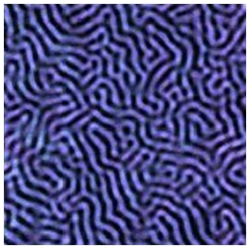
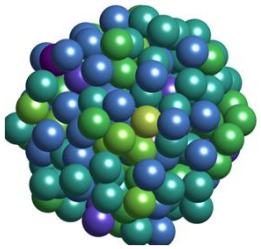
Future of Coherent X-ray Scattering at XFELO

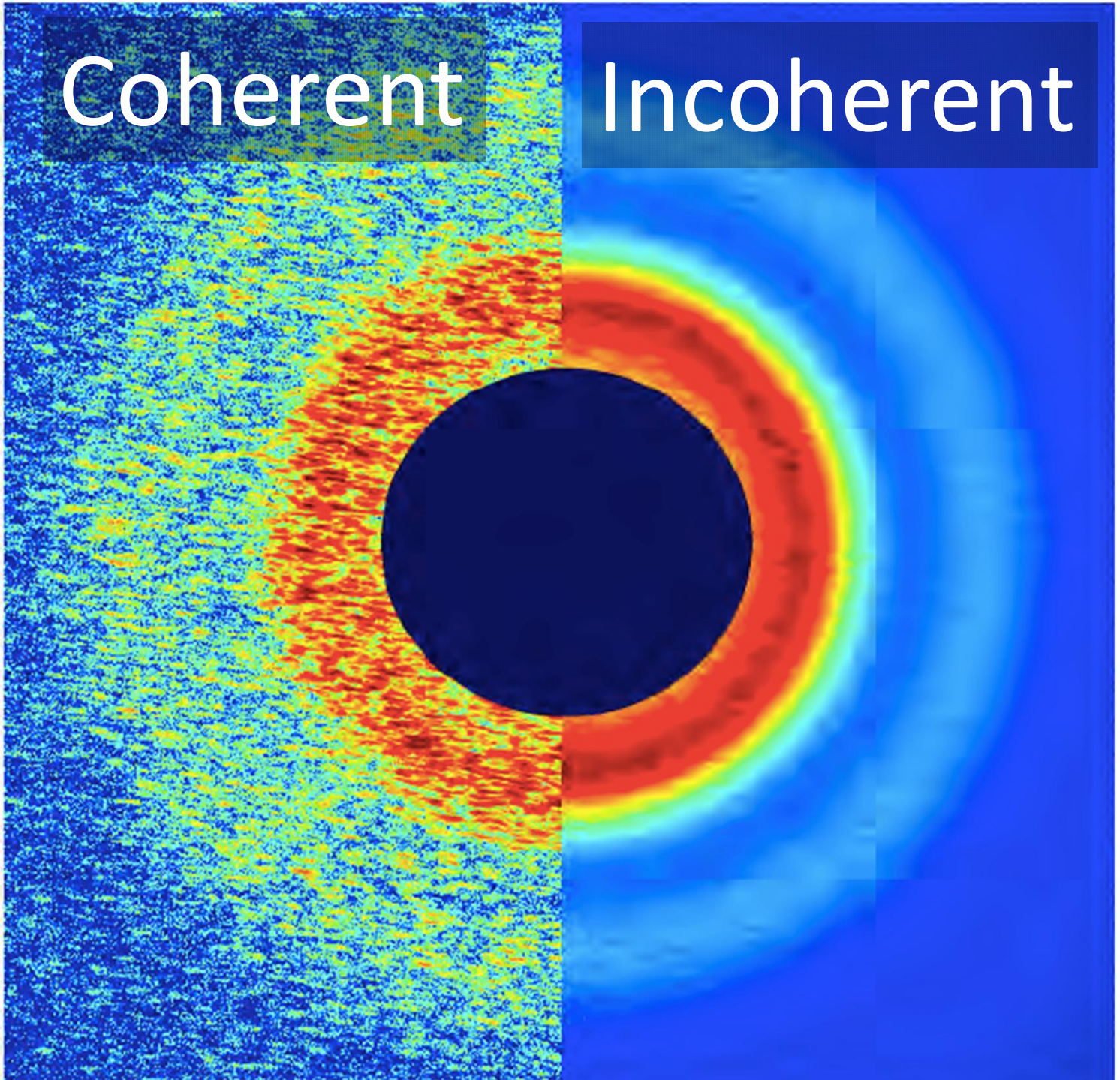




Oleg Shpyrko
UC San Diego

Tentative Talk Schedule

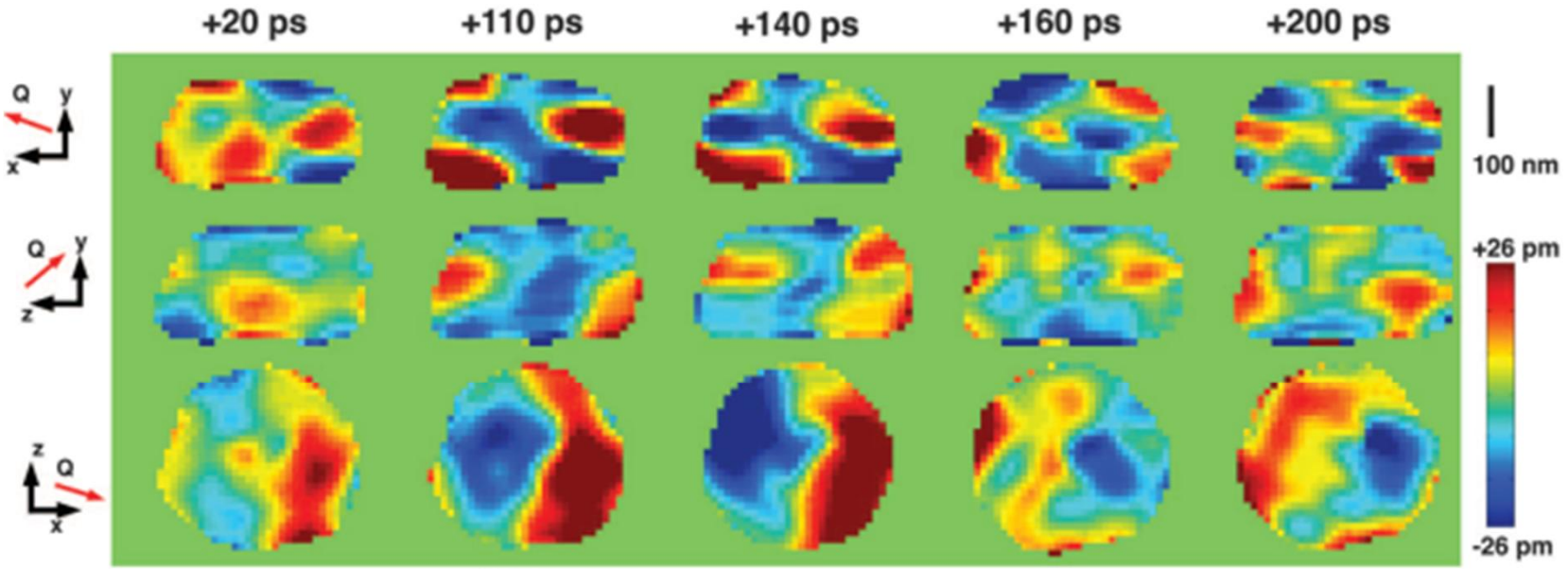
- Oleg Shpyrko, UC San Diego (~10min)
- Brian Stephenson, Argonne (~10min)
  (or Anders Madsen if Brian is too jetlagged/asleep)
- Mark Sutton, McGill (10-15min)
- Andrej Singer, UC San Diego (10-15min)
- Gerhard Grubel, DESY (10-15min?)
- Everyone + discussion (till dinner and beyond)

