Bragg Coherent X-ray Diffraction for Nanocrystal Structure and Dynamics

Ian Robinson
Jesse Clark
Johannes Ihli
Ana Estandarte
Ross Harder
Matt Cherukara
I-16 Diamond
I-07 Diamond
XPP LCLS

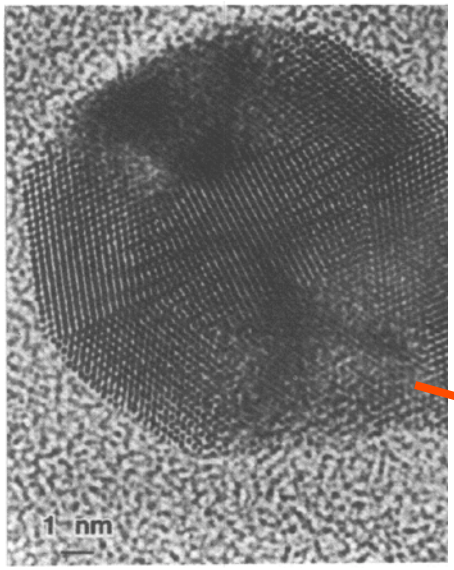
Condensed Matter Physics and Materials Science Department
Brookhaven National Lab
London Centre for Nanotechnology

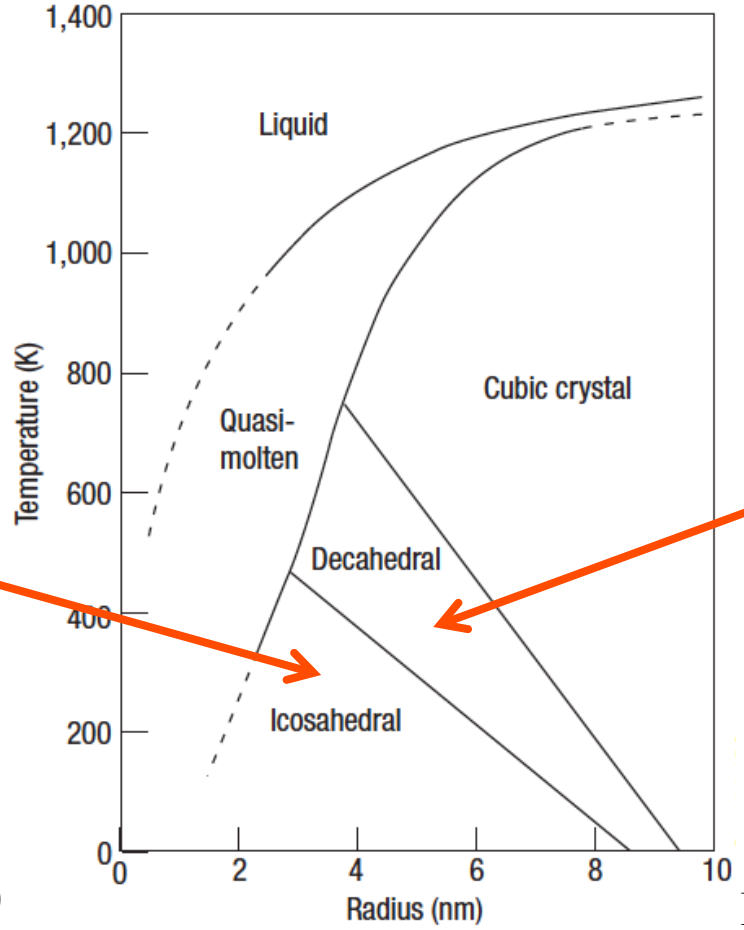
Materials and their Dynamics by Coherent X-ray Scattering
NSLS-CFN Users Meeting
May 2017

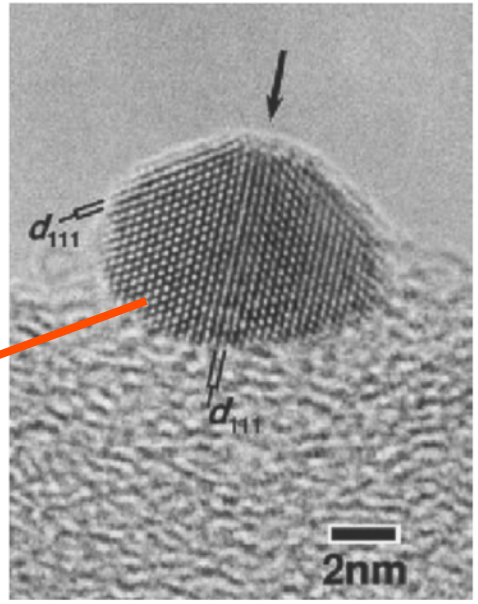
Outline

- Nanocrystal structures
- Bragg Coherent X-ray diffraction
- Dislocations during crystal growth
- Nanoscale alloying
- Ultrafast snapshots of moving matter

Phase Diagram of Gold vs Size



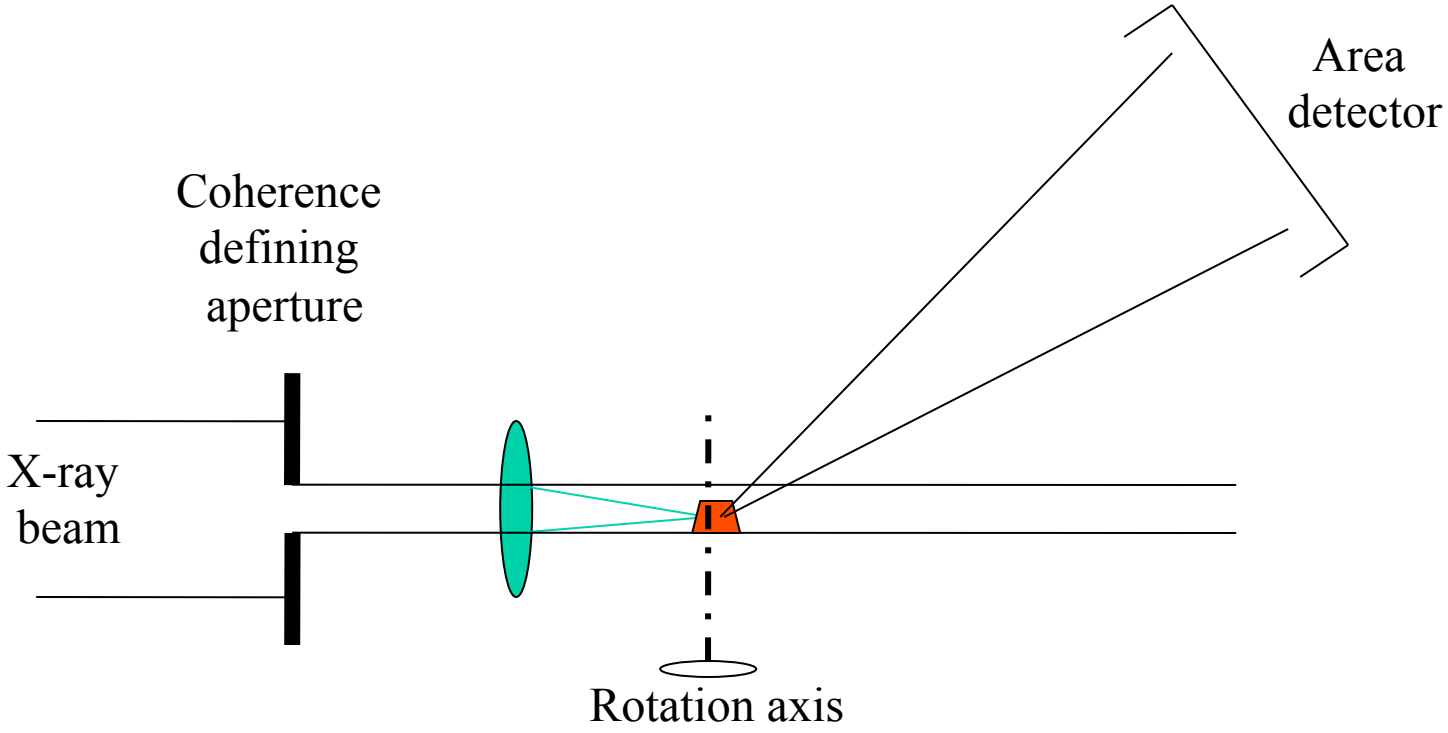


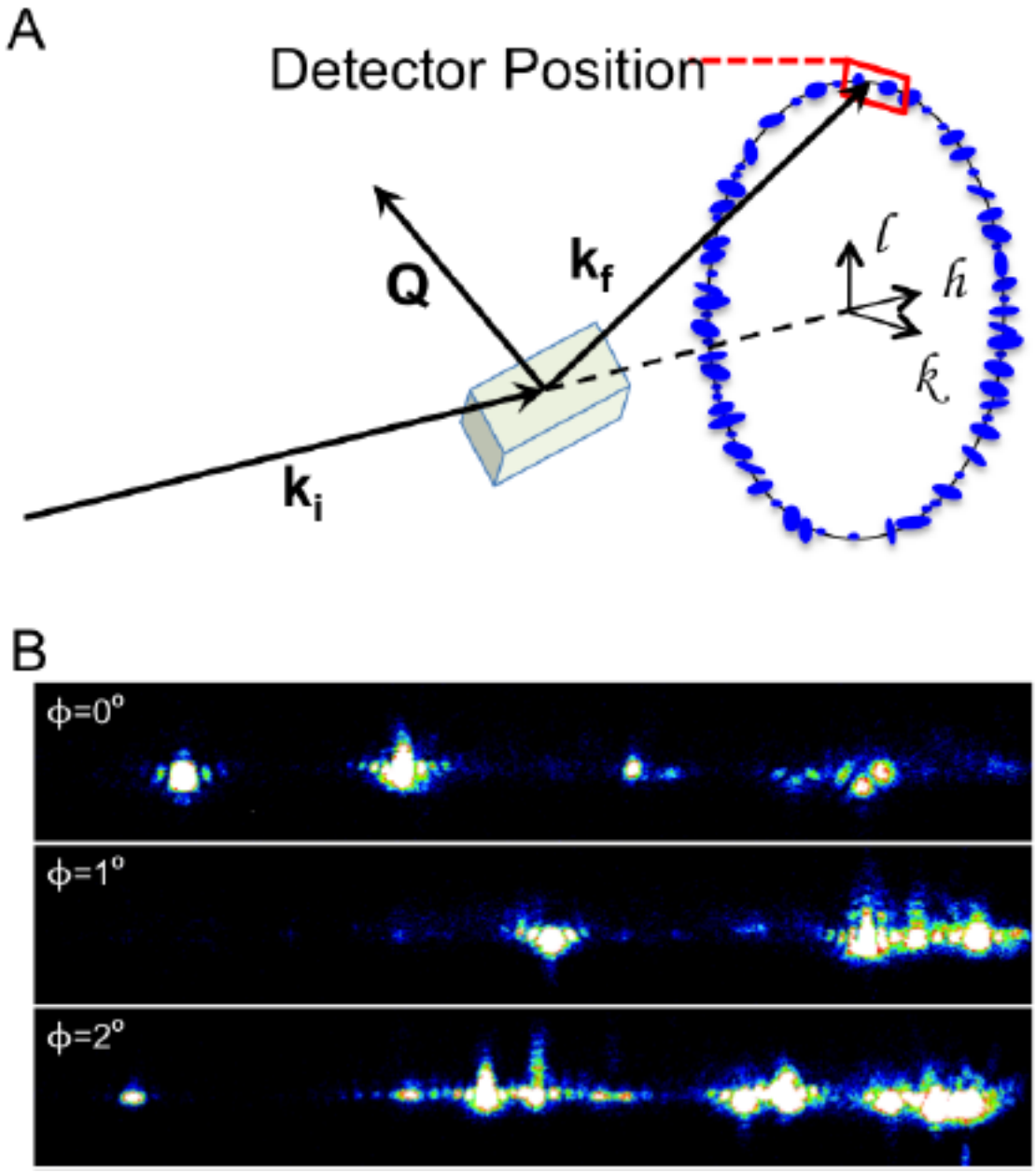


L. D. Marks, RPP (1994)

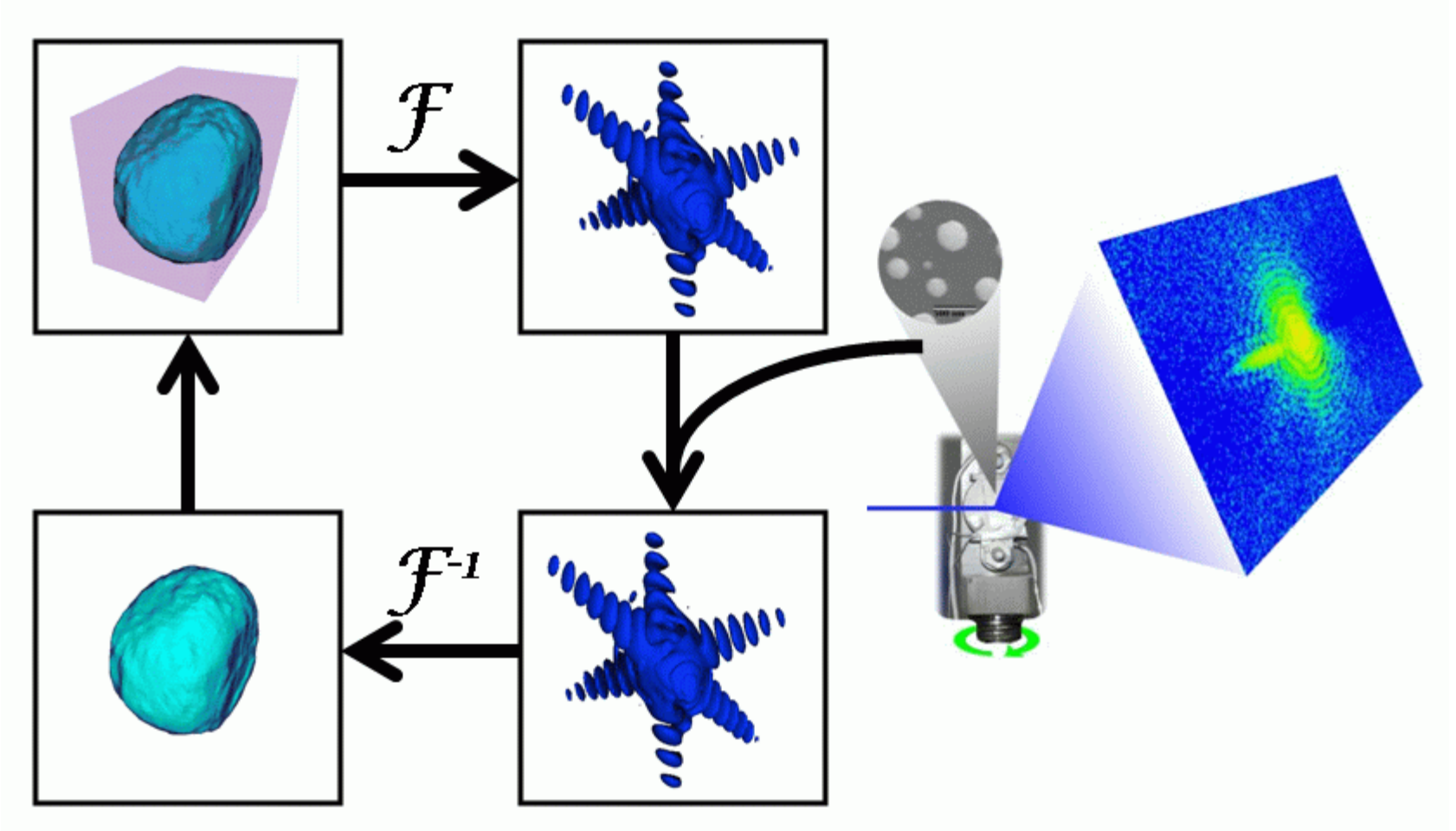
Koga and Sugawara (2003)

