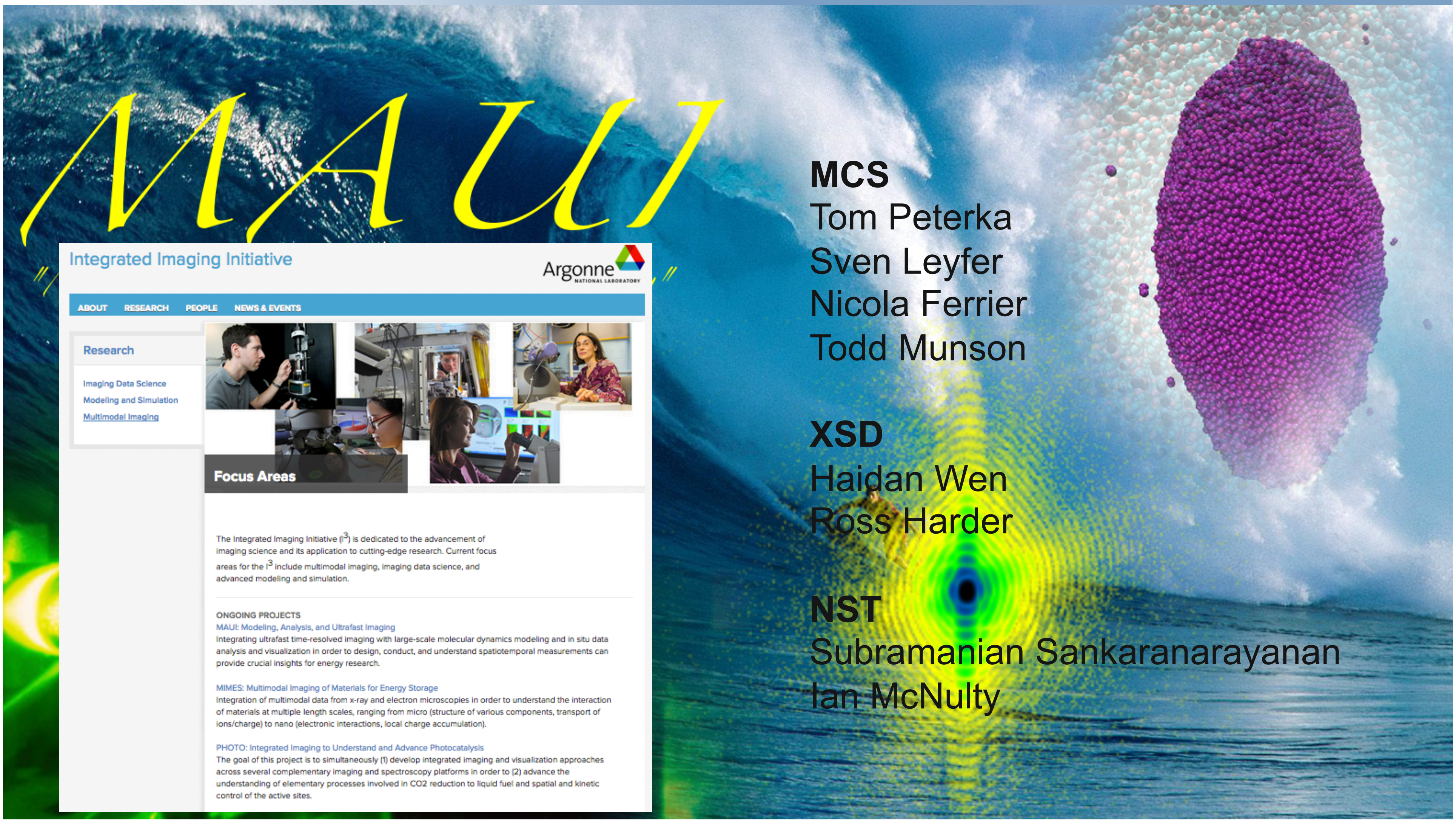


MAUI
Integrated Imaging Initiative
Argonne NATIONAL LABORATORY
ABOUT RESEARCH PEOPLE NEWS & EVENTS
Research
Imaging Data Science
Modeling and Simulation
Multimodal Imaging
Focus Areas
The Integrated Imaging Initiative (I^3) is dedicated to the advancement of imaging science and its application to cutting-edge research. Current focus areas for the I^3 include multimodal imaging, imaging data science, and advanced modeling and simulation.
ONGOING PROJECTS
MAUI: Modeling, Analysis, and Ultrafast Imaging
Integrating ultrafast time-resolved imaging with large-scale molecular dynamics modeling and in situ data analysis and visualization in order to design, conduct, and understand spatiotemporal measurements can provide crucial insights for energy research.
MIMES: Multimodal Imaging of Materials for Energy Storage
Integration of multimodal data from x-ray and electron microscopies in order to understand the interaction of materials at multiple length scales, ranging from micro (structure of various components, transport of ions/charge) to nano (electronic interactions, local charge accumulation).
PHOTO: Integrated Imaging to Understand and Advance Photocatalysis
The goal of this project is to simultaneously (1) develop integrated imaging and visualization approaches across several complementary imaging and spectroscopy platforms in order to (2) advance the understanding of elementary processes involved in CO2 reduction to liquid fuel and spatial and kinetic control of the active sites.
MCS
Tom Peterka
Sven Leyfer
Nicola Ferrier
Todd Munson
XSD
Haidan Wen
Ross Harder
NST
Subramanian Sankaranarayanan
Ian McNulty

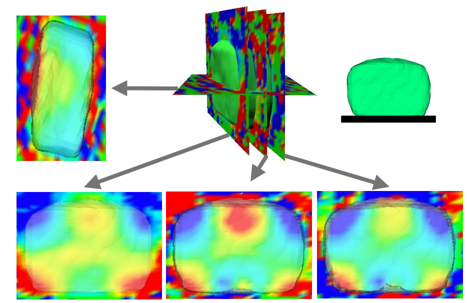
Argonne NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

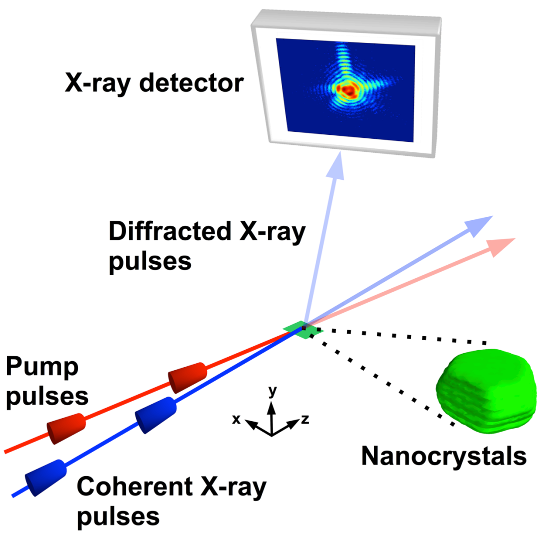
Science Impact High resolution imaging of structure

In-situ and operando characterization of materials evolution

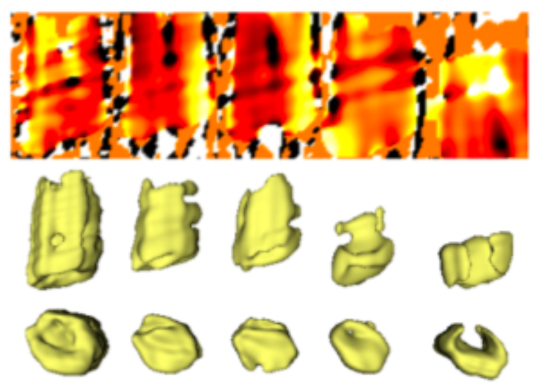
- Mechanical response at nanometer length scales
  - Structural response to chemical reactions & in-situ catalysis
  - Decomposition of semiconductors in contact with noble metals
  - Structural changes in crystals due to defect formation and removal
  - Alloying and dealloying
  - High temperature and pressure
- Domain wall (magnetic, orbital, charge) structure in the complex oxides and multi-layer
- Phase transitions vs temperature and magnetic field



Cha, Wonsuk, et. al 2013
Nat Mater 12 (8) 729–34.



