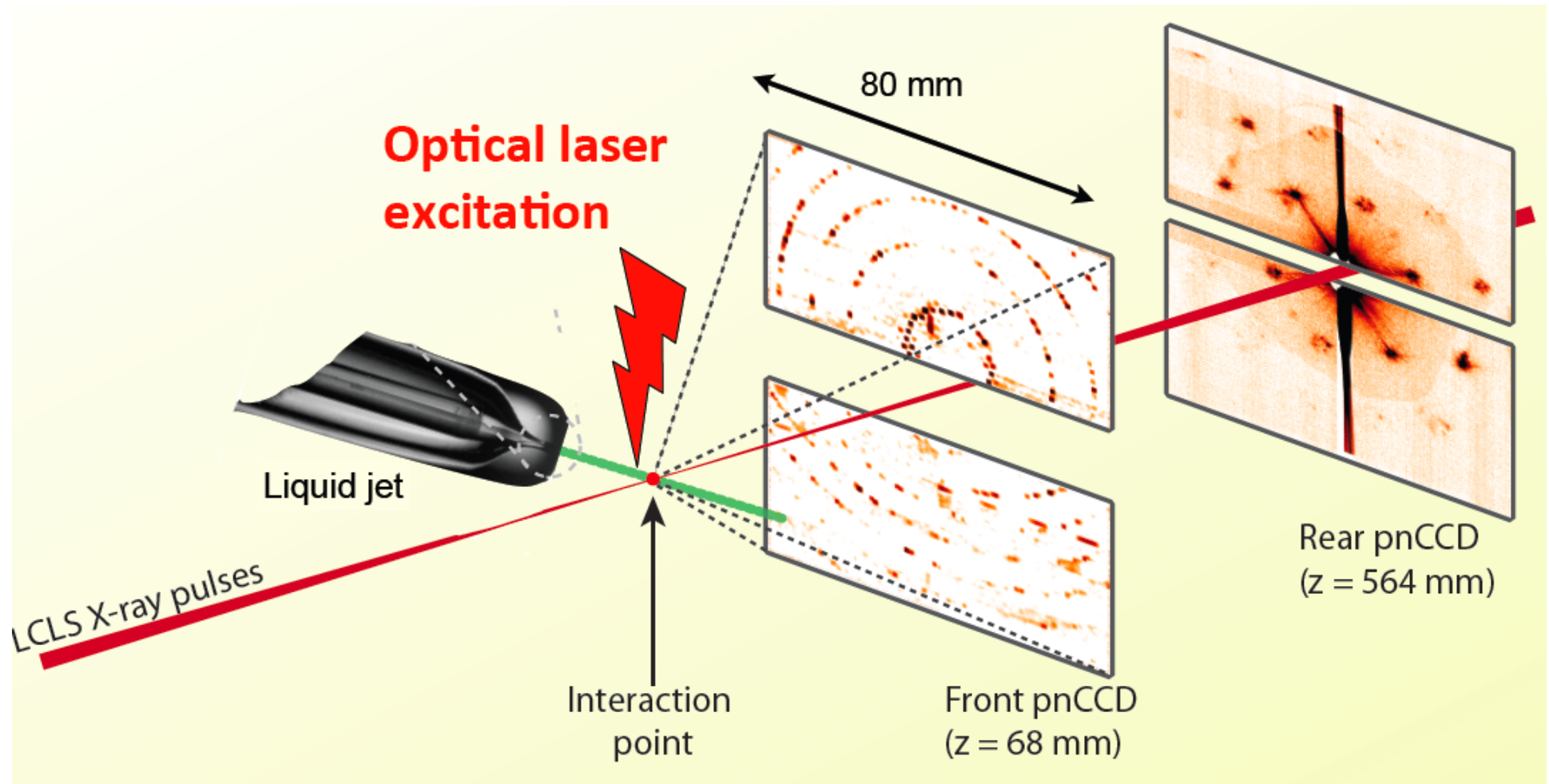


# Materials Science using XFELs

- Ground rule #1: €13,000 per **hour**
- Ground rule #2: fully automated experiment
- Ground rule #3: non-toxic, safe samples
- Ground rule #4: nanoparticles by the kg
- 30,000 pulses/sec at E-XFEL,  $3000 \times 10$
- 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
- Veto frames where no “hit” or diffraction
- Pump-Probe has two state variables
  - Optical fluence = sample temperature
  - Delay time after ‘instantaneous’ heating
- Pressure accessible using “tamper”
- Explore phase diagrams eg spinodals
- Nanoparticle sample format = synthesis

# MID design considerations

- 6m detector arm for Bragg
- 200 $\mu\text{m}$  pixels on AGIPD
- 2.5 $\mu\text{m}$  maximum sample size
- Detector bank around powder ring
- Self-veto on threshold

# Coherent x-ray diffraction (CXD)

- Complex density can image strain
- Strain associated with nano-shape
- Time resolved strain patterns
- Materials Science by XFEL?
- Conditions favorable at MID