Bragg Coherent Diffraction Imaging "Lensless" X-ray Microscope, 2003




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

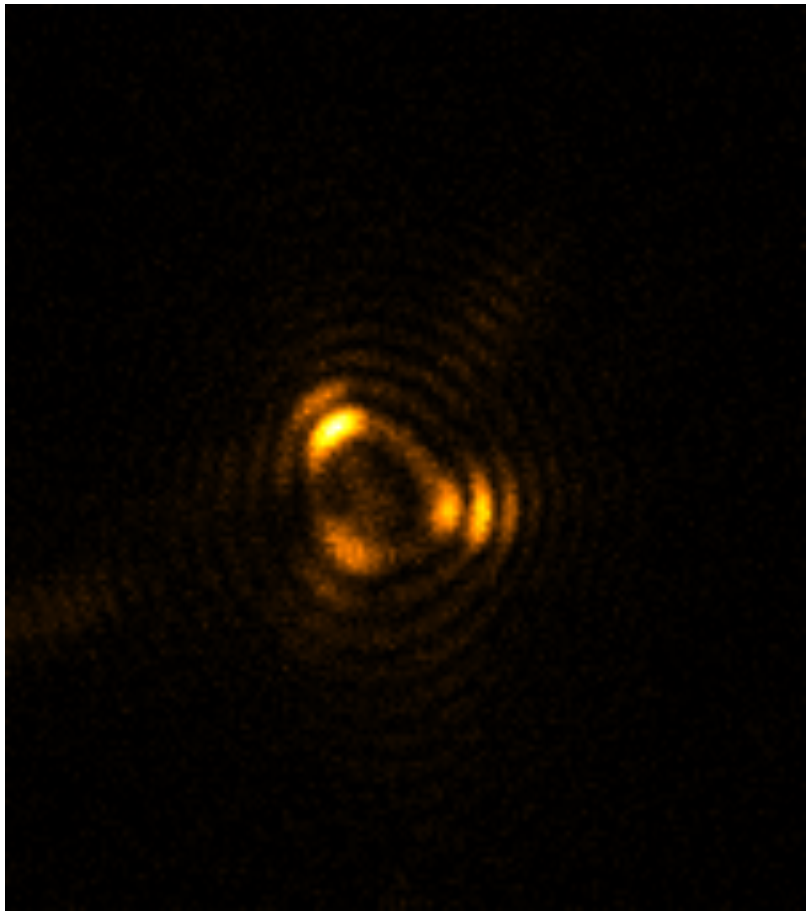
Generic "Error Reduction" method

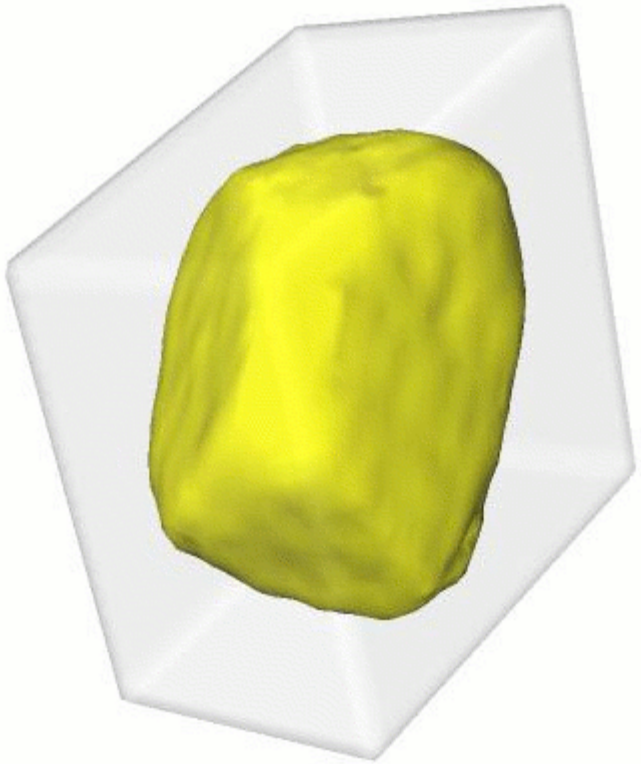


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

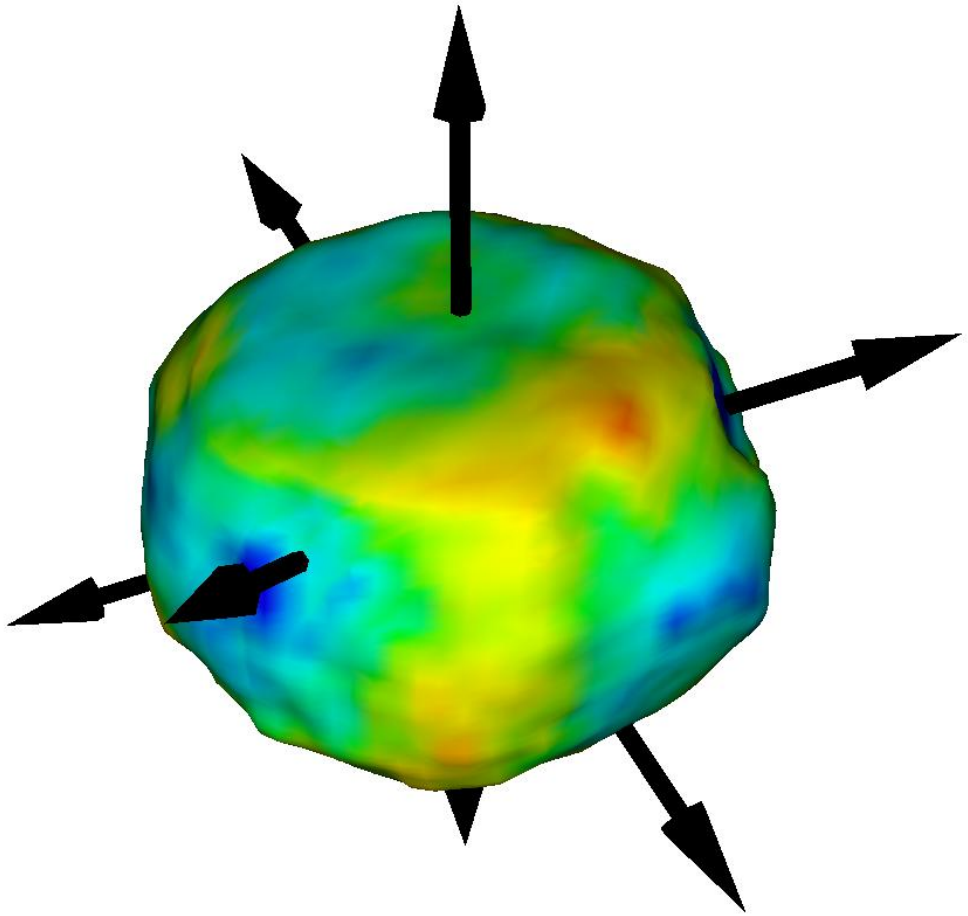
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