J. N. Clark, et al.
Science 341 (6141): 56–59.



Coherent diffractive imaging of solid state reactions in zinc oxide crystals.
Leake, S. J., Harder, R., & Robinson, I. K. (2011) *New Journal of Physics*, *13*(11), 113009

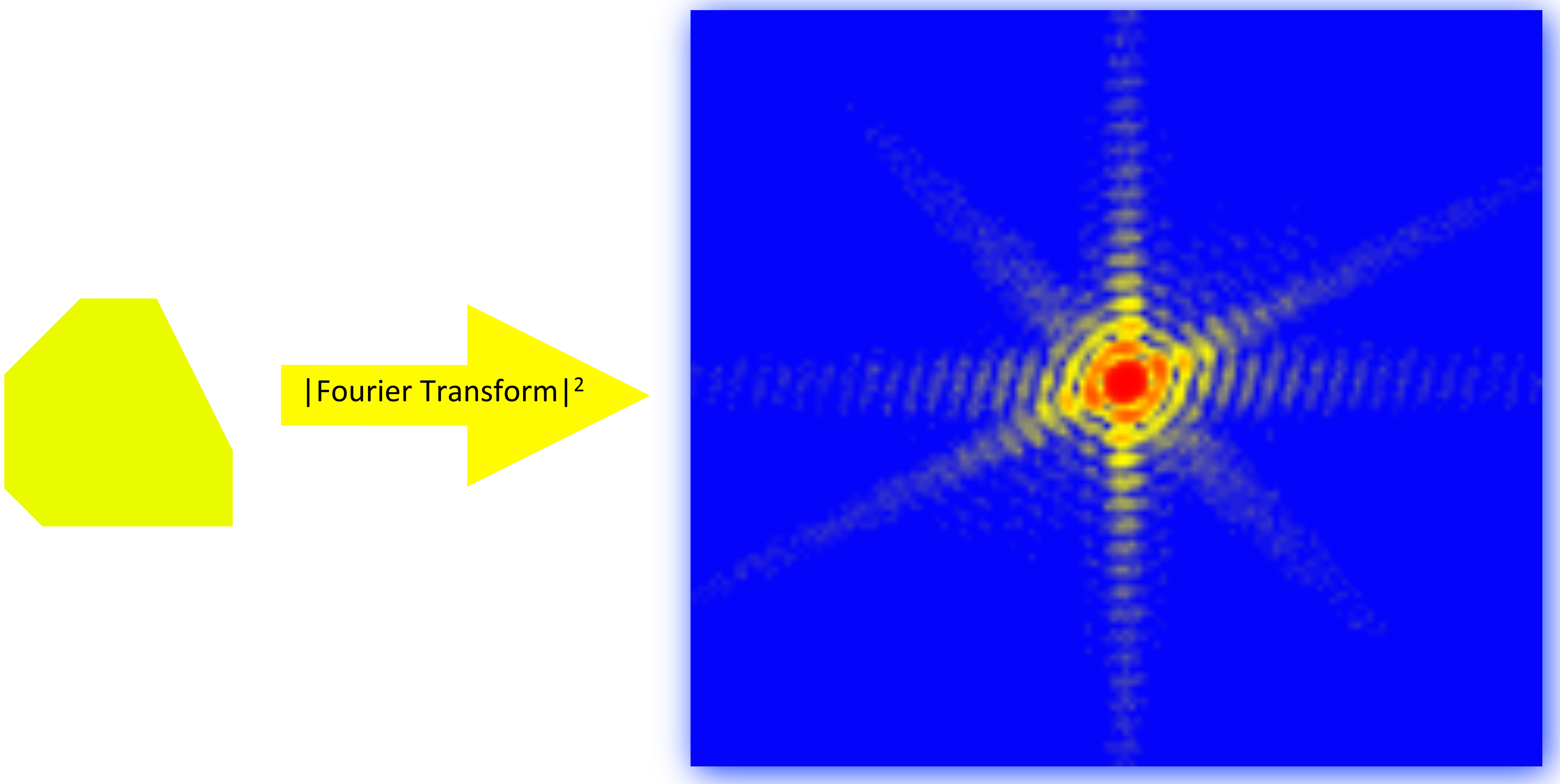
Watari, M., Harder R., et al. (2011).
Nat Mater, *10*(11), 862–866.

chain thiols, the large stress cannot arise from the va
chain–chain interactions or other weak forces alone, bu
least ionic or covalent rearrangements. Indeed the Au–S
plays a crucial role in SAM formation: the structure c
(1.6 nm) thiolated nanocrystals has its Au–Au spaci
disrupted and sulphur intermixed with gold in the o
Our findings support this model and show strong th
deformations of our 300 nm crystals with strains penet
than 20 nm from the outer surface towards the crystal
strains are absent. The tight-radius spherical parts of
nanocrystals might also undergo strong Au–S inter
would indeed be able to provide sufficient stress.
reactions involving atomic diffusion of Au at room
would also be an attractive explanation of the relatively s
seen in both our X-ray and the cantilever experiments.
Our observation of relative contraction of the
expansion of the curved surface regions of Au n
illustrated in Fig. 3e, leads to the conclusion that the

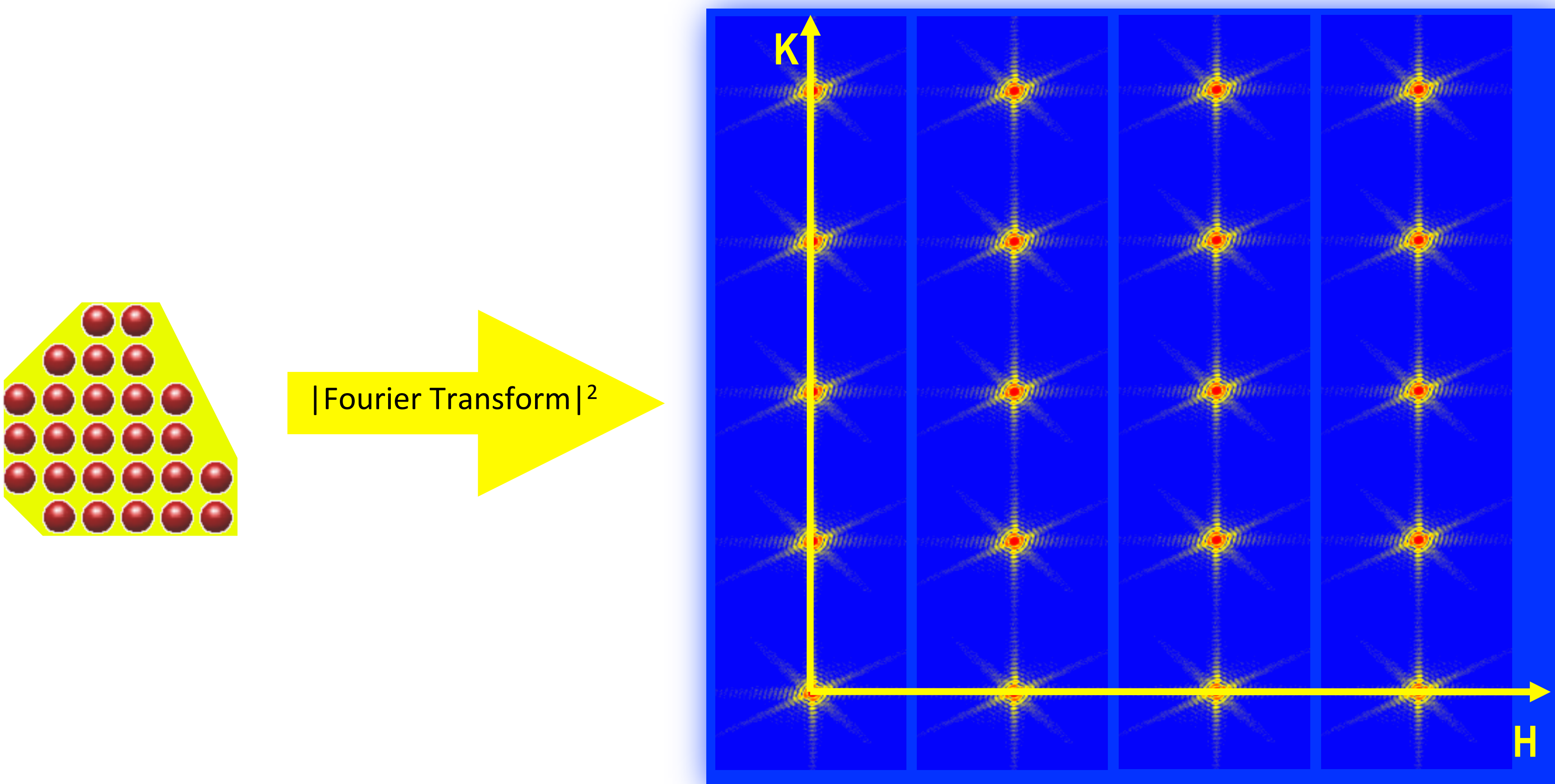
NATURE MATERIALS | VOL 10 | NOVEMBER 2011 | www.nature.com/

© 2011 M

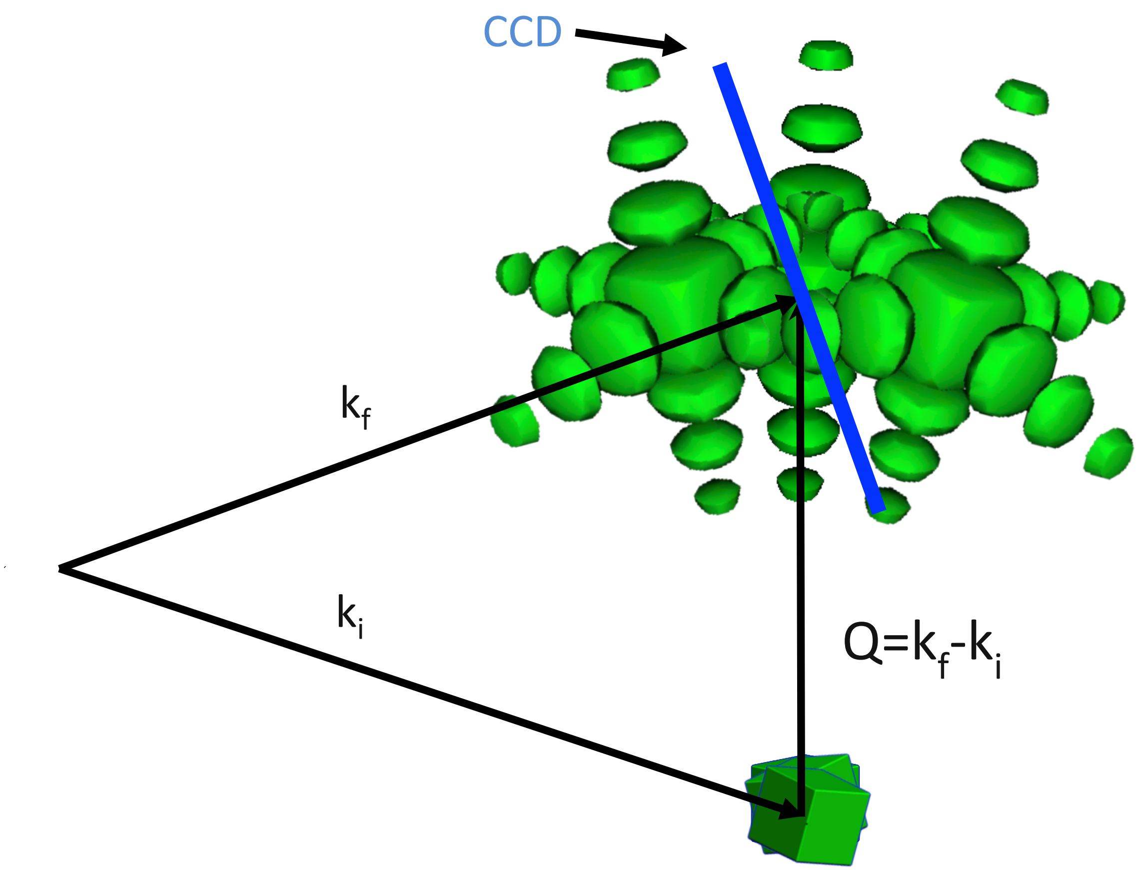
Coherent Diffraction from Crystals



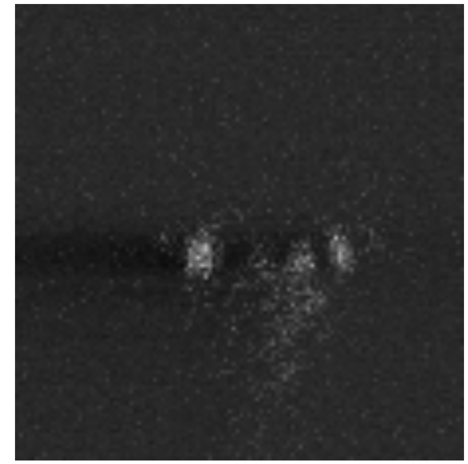
Coherent Diffraction from Crystals

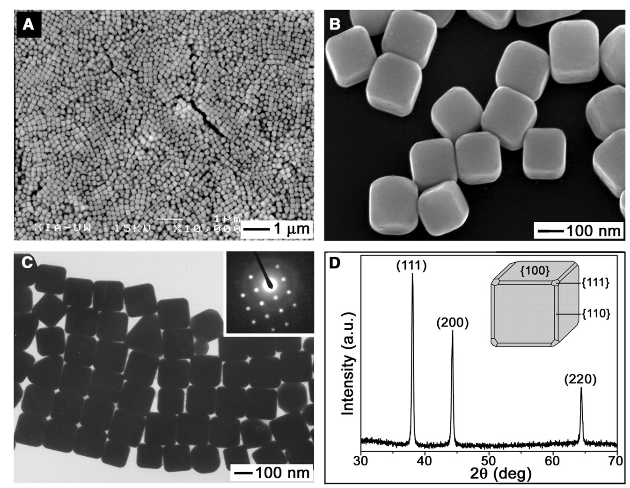


Measuring 3D CXD



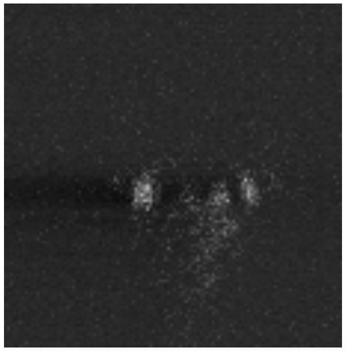
Silver Nano Cube (111)

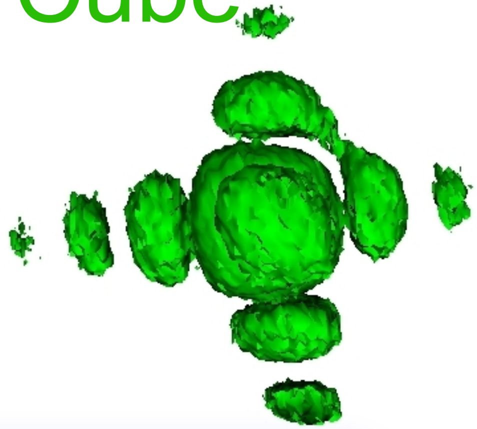


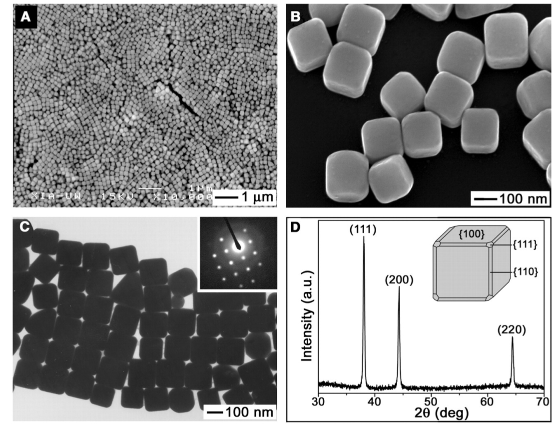


Yugang Sun and Younan Xia, Science 298 2177 (2003)