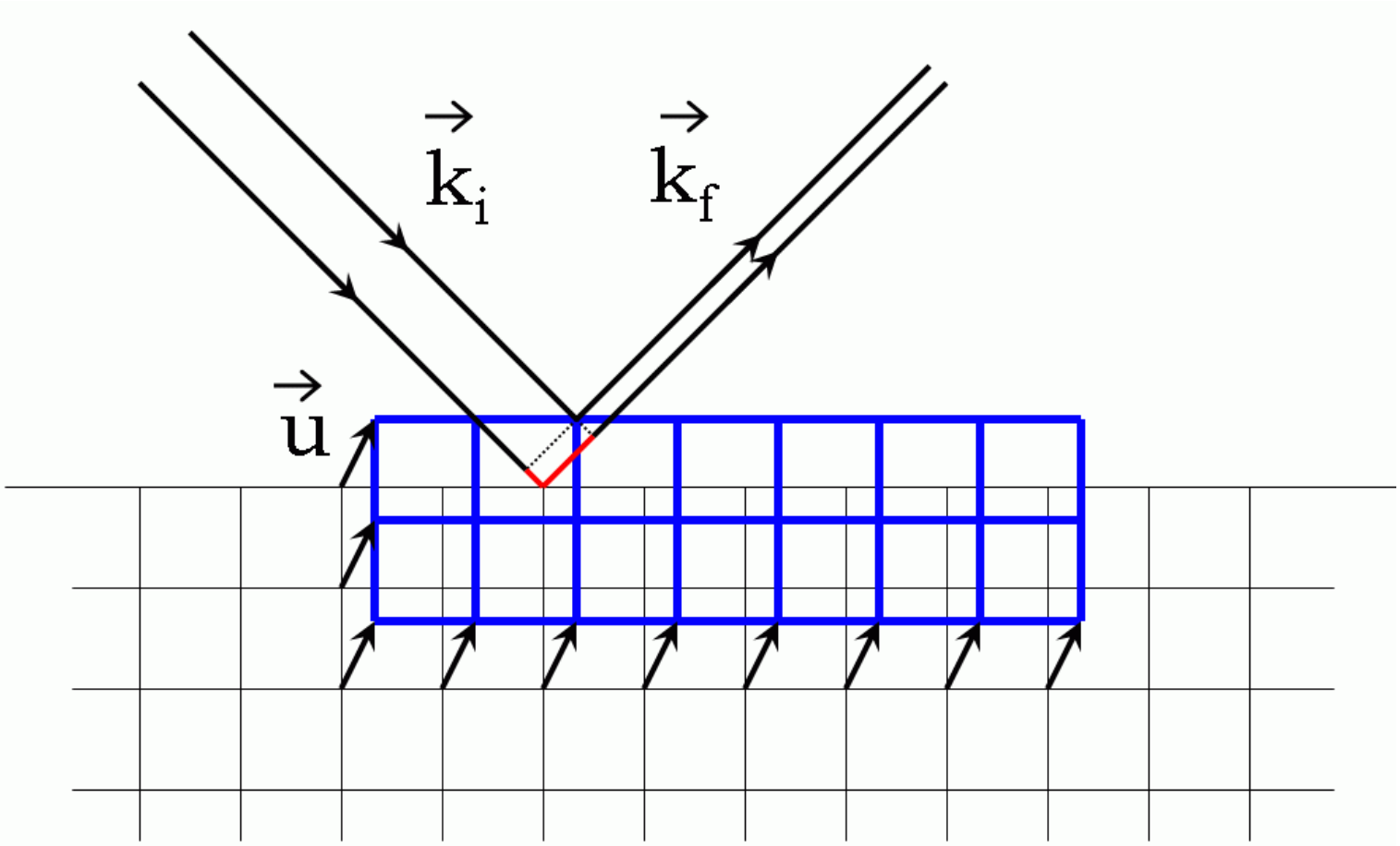


Phase isosurface of residual strain



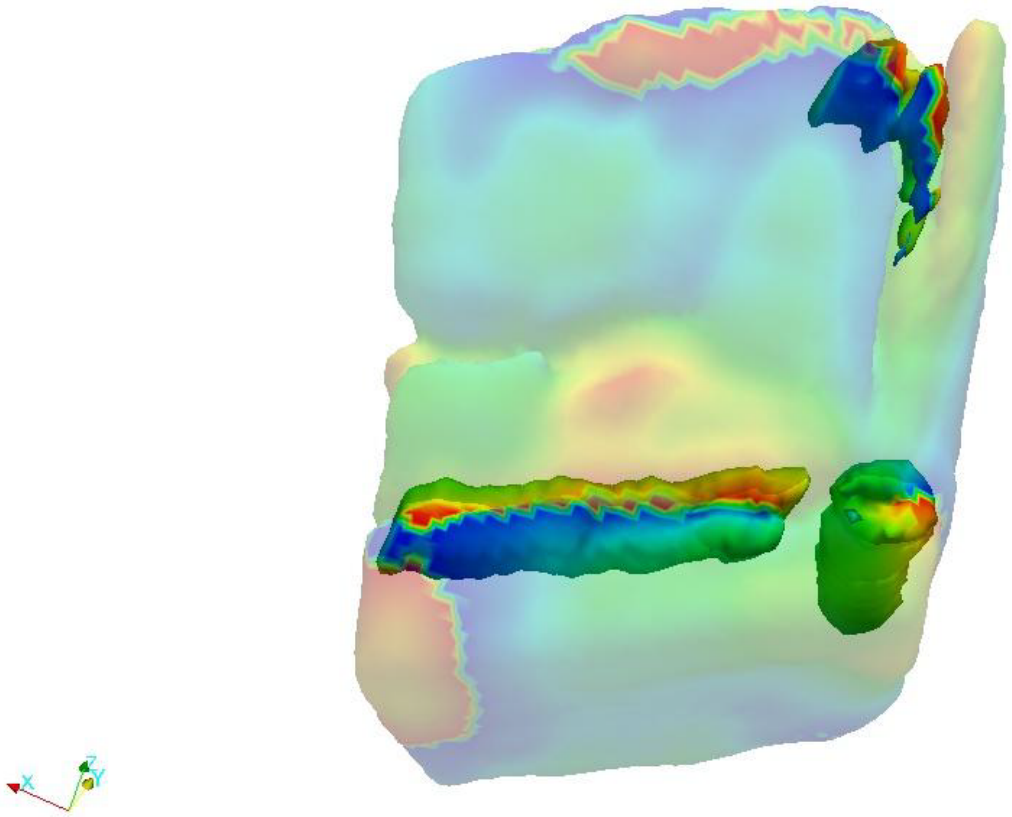
Sensitivity to strain

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



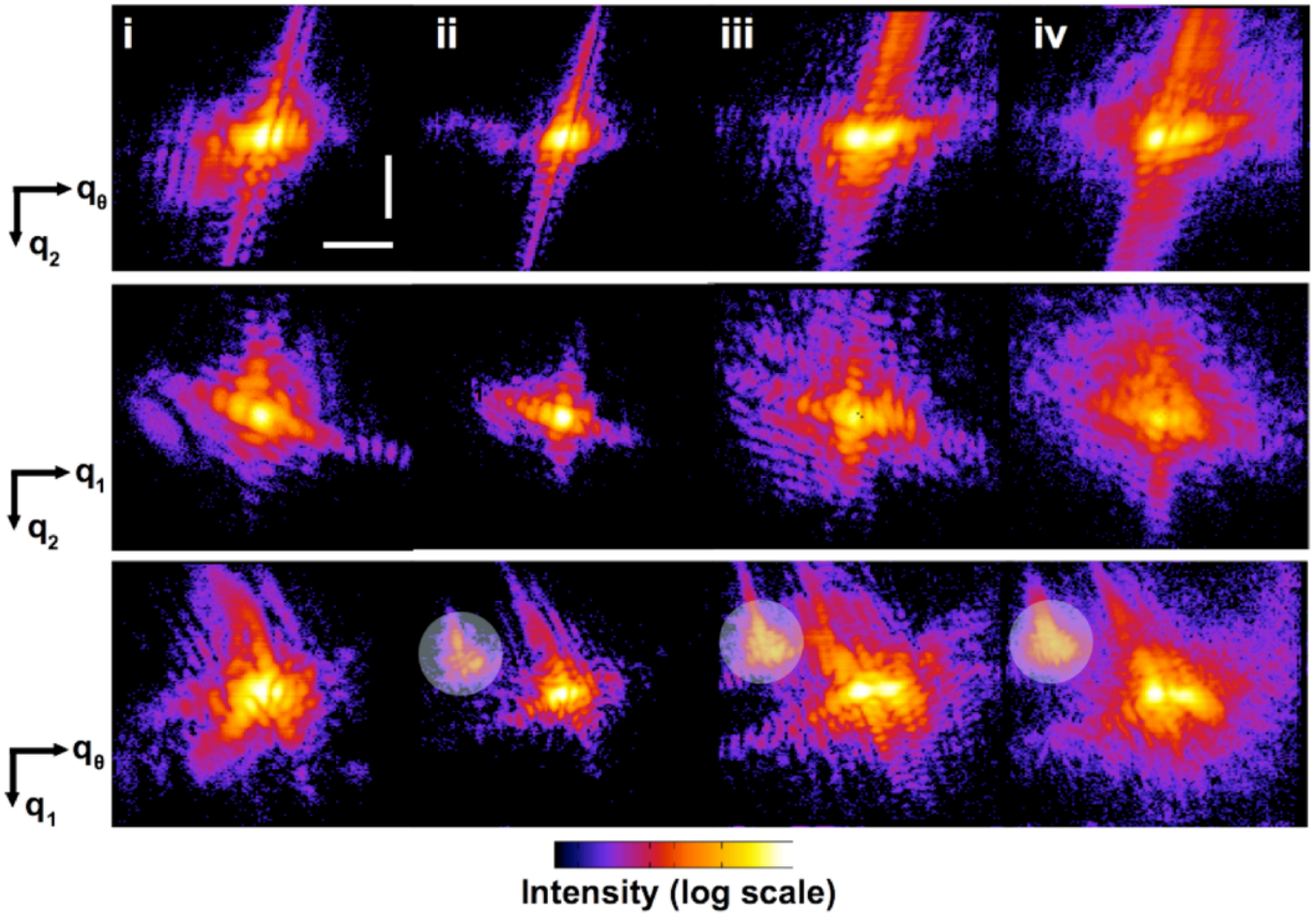
Screw dislocations in Calcite

Jesse Clark, Johannes Ihli et al, Nat. Matls **14** 780 (2015)



Dissolution and Growth

J. Clark, J. Ihli, A. Schenk, Y. Kim, A. Kulak, J. Campbell, G. Nisbet, F. Meldrum, I. Robinson, Nat Matls **14** 780 (2015)



Dissolution and Growth

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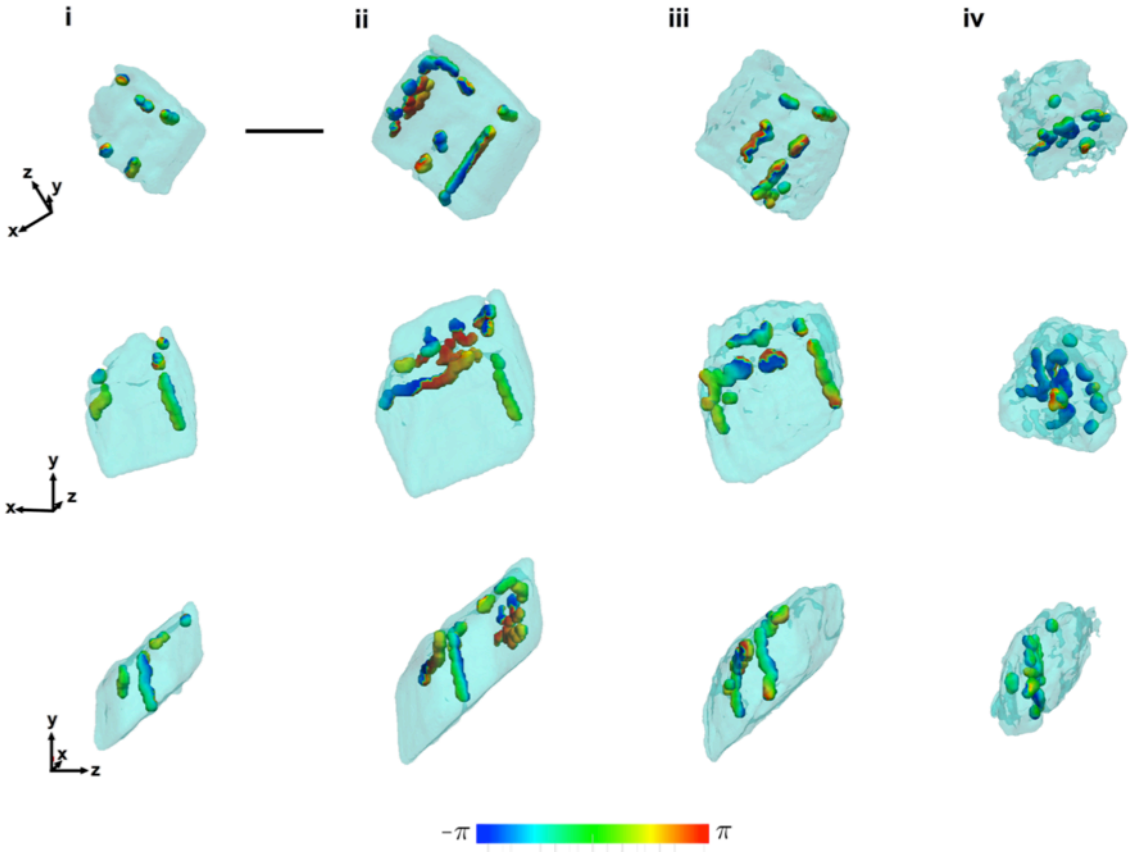
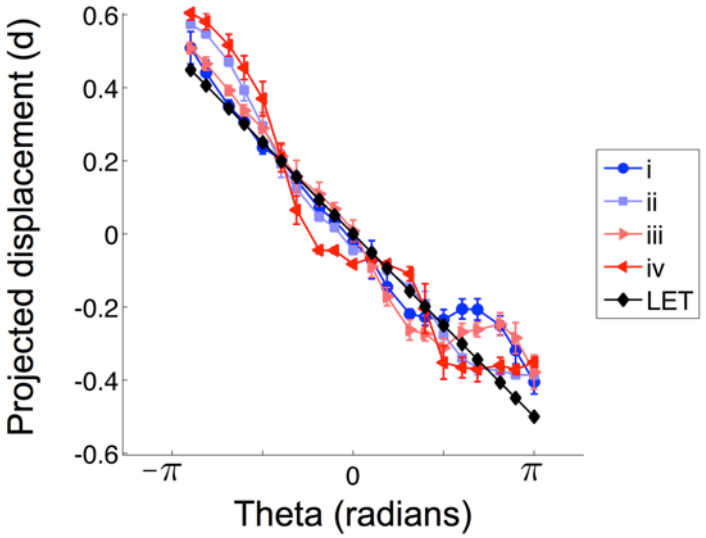
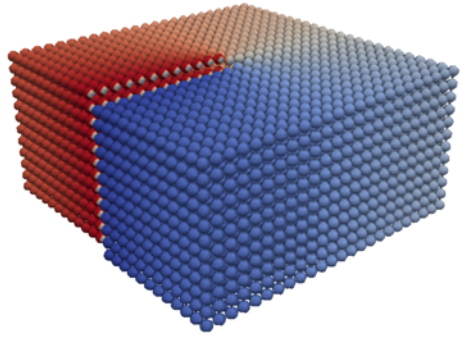
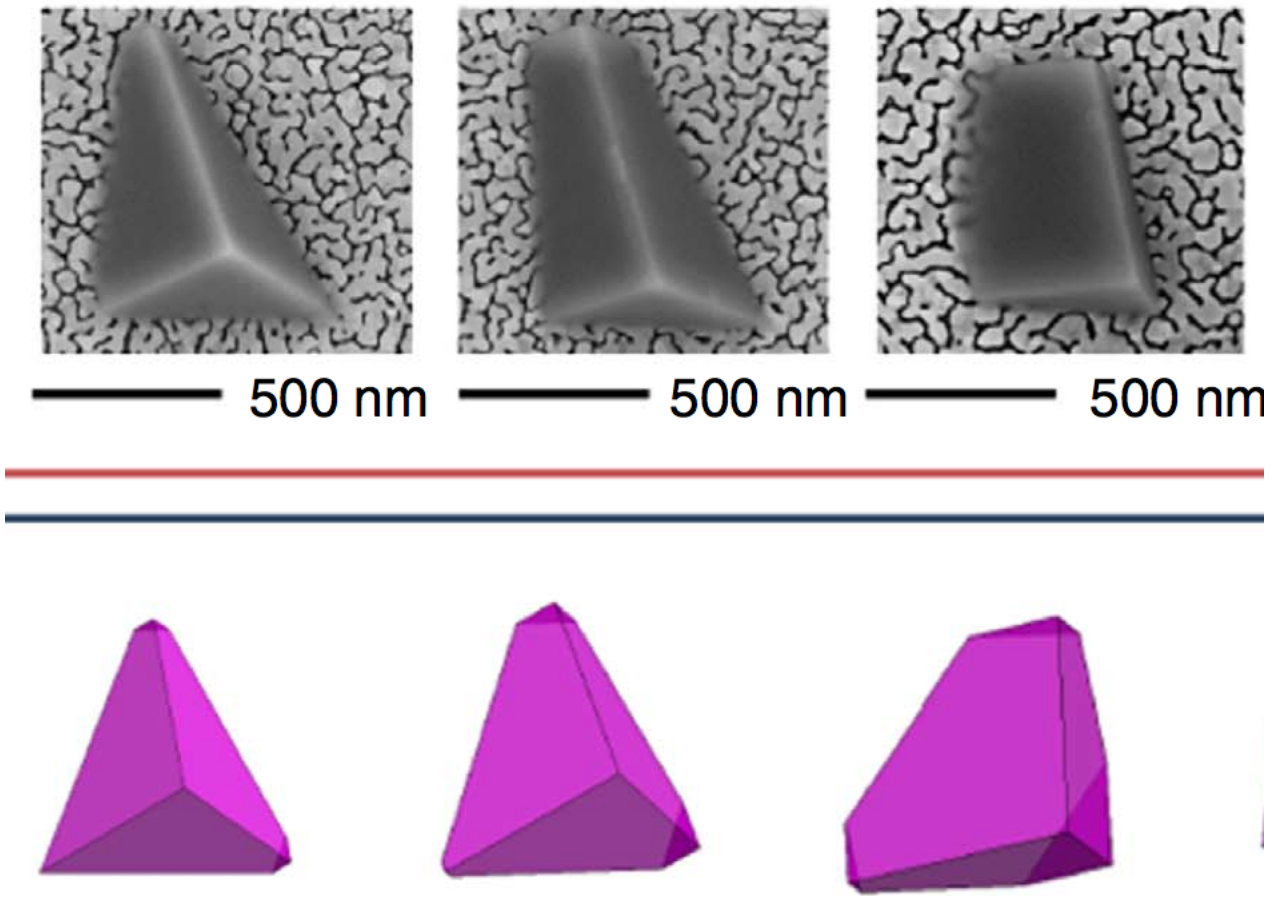






Calcite growth on SAM/Au(111)