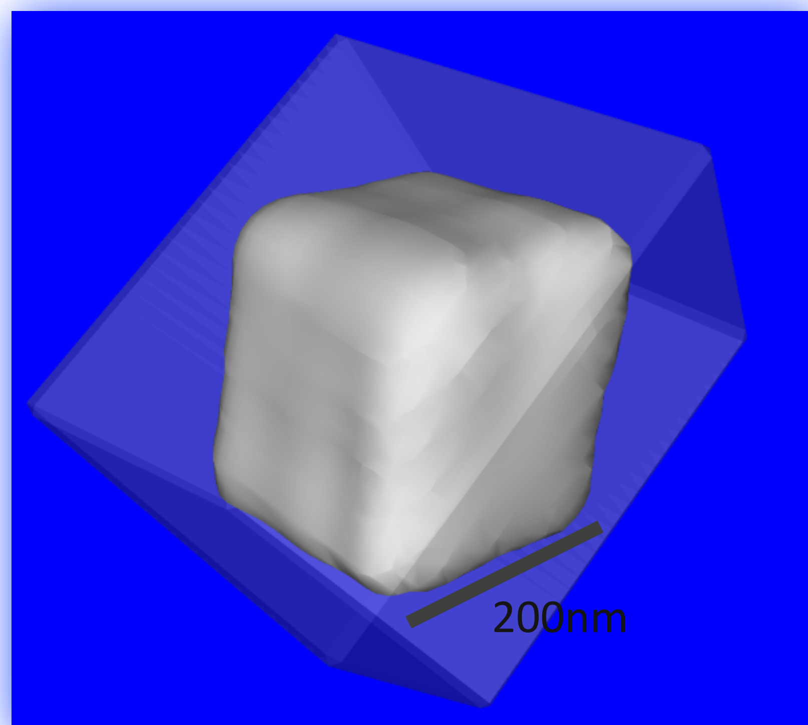
3D Ag Nano Cube

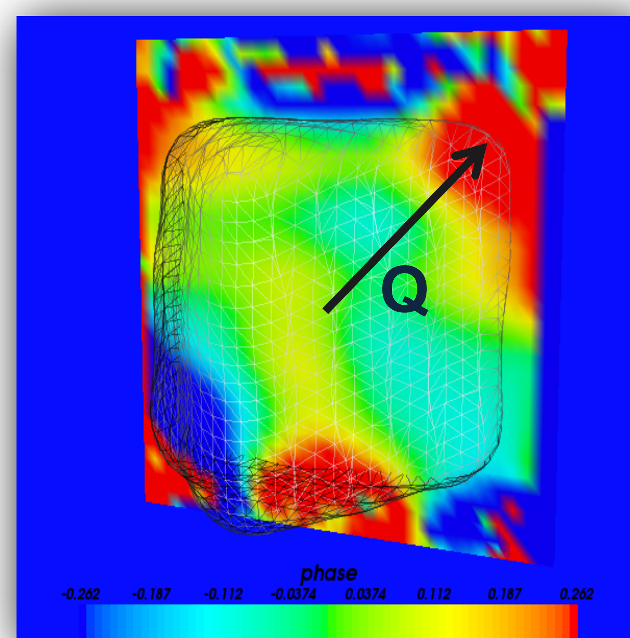




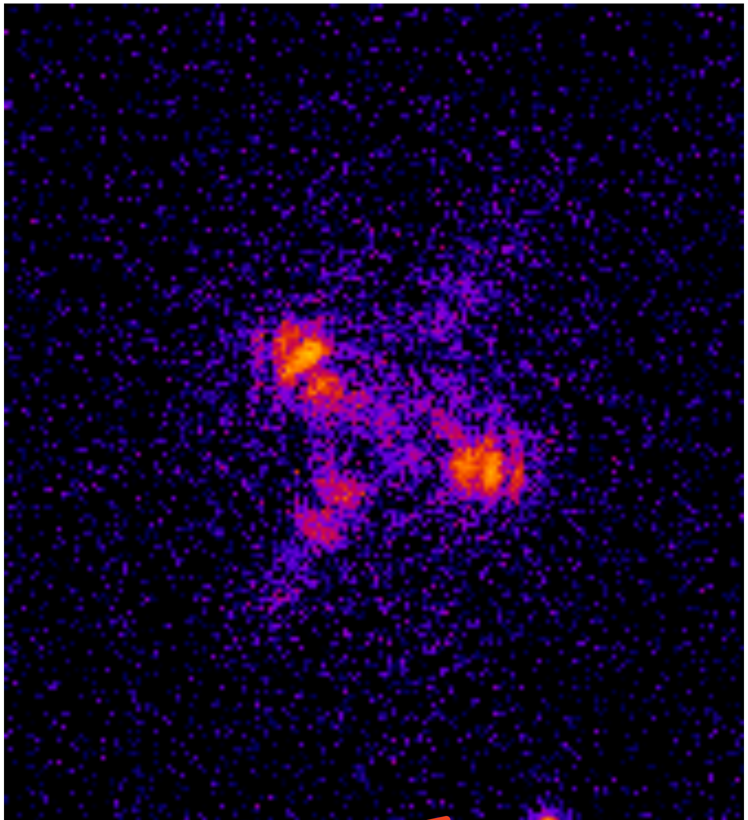


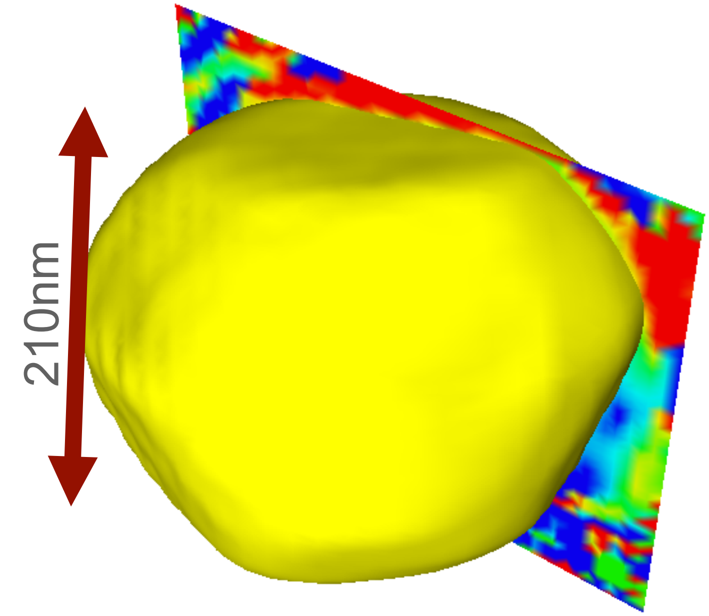
Yugang Sun and Younan Xia, Science 298 2177 (2003)

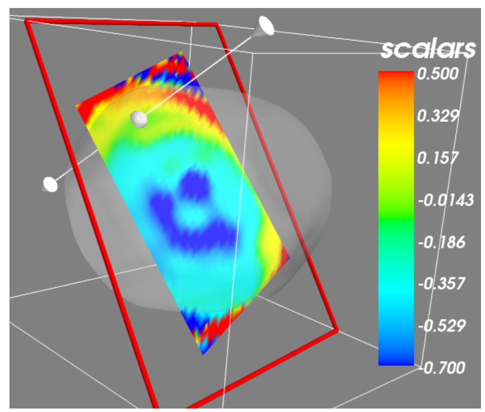


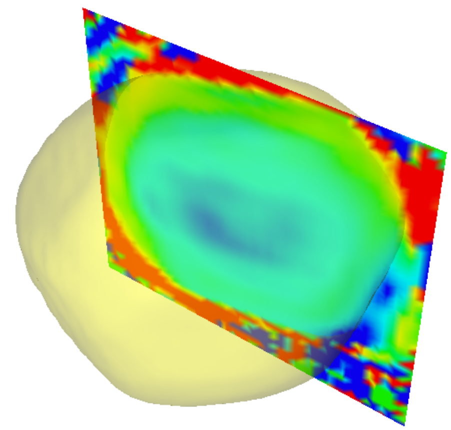


Hi Resolution Imaging?









~7nm data

At APS 34-ID-C:
9.25 hours of scanning
0.64 hours of x-ray exposure

APS-MBA (100x) → 25 sec?

Water Purification

http://www.wssinfo.org/

http://water.org/water-crisis/water-facts/water/

Million Atom MD simulations
Gold in water

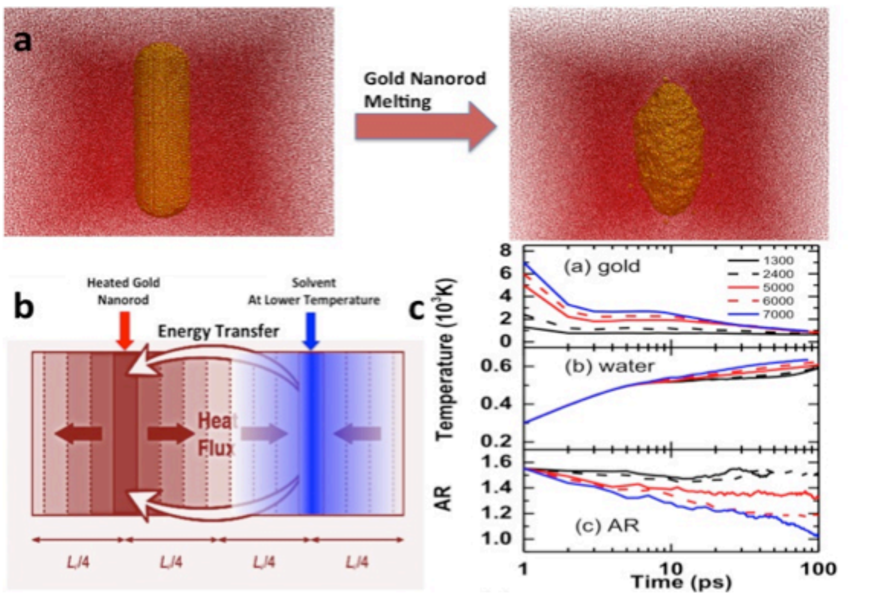
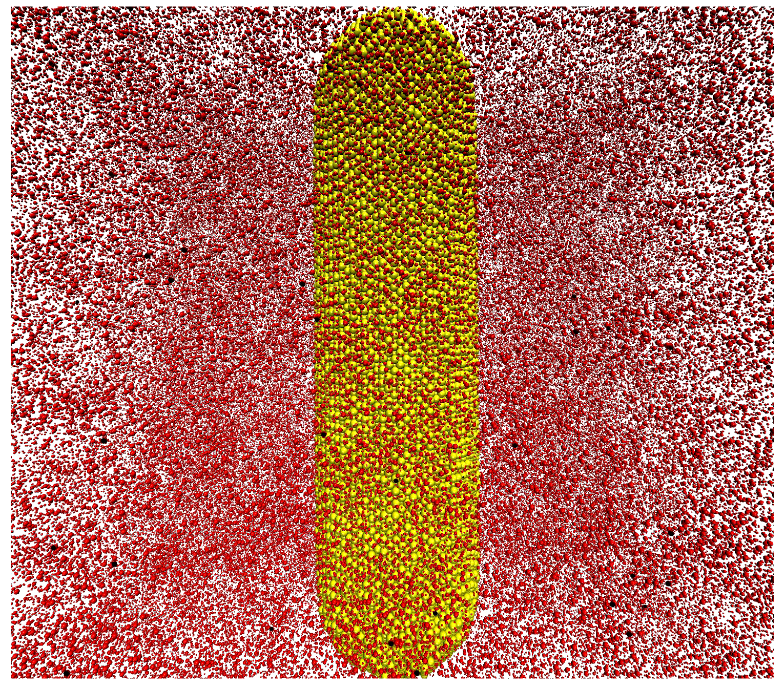