J. Ihli, J. N. Clark, et al, N. Comms **7** 11878 (2016)



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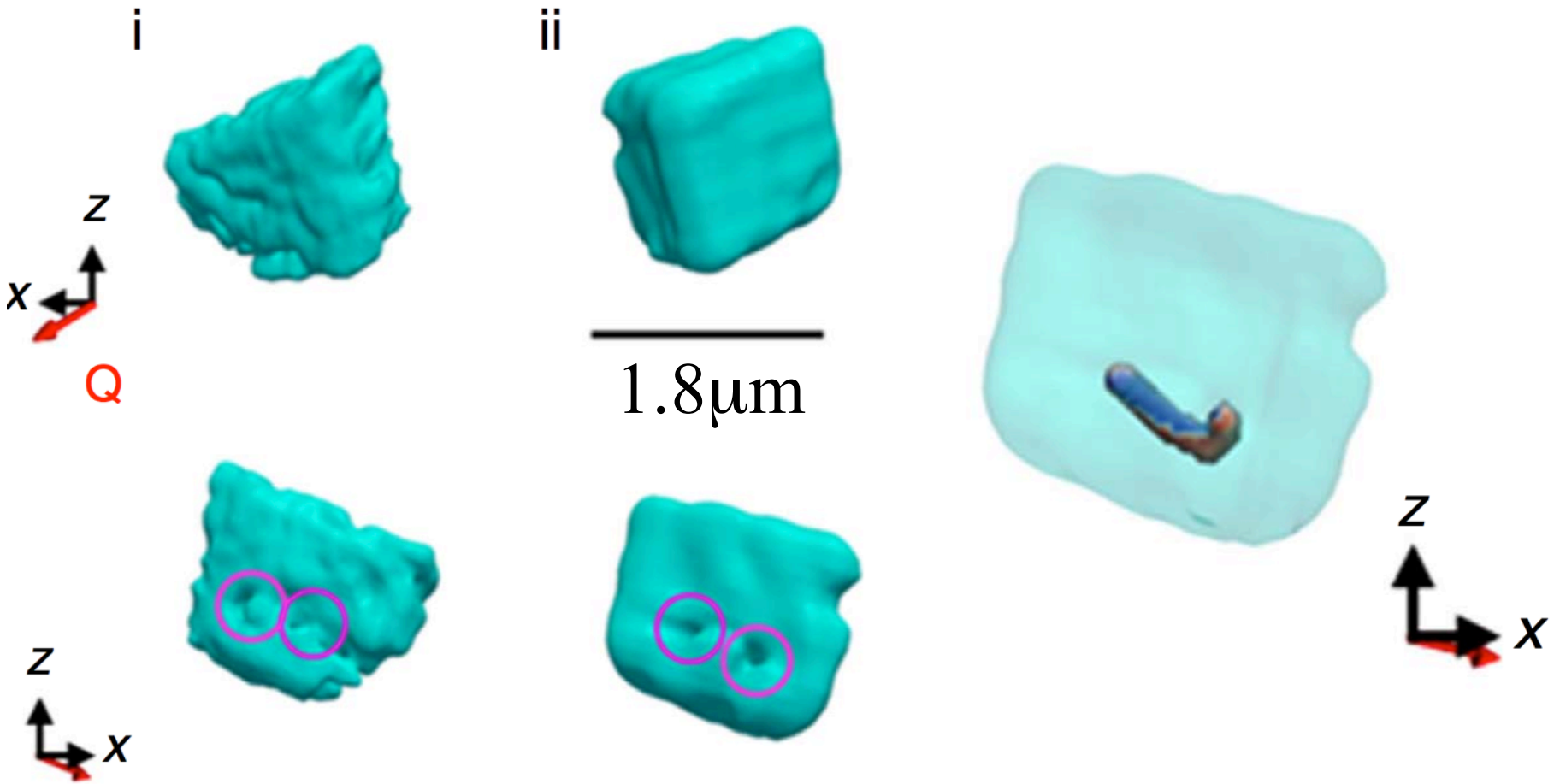

Calcite growth on SAM/Au(111)

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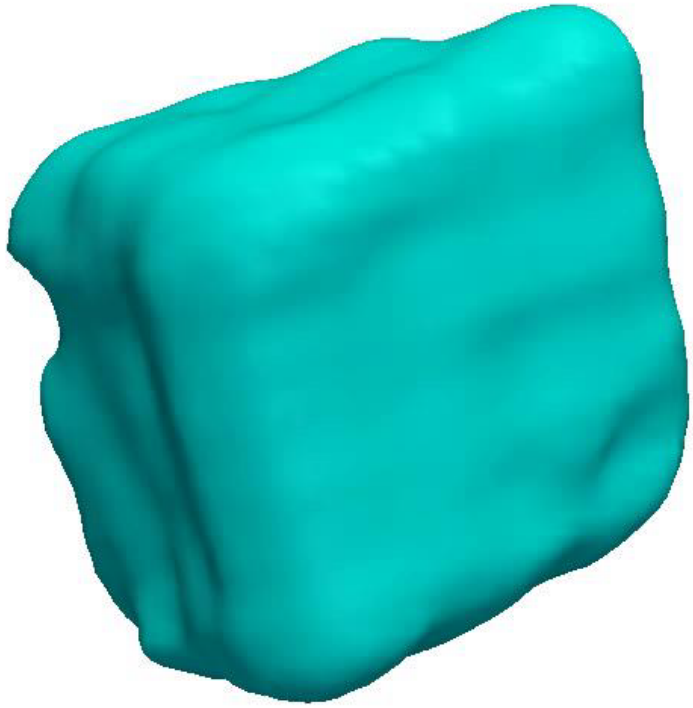
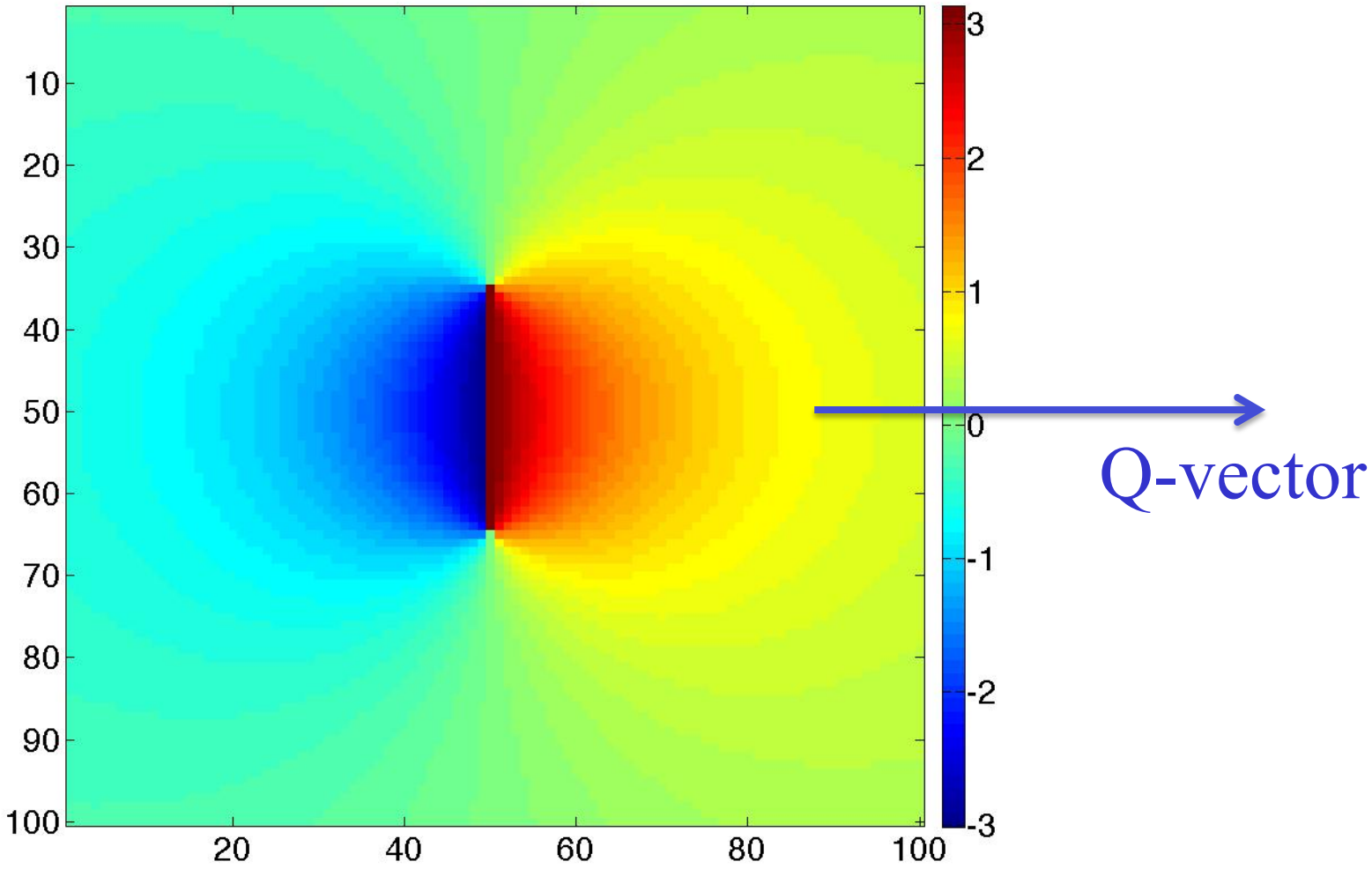
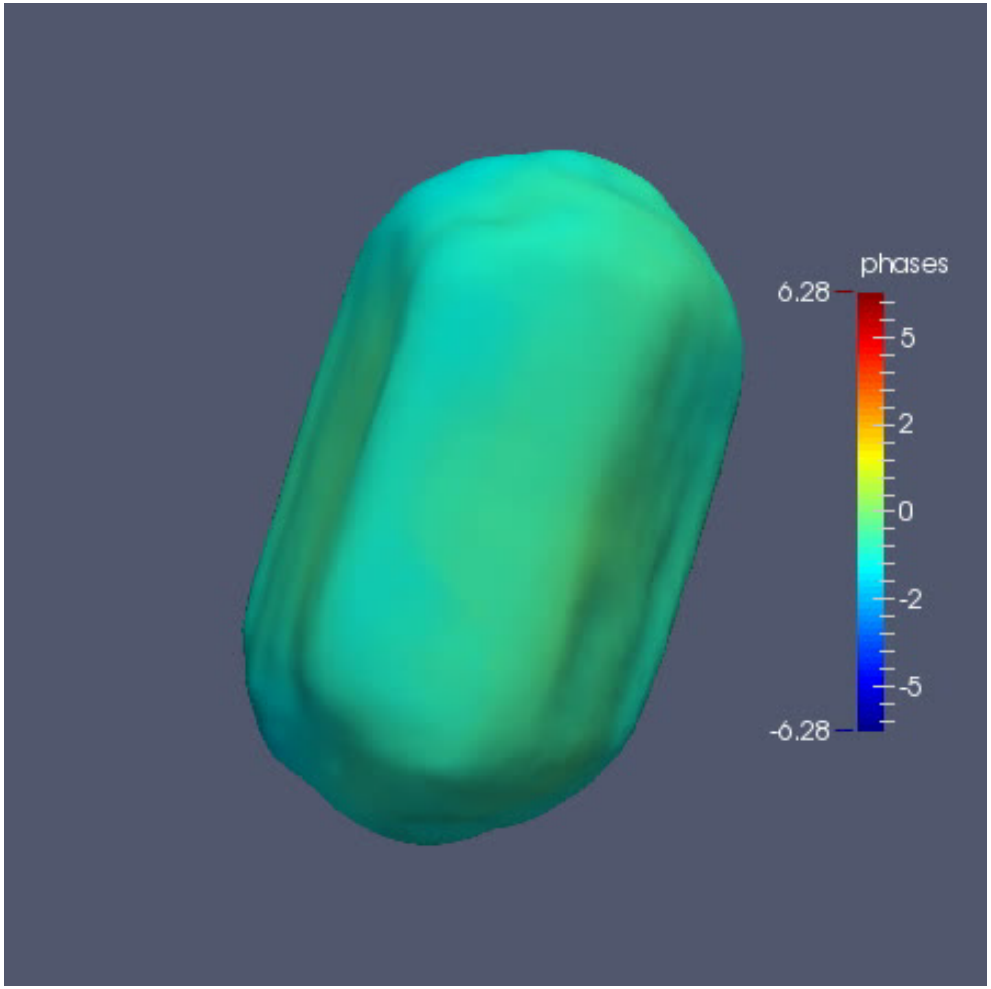


Strain field of Edge Dislocation Loop



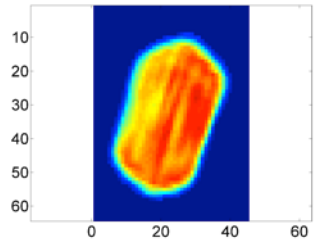
Au NC before Fe deposition

Ana Estandarte, to be published



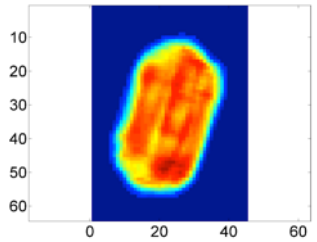
Amplitude: xz-cut plane, T=400°C

Before Fe dose

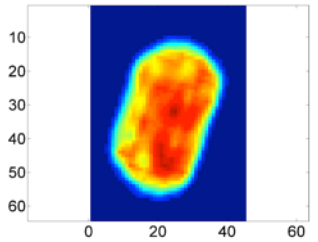


After 1st Fe dose,

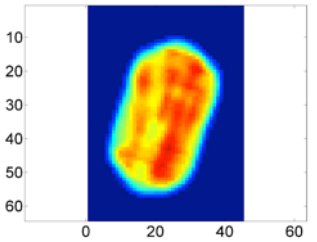
t=10min



t=1hr



t=2hrs



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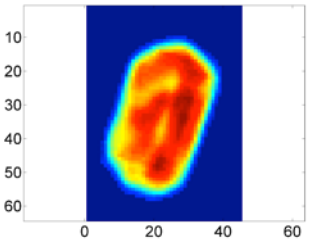
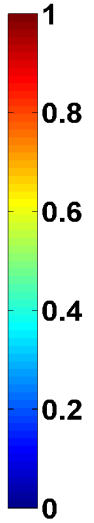
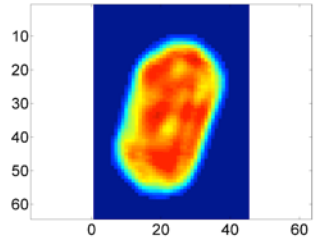


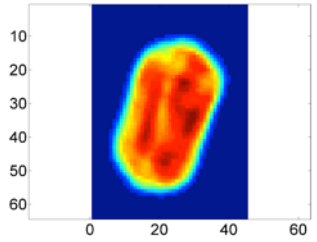


After 2nd Fe dose,

t=4hrs



t=5hrs



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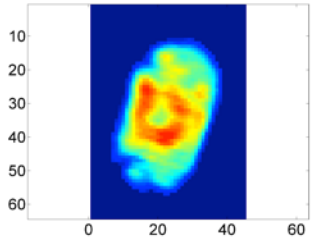

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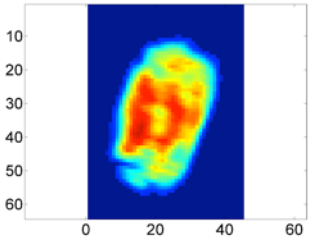
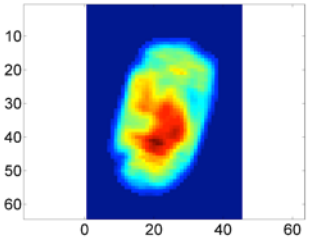
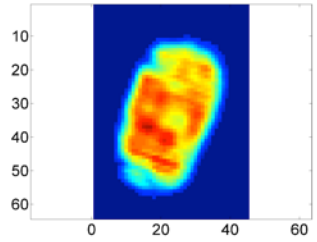


t=2hrs



After 3rd Fe dose,

t=3hrs



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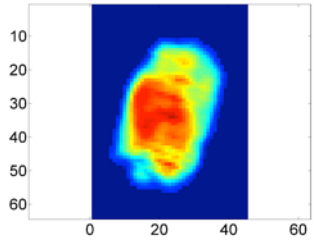
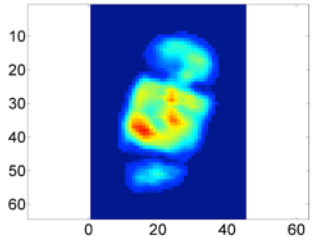
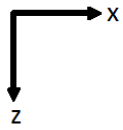


t=20min

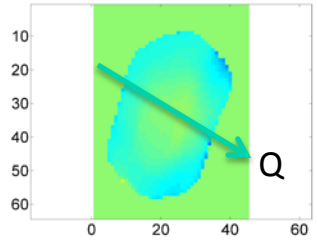




667 nm

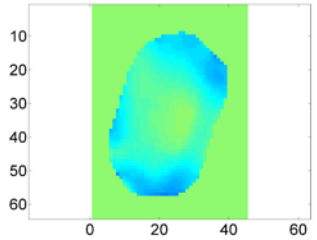
Phase: xz-cut plane, T=400°C

Before Fe dose

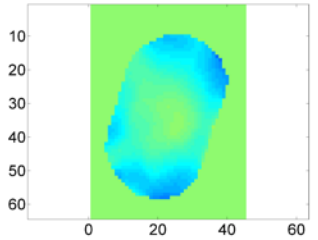


After 1st Fe dose,

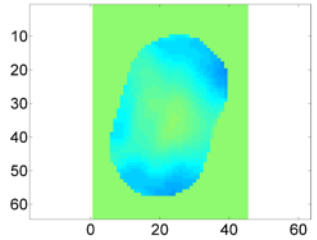
t=10min



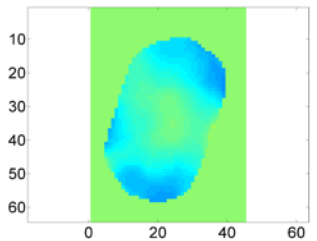
t=1hr



t=2hrs

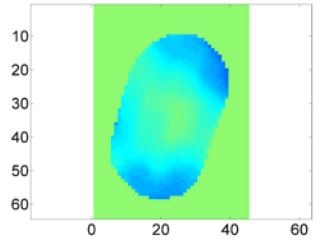


t=3hrs

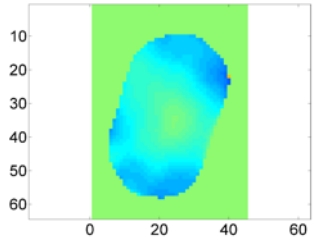


After 2nd Fe dose,

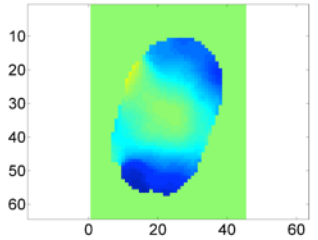
t=4hrs



t=5hrs



t=10min



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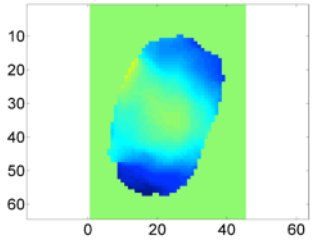
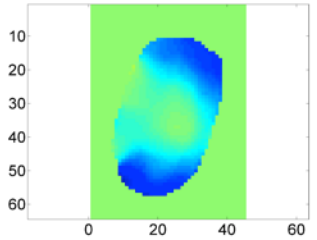
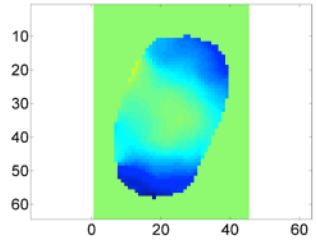