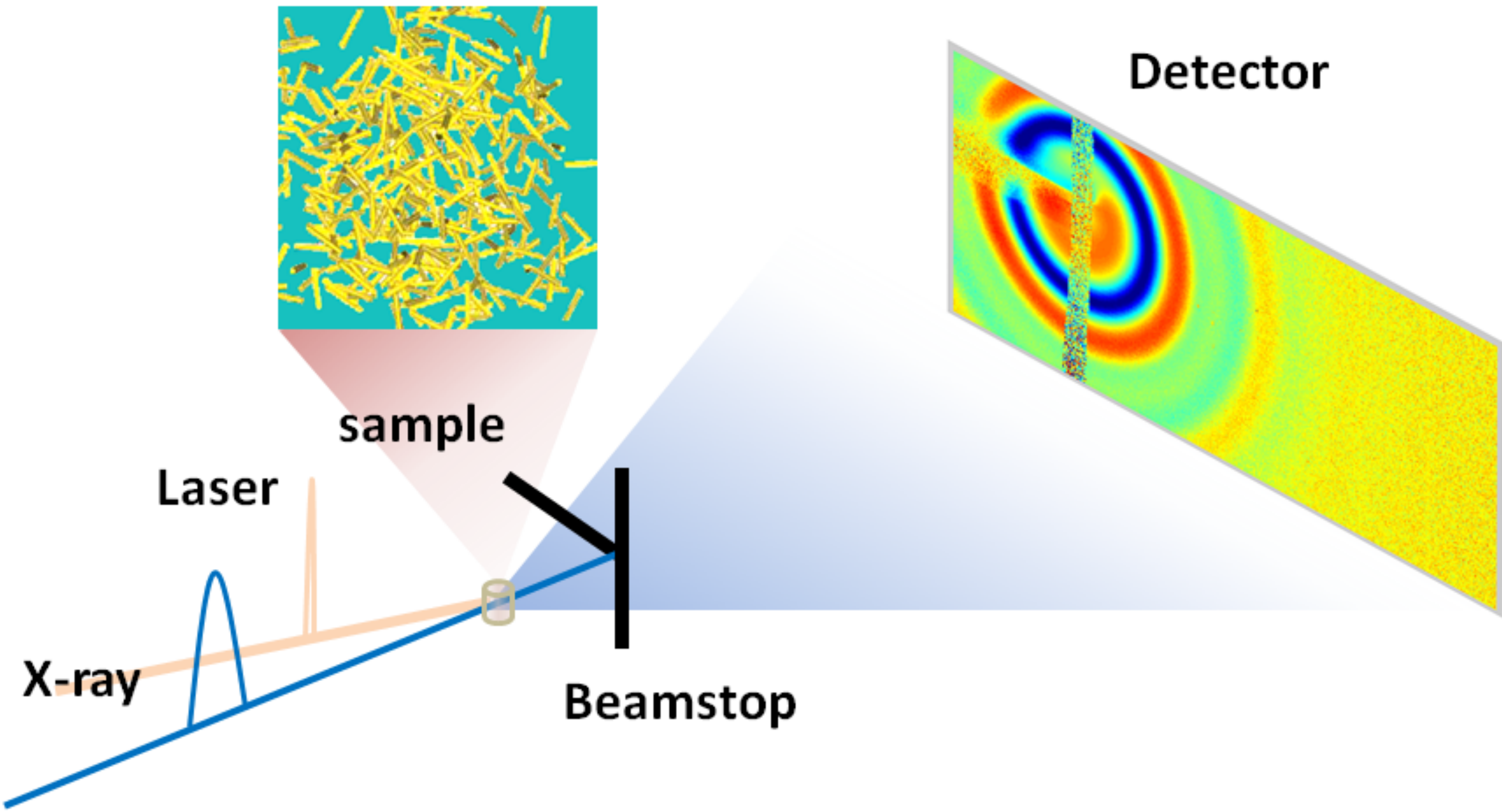
Figure 3: (a) Million-atom MD simulation showing a laser-heated gold nanorod in water (b) Typical schematic of an NEMD simulation to compute heat transport (c) Temperature dissipation and aspect ratio in our preliminary MD calculations.



Courtesy: Subramanian Sankaranarayanan (ANL-NST)

Li, Yuelin, Haidan Wen, Subramanian K R S Sankaranarayanan, et al.. 2015. *Scientific Reports* 5.

Nanorod melting in small angle x-ray scattering



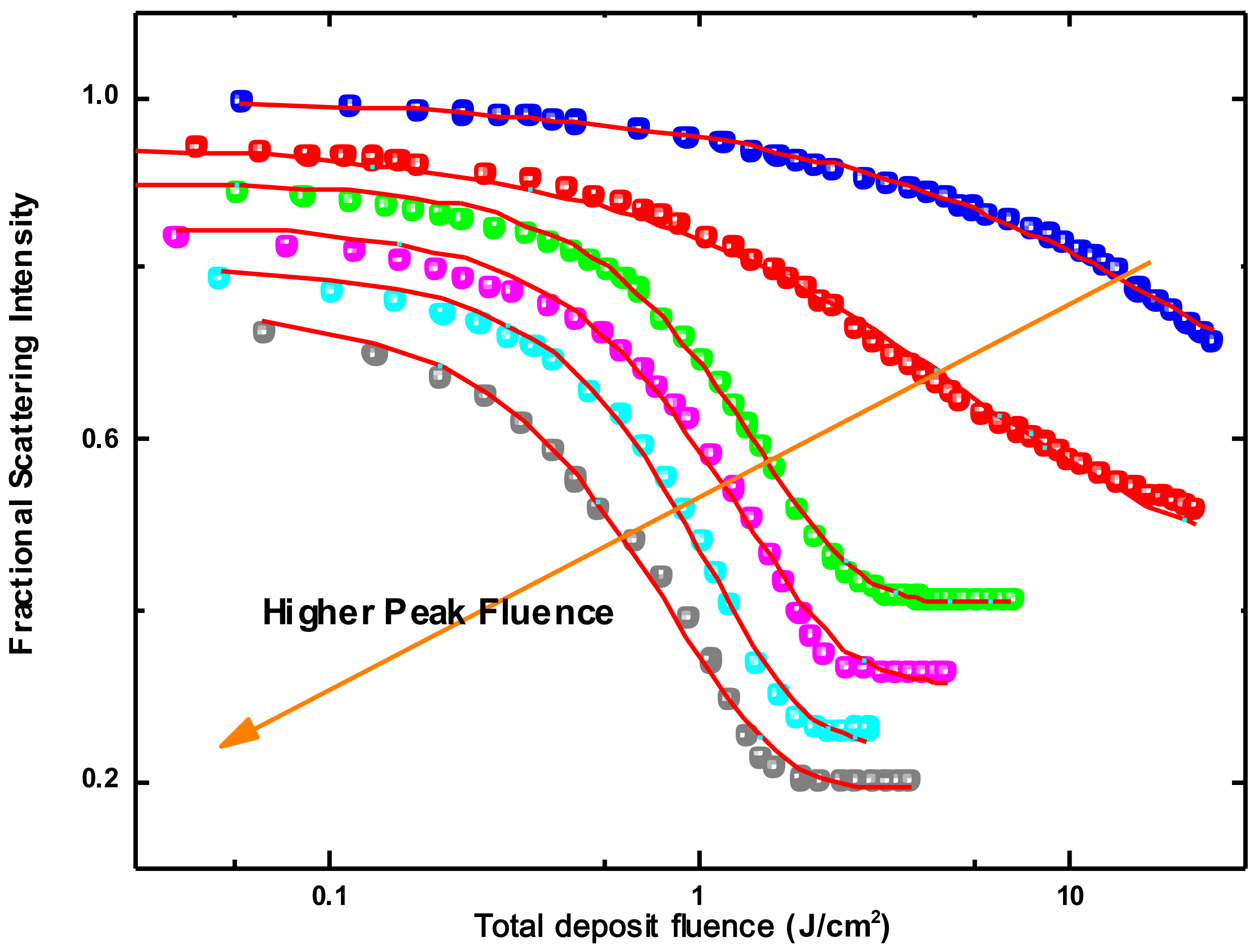
Li, Yuelin, Haidan Wen, Subramanian K R S Sankaranarayanan, et al.. 2015. *Scientific Reports* 5.