t=2hrs

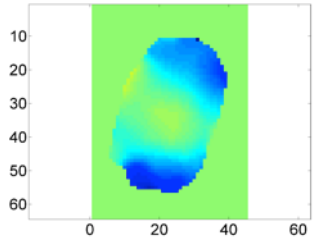


After 3rd Fe dose,

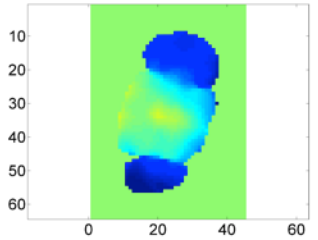
t=3hrs

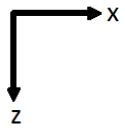


t=6hrs



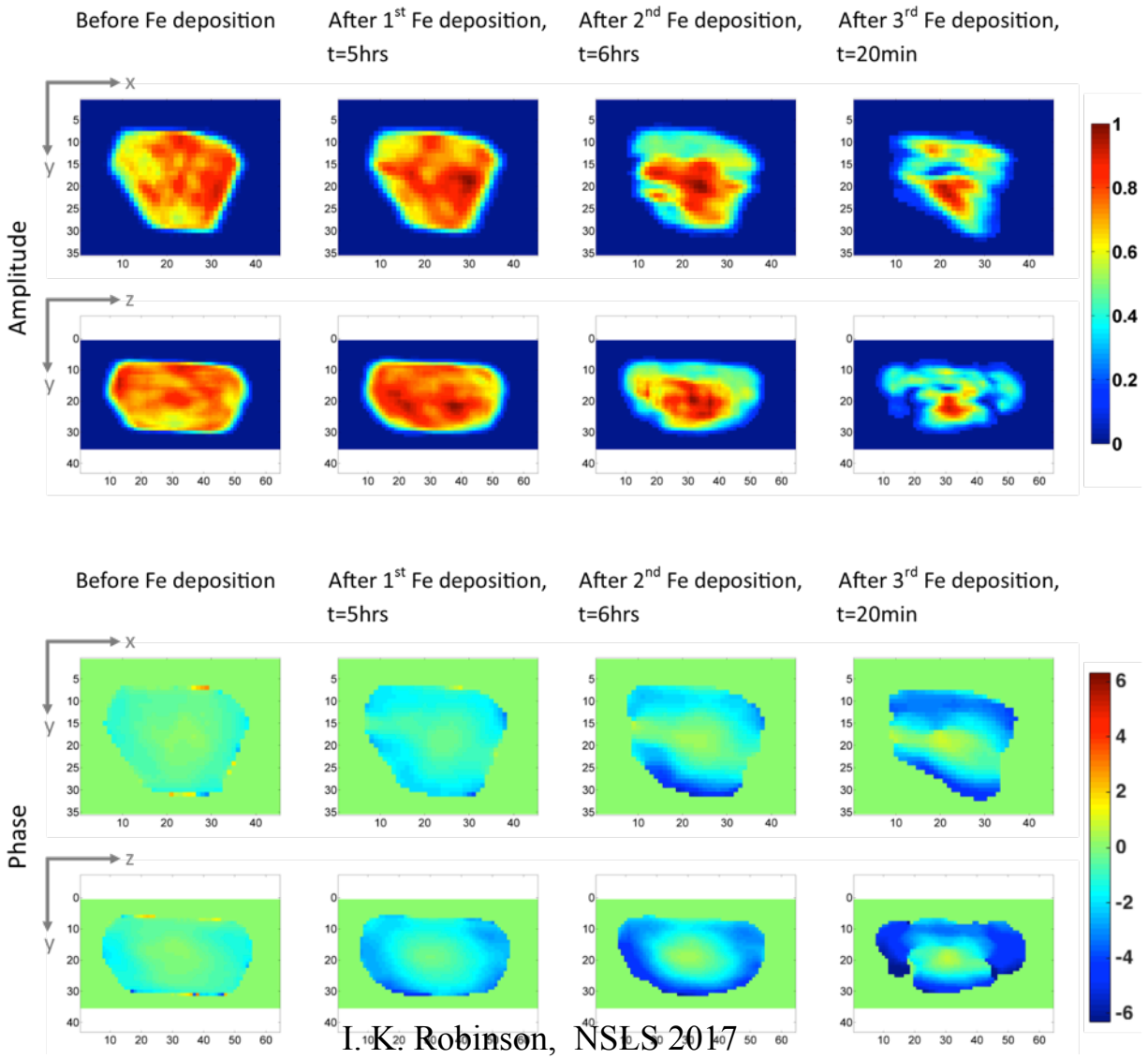
t=20min





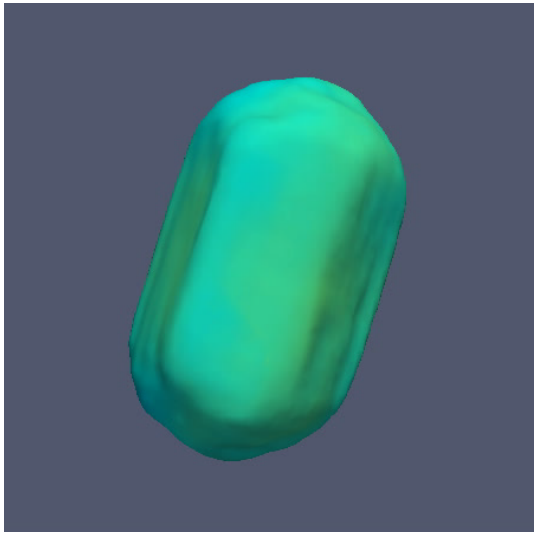
667 nm

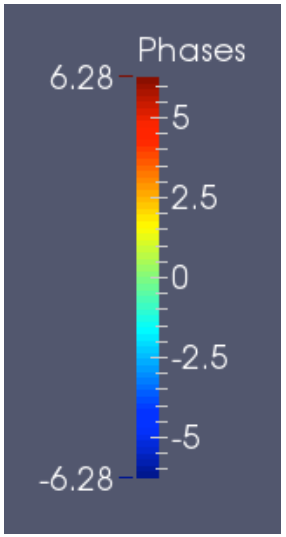
xy- and zy-cut planes, T=400°C



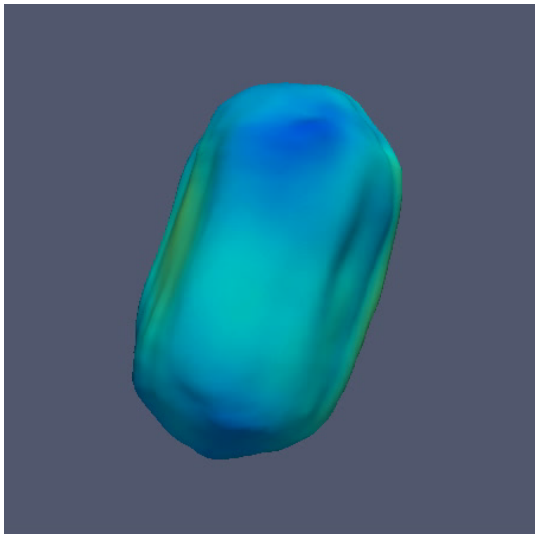
Phase Isosurface Images

Control

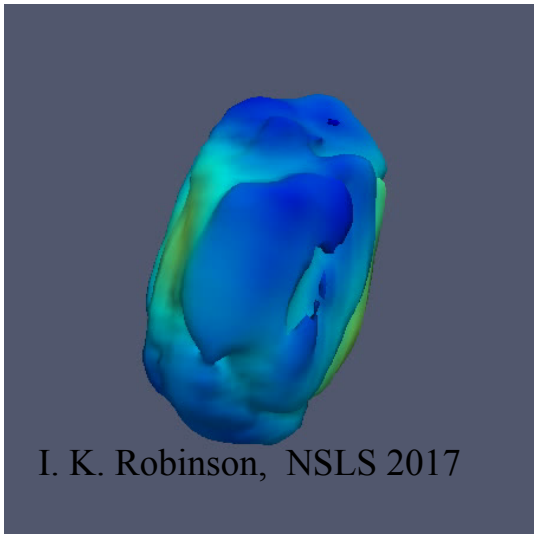




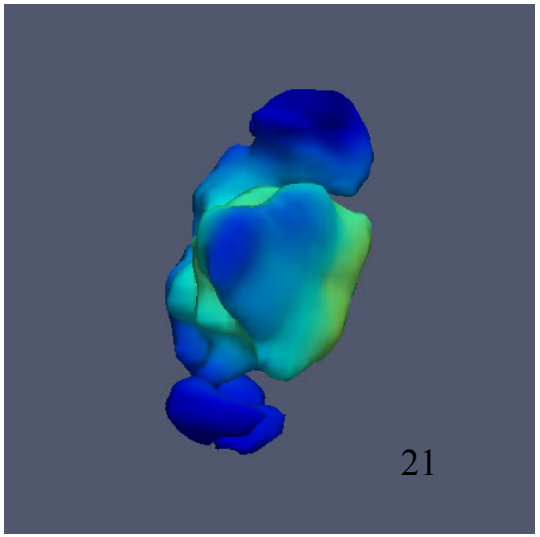
After 1st Fe dose



After 2nd Fe dose



After 3rd Fe dose



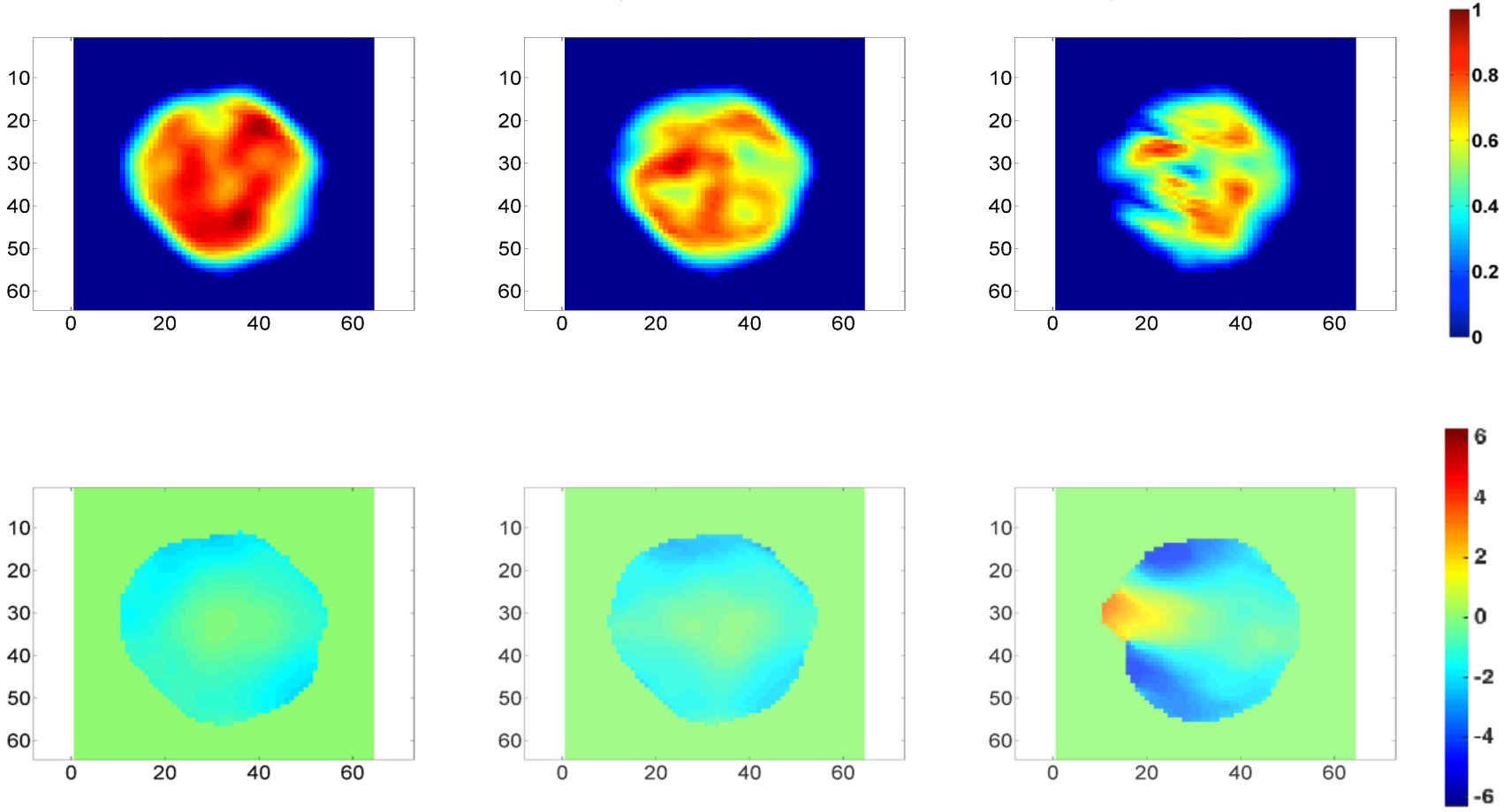
Amplitude and Phase, T=300°C

Ana Estandarte, to be published

Before Fe dose

1st Fe dose, t=6hrs

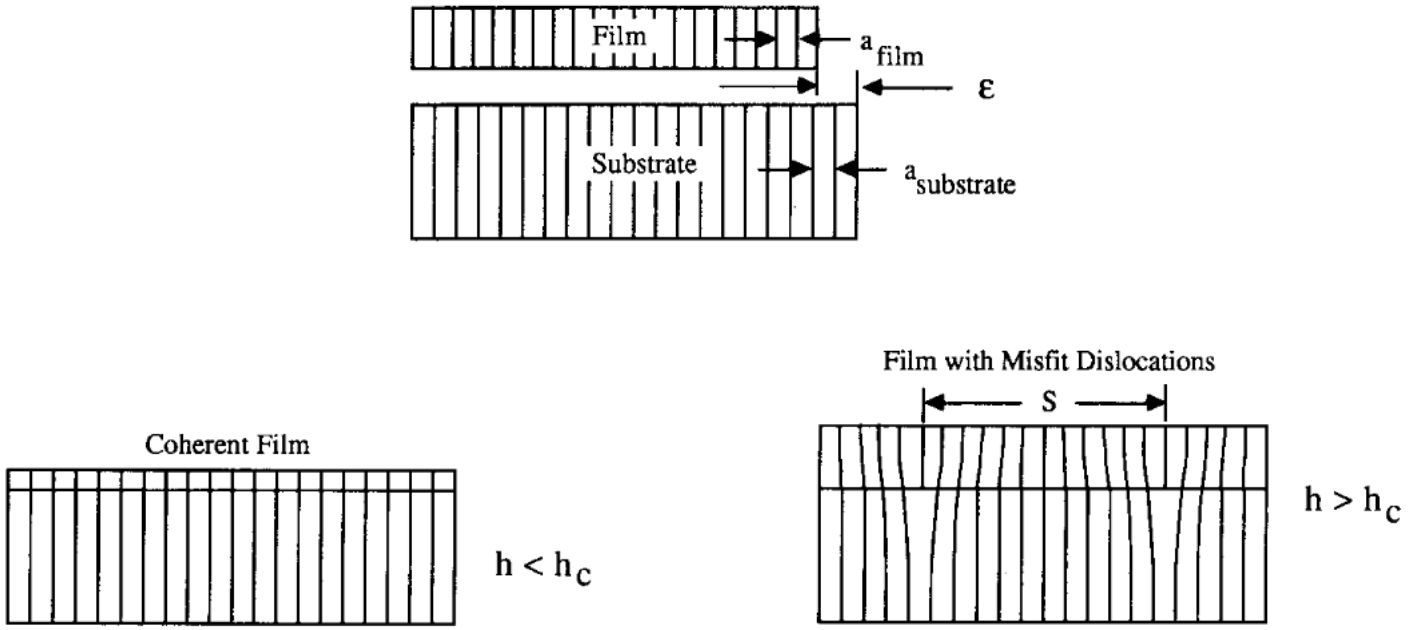
2st Fe dose, t=8hrs



Misfit Dislocations and Stacking Faults

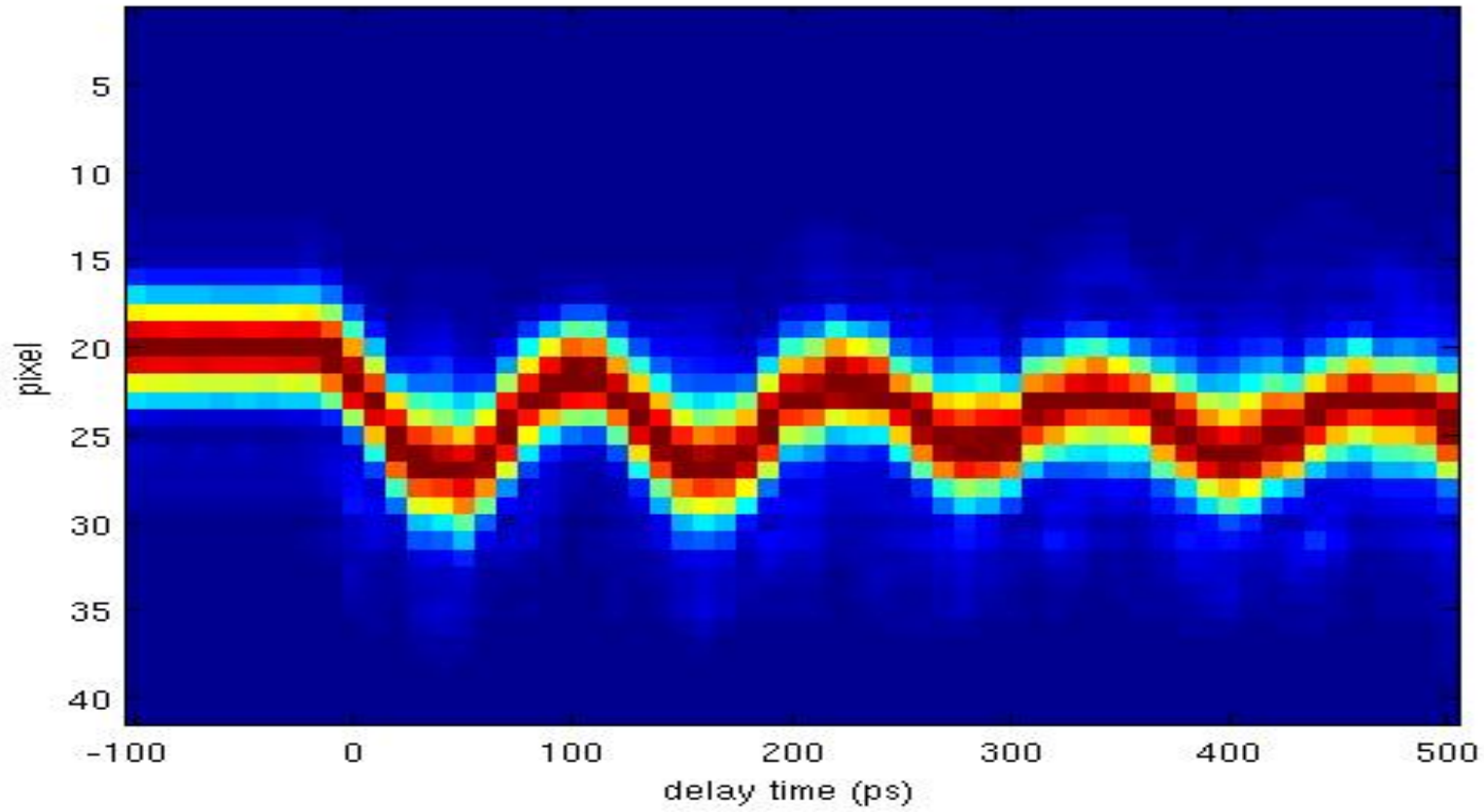
Ana Estandarte, to be published

- Alloying of Fe with Au → contraction of the nanocrystal lattice
- Lattice misfit between AuFe shell and Au core → formation of misfit dislocations



Au Pump-probe at LCLS (XPP)

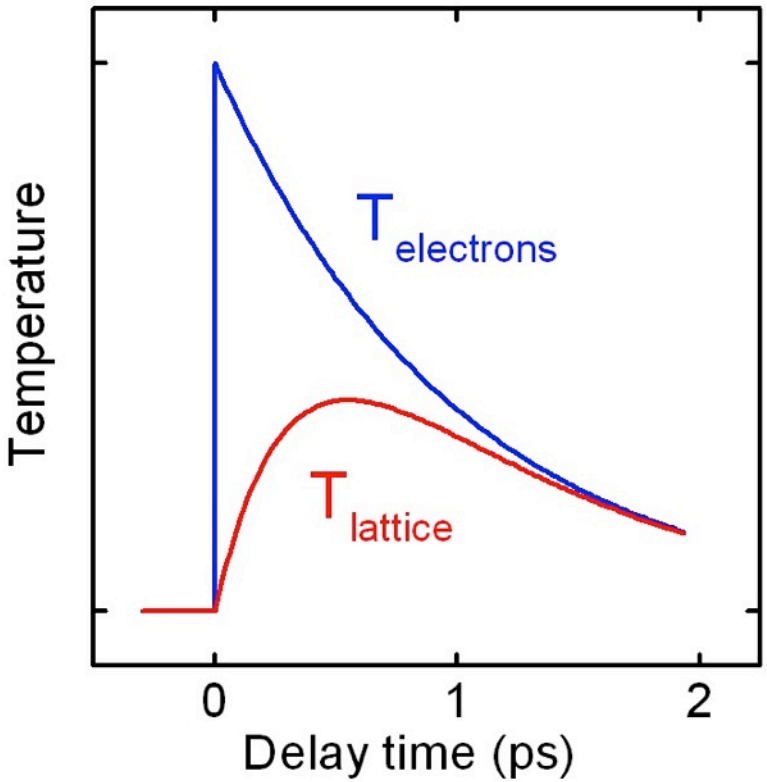
Justin Wark, Loren Beitra, Alexander Korsunsky, Ross Harder, David Fritz ,
Sebastien Boutet, Jesse Clark, Garth Williams, Brian Abbey, Andy Higginbotham,
Diling Zhu, Henrick Lemke, Mattieu Chollet, Marc Messerschmidt



"Two-temperature" model

I.K. Robinson et al, Journal of Optics **18** 054007 (2016)