Nanorod melting in small angle x-ray scattering

SAXS of melting nanorods

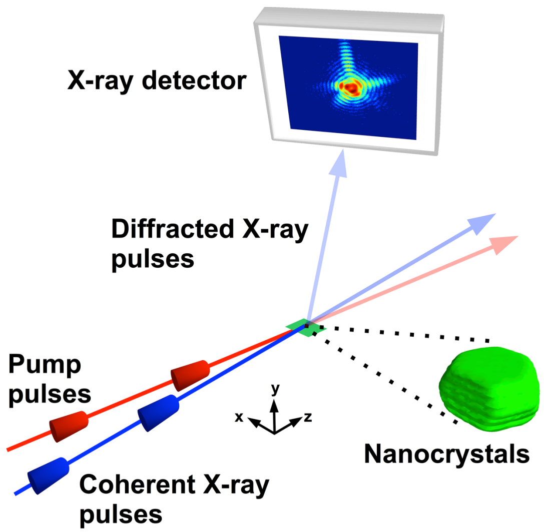
Li, Yuelin, Haidan Wen, Subramanian K R S Sankaranarayanan, et al.. 2015. *Scientific Reports* 5.

Nanorod melting in small angle x-ray scattering



Li, Yuelin, Haidan Wen, Subramanian K R S Sankaranarayanan, et al.. 2015. *Scientific Reports* 5.

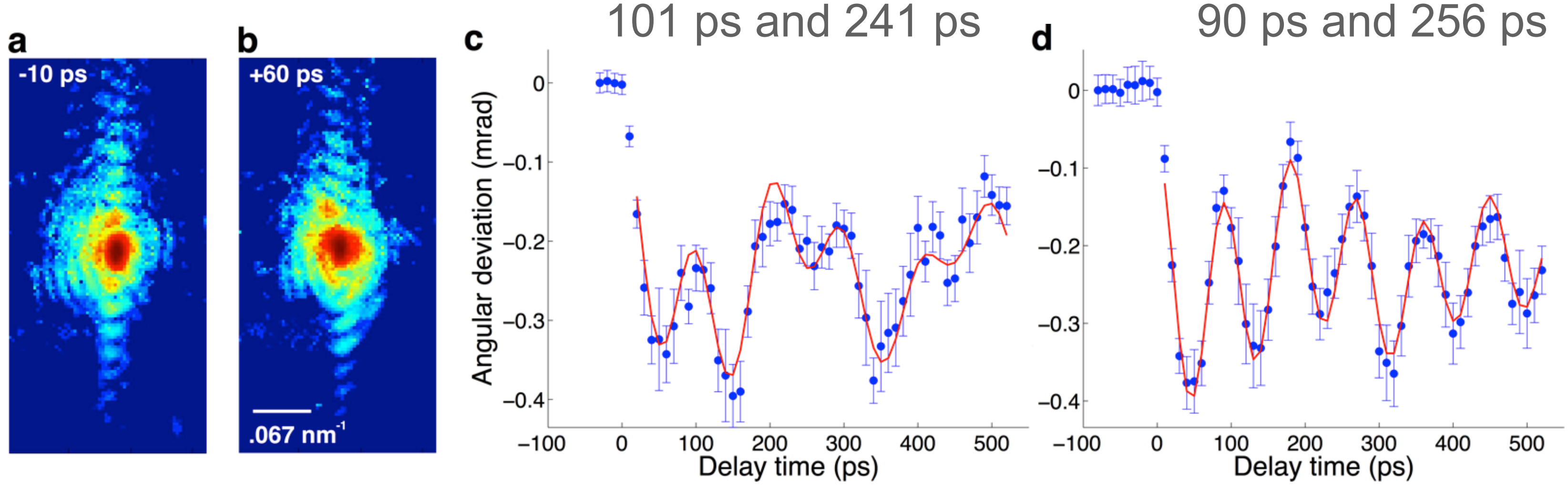
Imaging Lattice Dynamics
Laser Pump - CXD Probe@LCLS



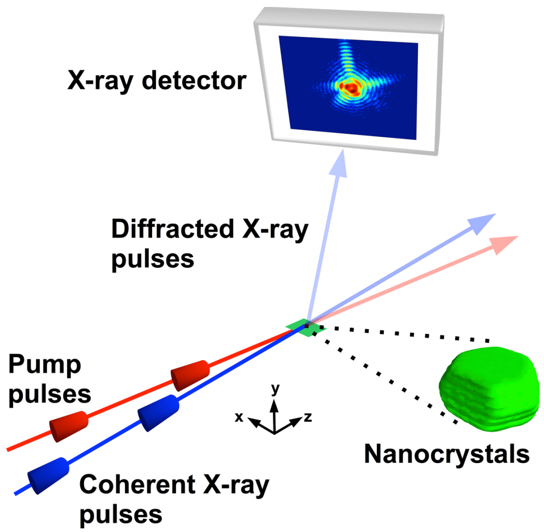
600 pm "breathing modes"

Crystal A
101 ps and 241 ps

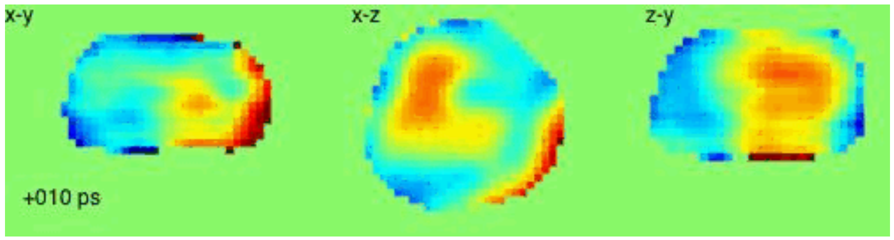
Crystal B
90 ps and 256 ps

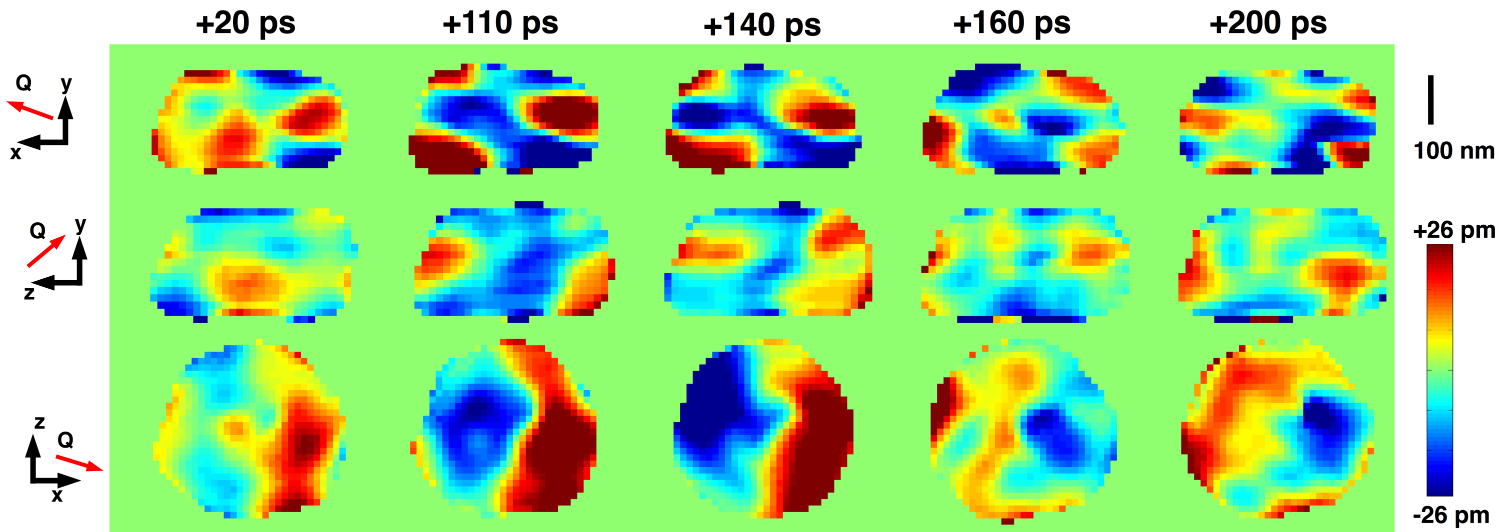


Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals
J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu,
M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder,
A. M. Korsunsky, J. S. Wark & I. K. Robinson
Science 341 (6141): 56–59.



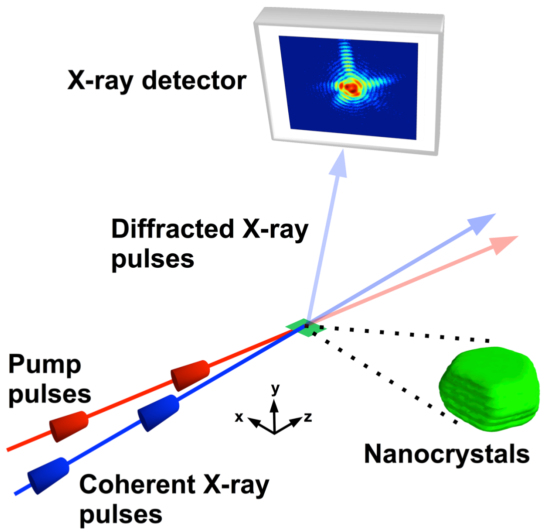
Imaging Lattice Dynamics
Laser Pump - CXD Probe@LCLS





Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals
J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu,
M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder,
A. M. Korsunsky, J. S. Wark & I. K. Robinson
Science 341 (6141): 56–59.

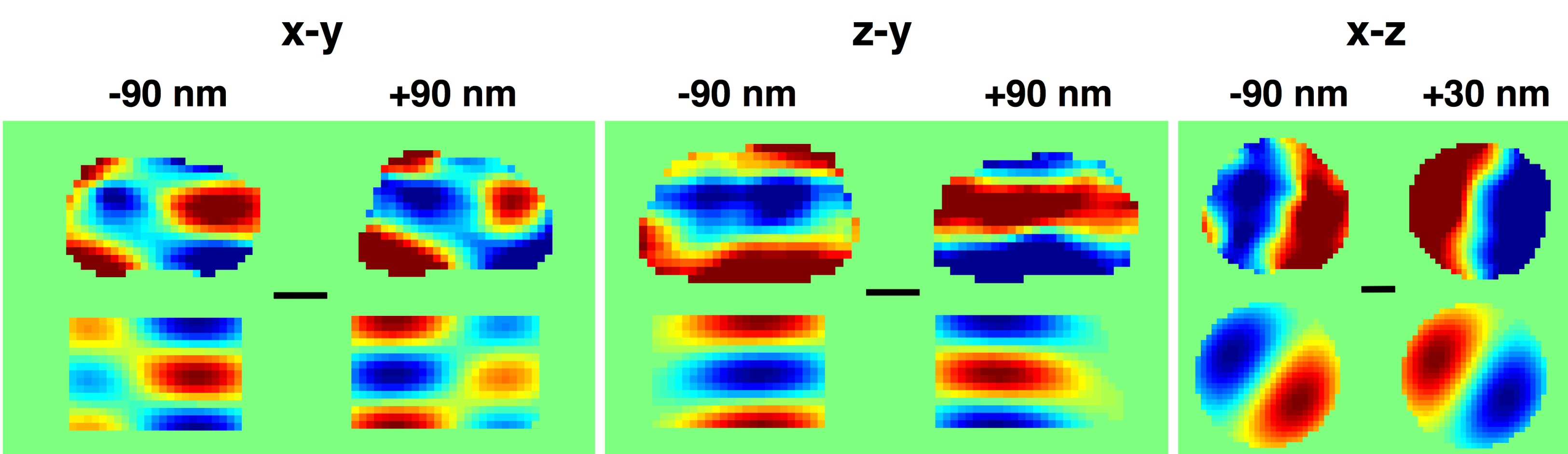
Imaging Lattice Dynamics
Laser Pump - CXD Probe@LCLS



Orthogonal slices
Through crystal density

3

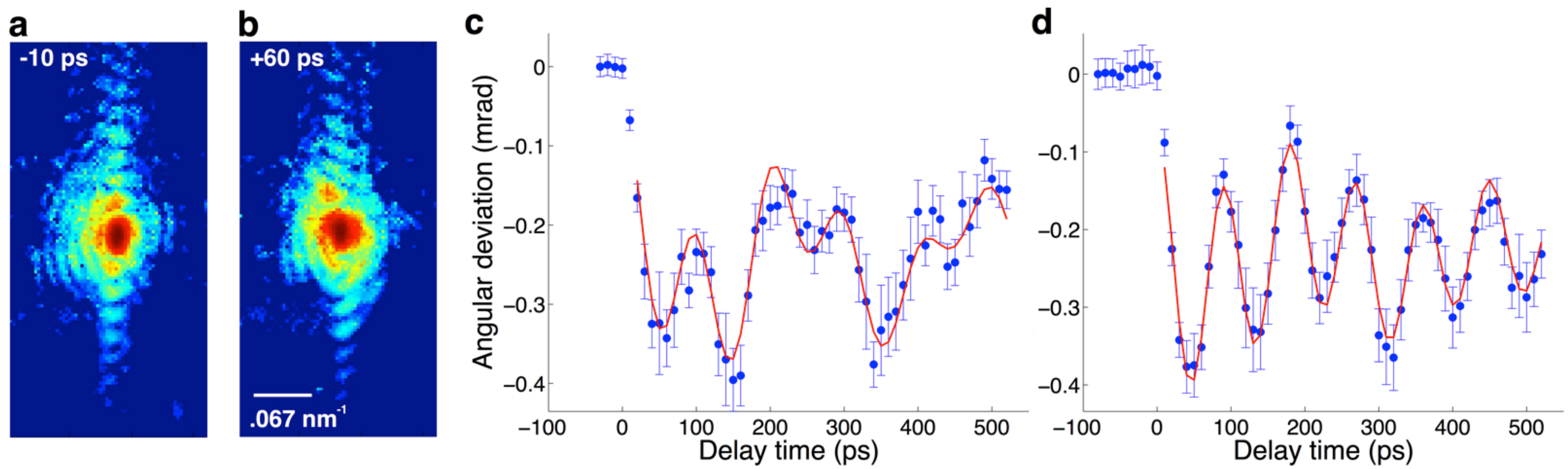
MD simulation
at +110ps



Ultrafast three dimensional imaging of lattice dynamics in individual gold nanocrystals
J. N. Clark, L. Beitra, G. Xiong, A. Higginbotham, D. M. Fritz, H. T. Lemke, D. Zhu, M. Chollet, G. J. Williams, M. Messerschmidt, B. Abbey, R. J. Harder, A. M. Korsunsky, J. S. Wark & I. K. Robinson
Science 341 (6141): 56–59.

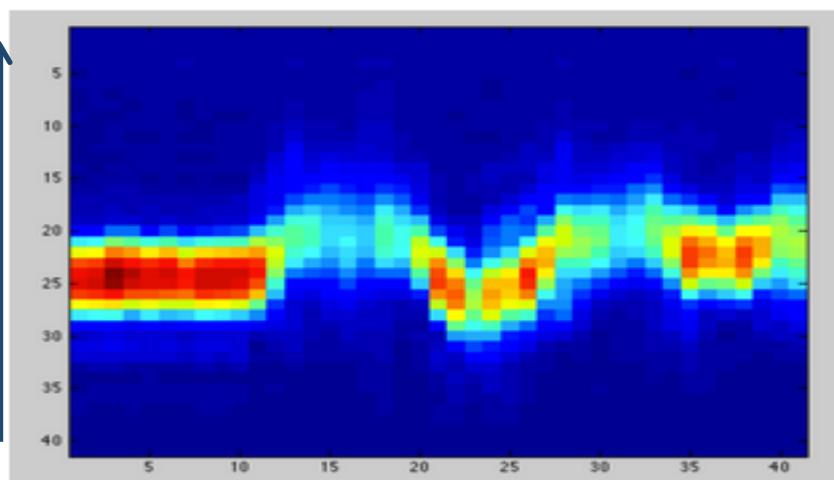
Non-electronic thermal response raw data from SACLA