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



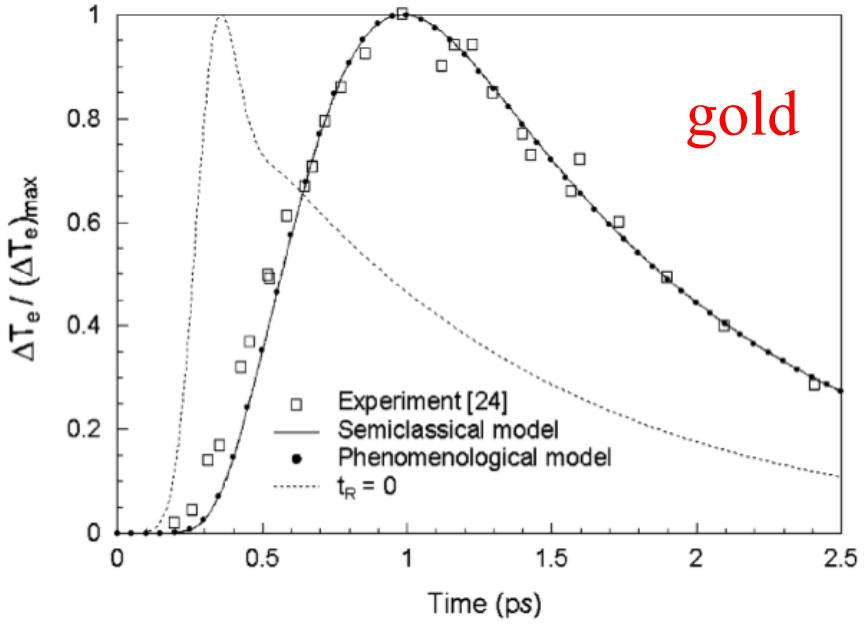
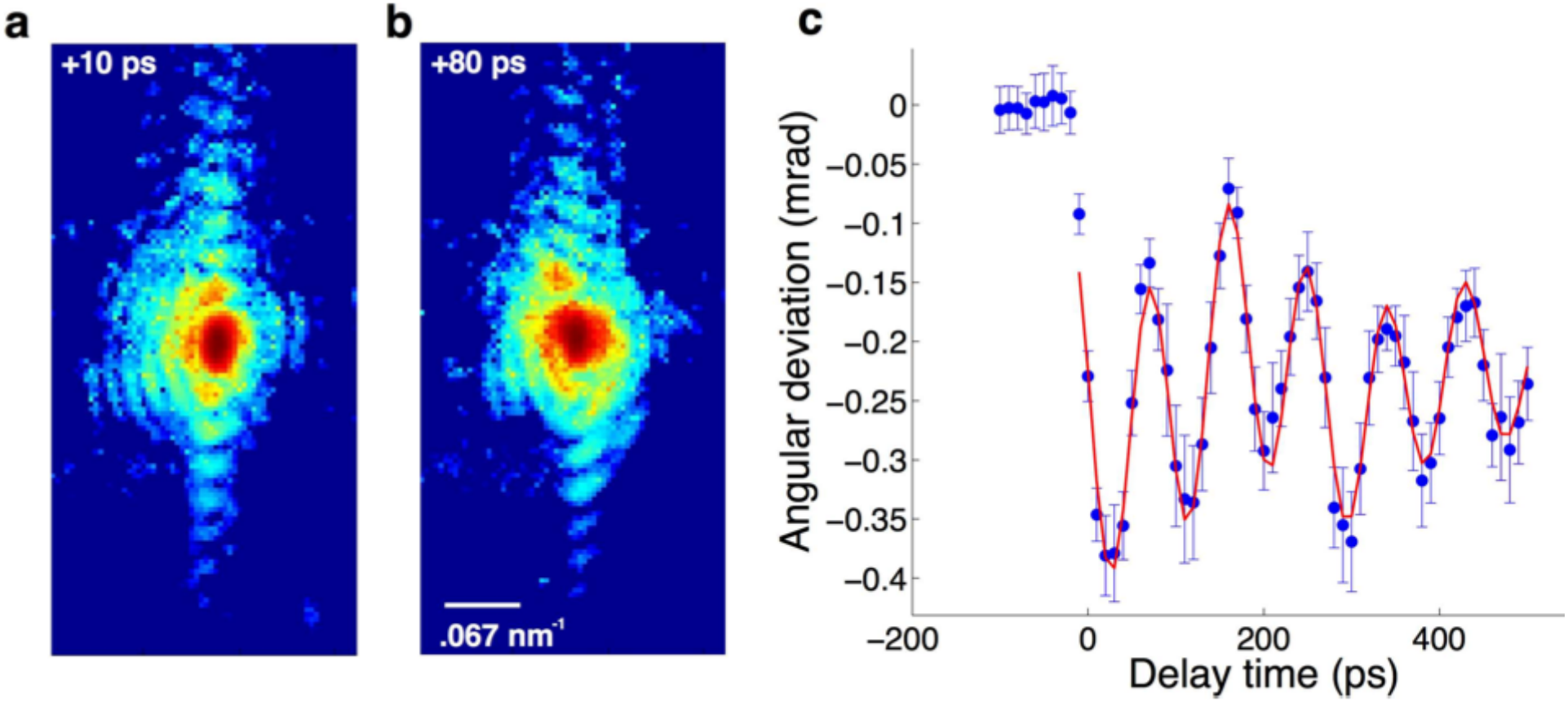


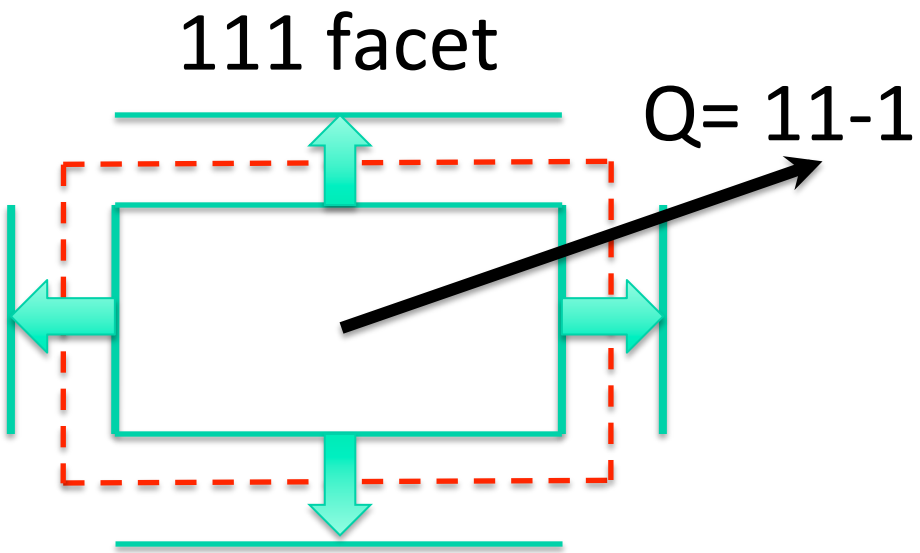
Fig. 2. Comparison of the change in electron temperature at the front surface of an 80-nm gold film irradiated by a 2.8 mJ/cm^2, 800 nm, 150-fs laser pulse.

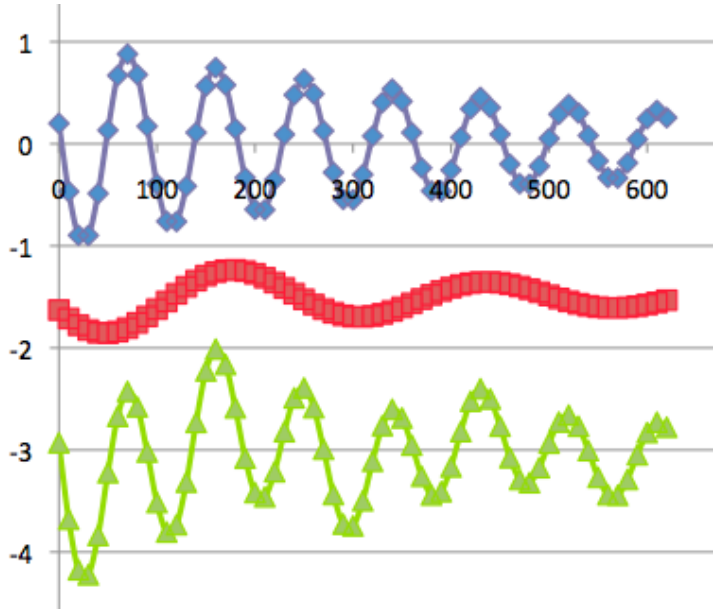
Time resolved Bragg peak position



Two Normal Modes of Vibration

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



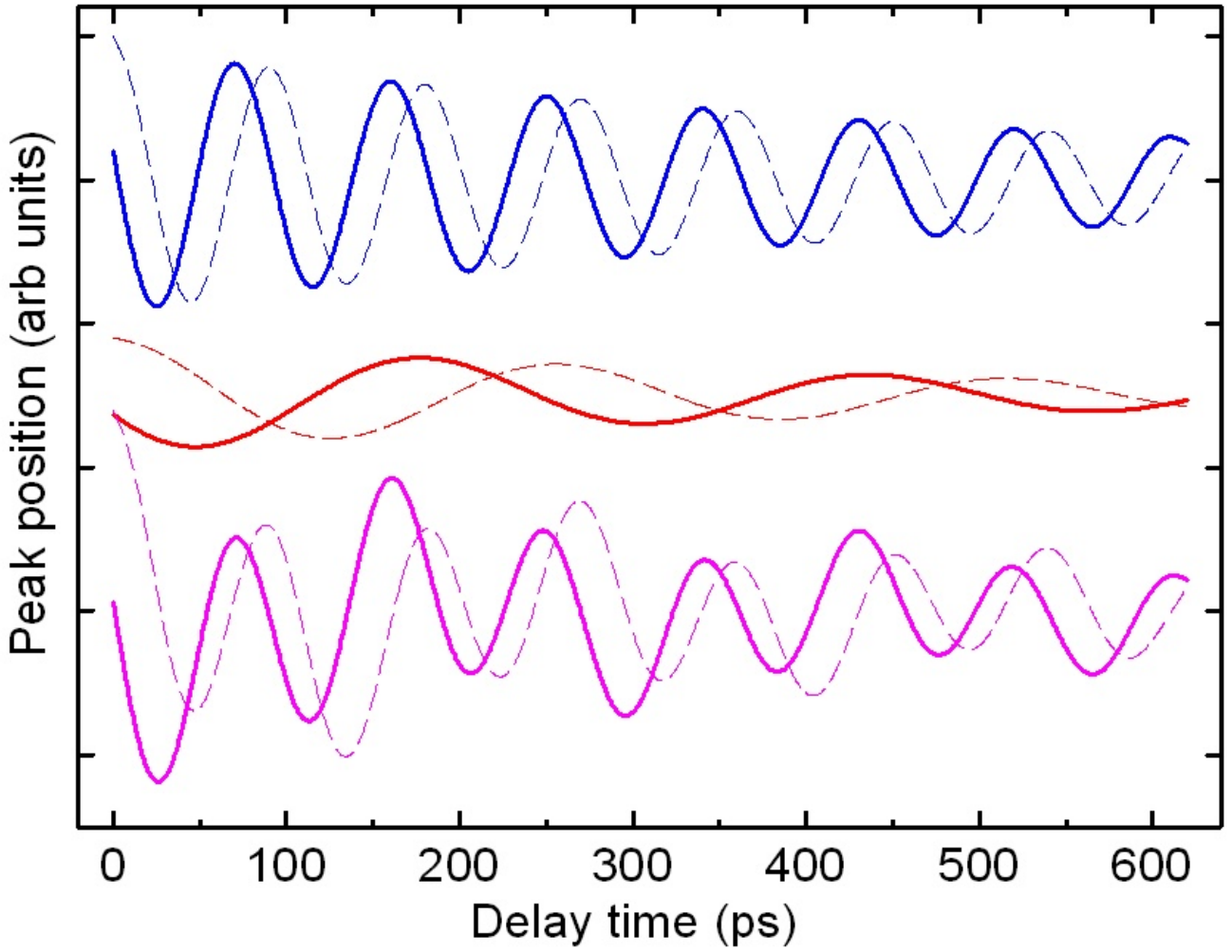


T_1 = 90ps h_1 = 145nm c_S = 3240 m/s

T_2 = 259ps h_2 = 420nm

Phase Origin of Vibrations

I.K. Robinson et al. Journal of Optics **18** 054007 (2016)

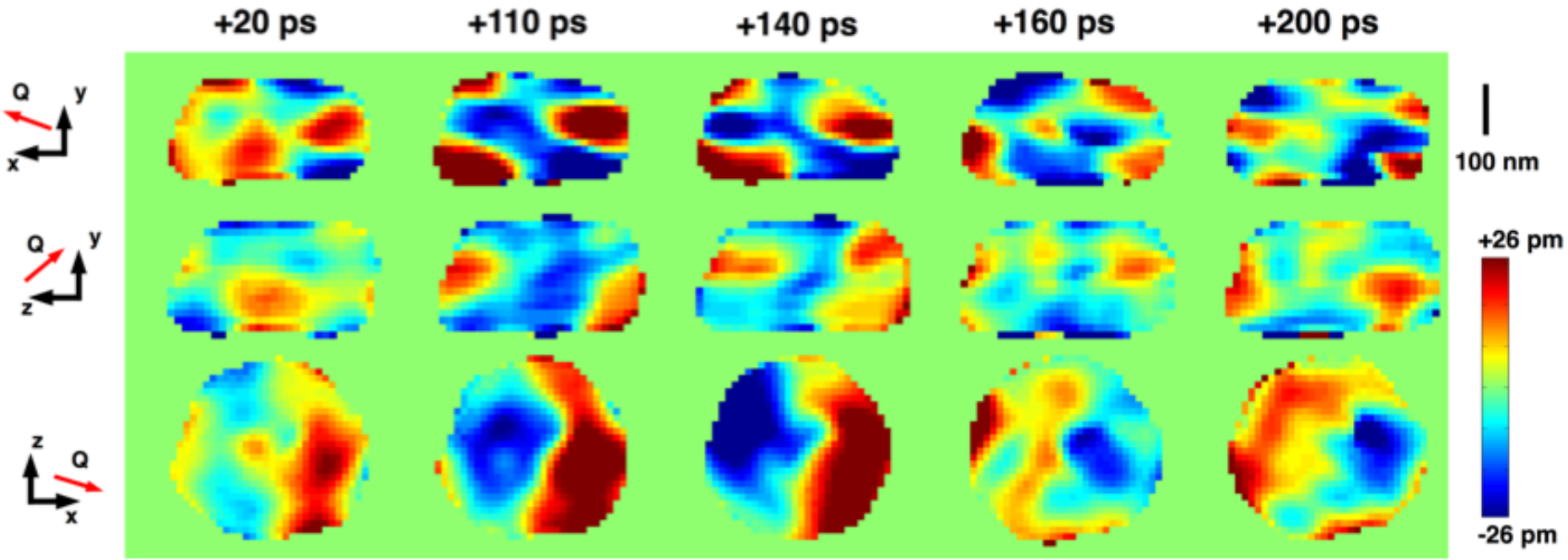


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

1000 frames averaged at each point of rocking curve

Jesse Clark et al, Science **341** 56 (2013)