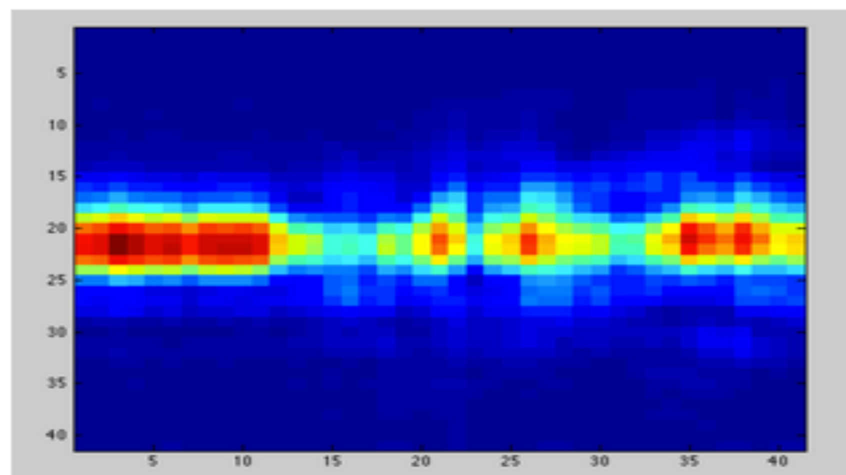
LCLS



SACLA

2theta

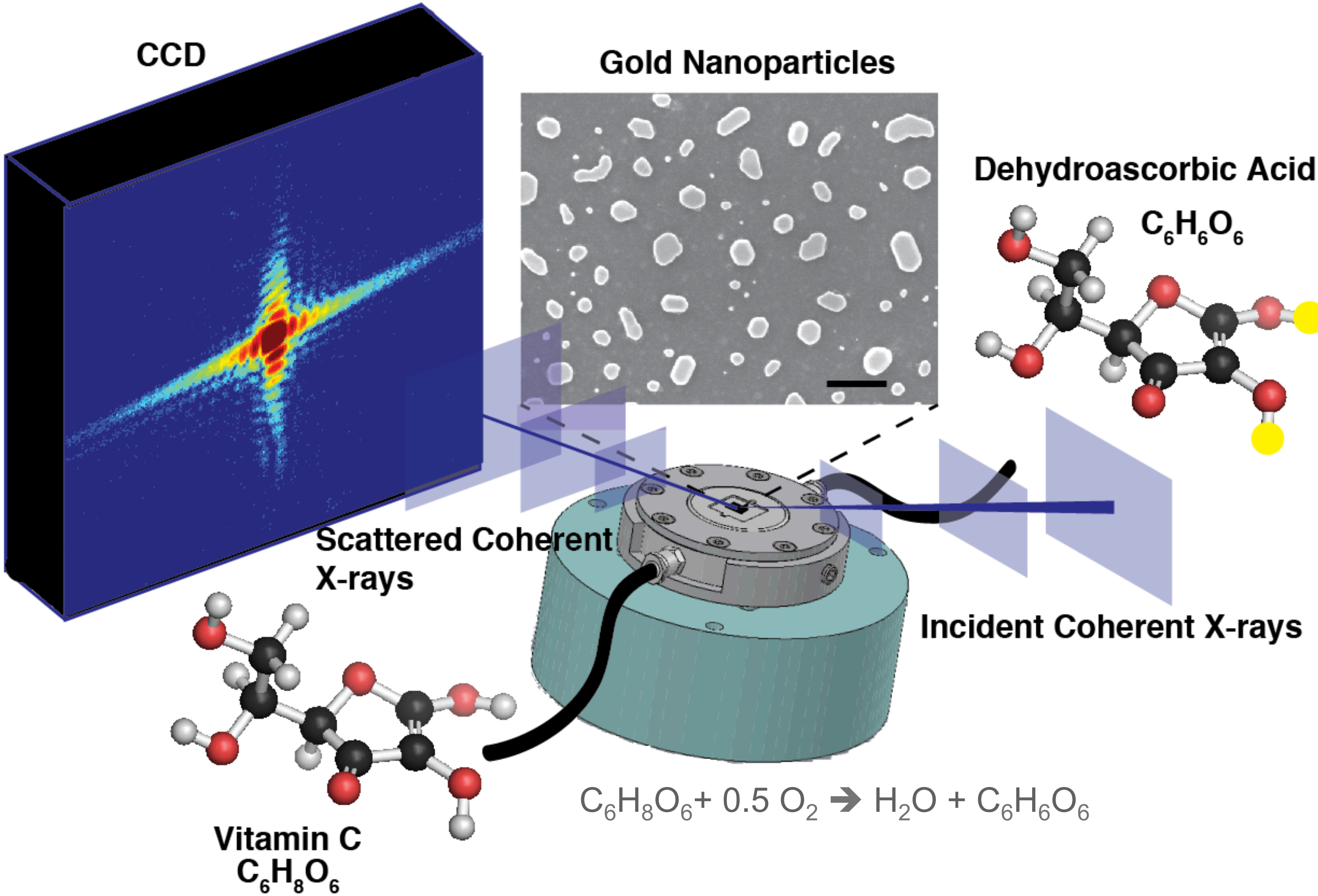




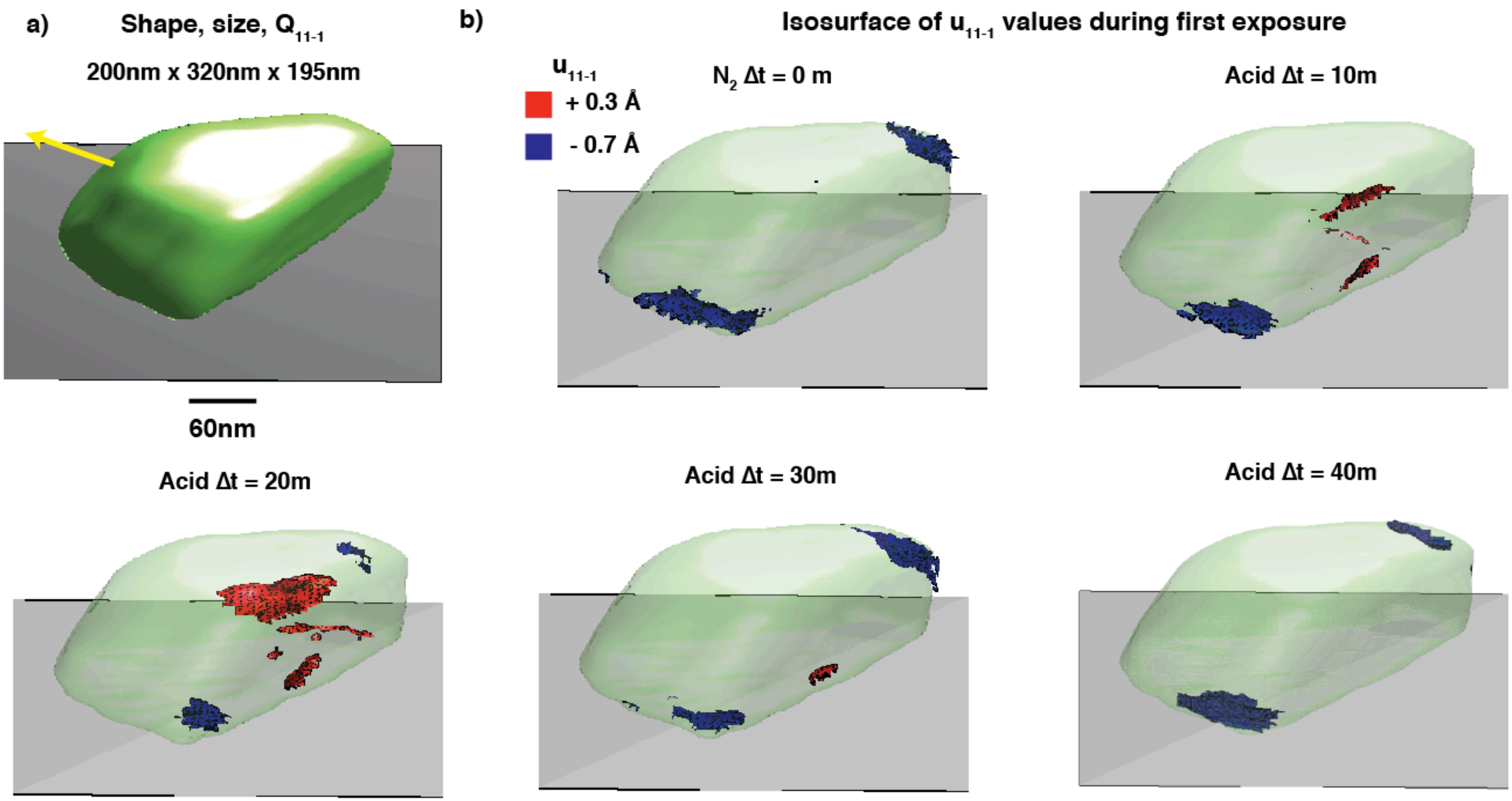
time

Bare

Nickle coated


CCD
Gold Nanoparticles
Dehydroascorbic Acid
$C_6H_6O_6$
Scattered Coherent
X-rays
Incident Coherent X-rays
Vitamin C
$C_6H_8O_6$
$C_6H_8O_6 + 0.5\ O_2 \rightarrow H_2O + C_6H_6O_6$

Ascorbic Acid decomposition on gold



- Lattice change occurs at junctions involving the flattest facet
- Electron injection should create largest electric field at crystallographic discontinuities or apexes, providing "hot spots" for the reaction

Courtesy: Andrew Ulvestad (UCSD)

MAUI - Workflow

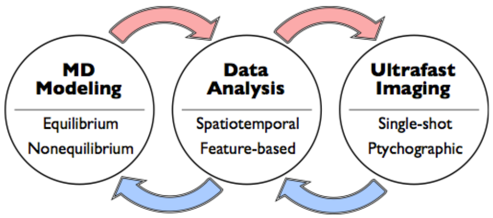


Figure 1. Simulation and experiment are integrated through a common language of data analysis.