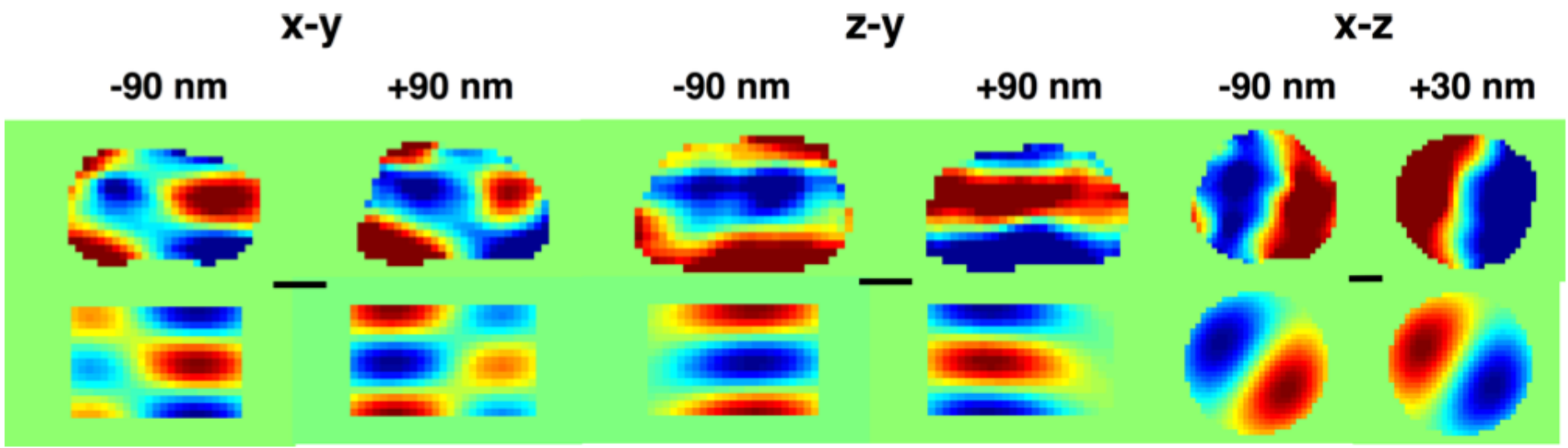


Dynamic imaging of displacements

CDI inversion of 3D diffraction patterns

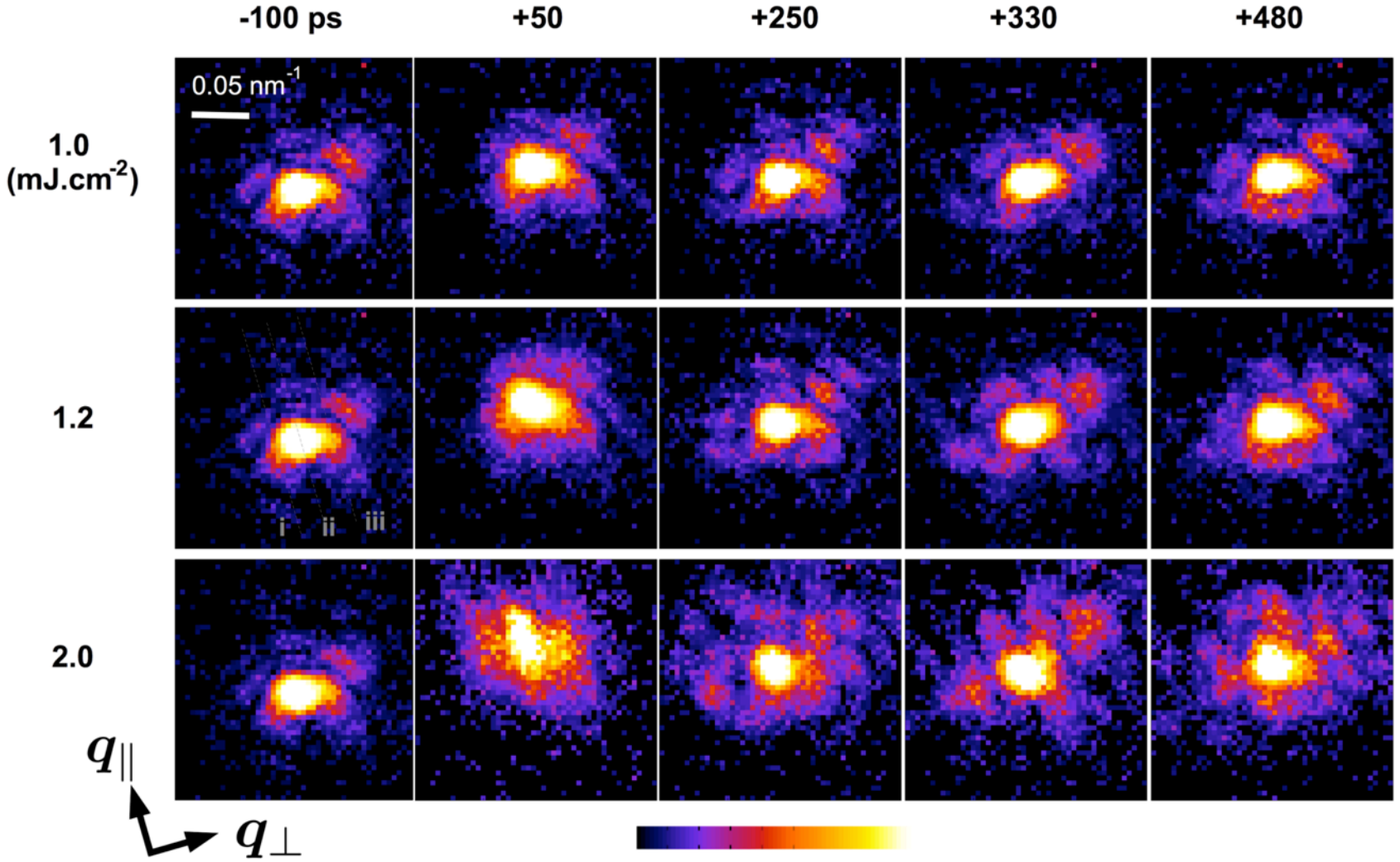
Comparison with (1,1) normal mode of cylinder

Jesse Clark et al, Science **341** 56 (2013)



Dependence on Laser Fluence

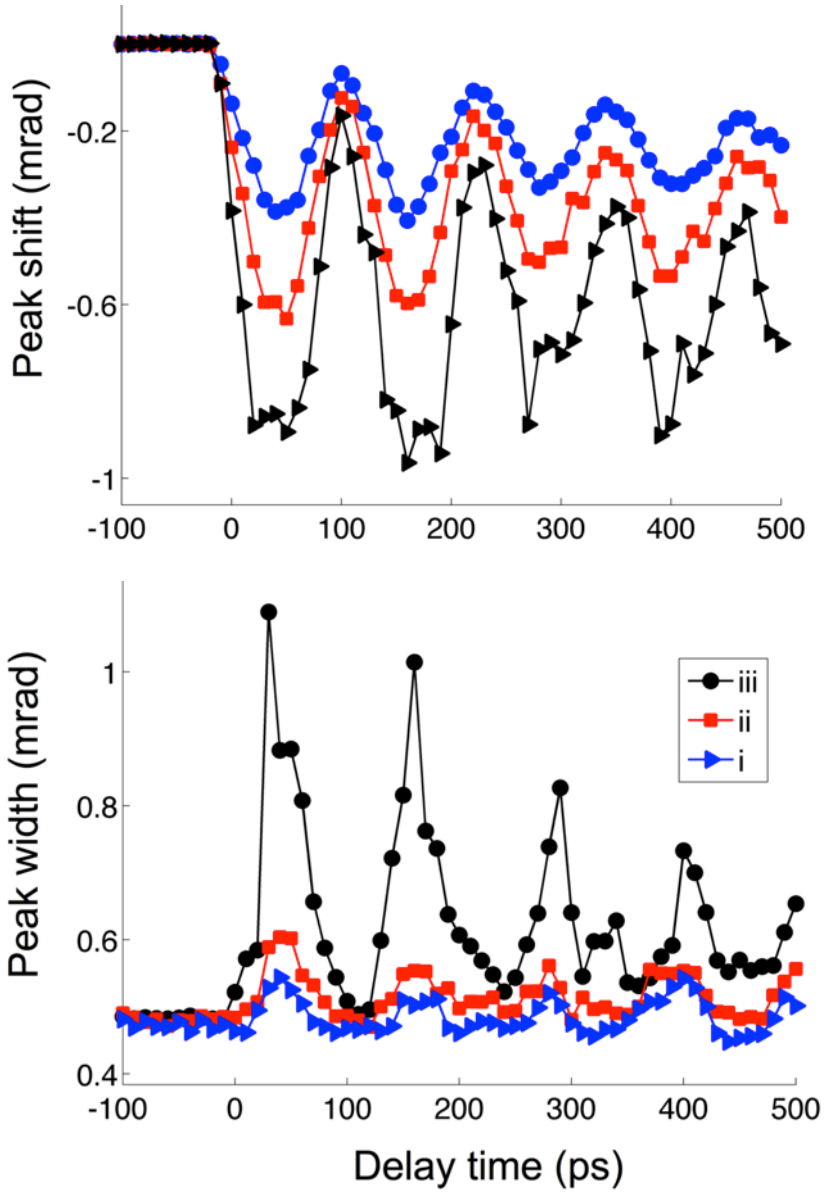
Jesse Clark et al, PNAS **112** 7444 (2015)



Dependence on Laser Fluence

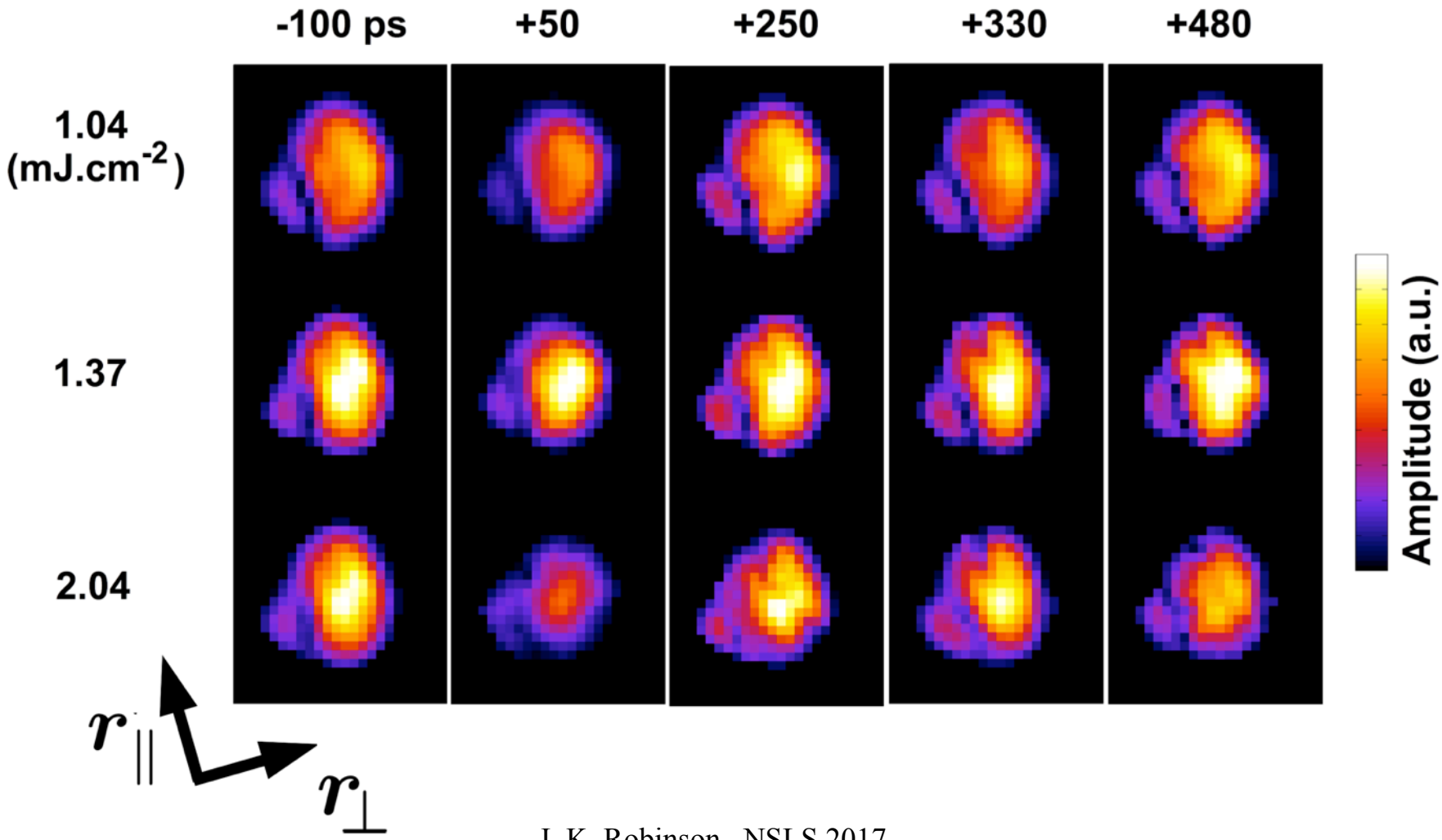
Jesse Clark et al, PNAS **112** 7444 (2015)

1.0 mJ cm^{-2}
1.4 mJ cm^{-2}
2.0 mJ cm^{-2}



Dependence on Laser Fluence

Jesse Clark et al, PNAS **112** 7444 (2015)



Bragg Coherent Diffraction Imaging

- Complex density can image strain
- Strain associated with nano-shape
- In-situ crystal growth of calcite
- Nanoscale alloy is core-shell
- Ultrafast snapshots of vibrations
- Transient melting of nanoparticles