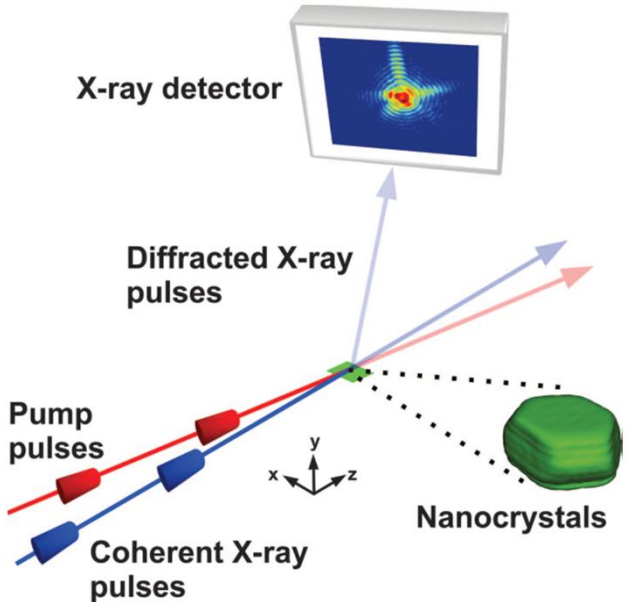

Coherent
Incoherent

How do we take advantage of Coherence of XFELO?

- Quasi-CW (1-2+ MHz)
- Short pulses (<1 ps)
- High energy (10-25 keV)
- HUGE Coherent flux ($10^{14\text{-}15}$ ph/s)
- Narrow Bandwidth (5meV) -> Longitudinal Coherence Length (~0.3-1mm)
- Pump – Probe, Probe, Probe…

Dynamics of reproducible processes (shock wave propagation) with CXDI at LCLS:



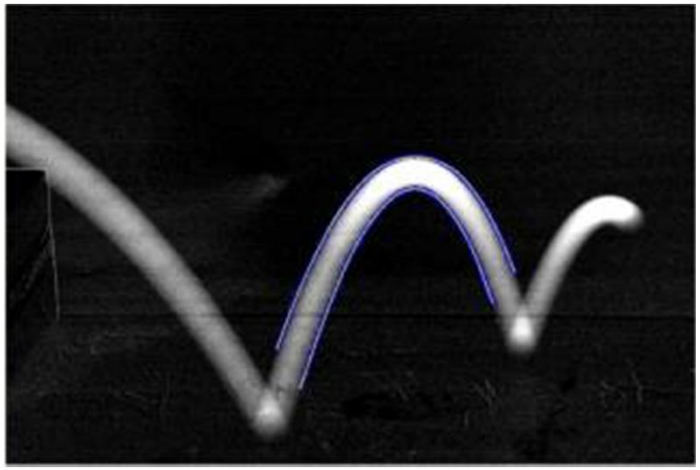


Clark et. al, Science, **341**, 56 (2013)

Grand Challenge:

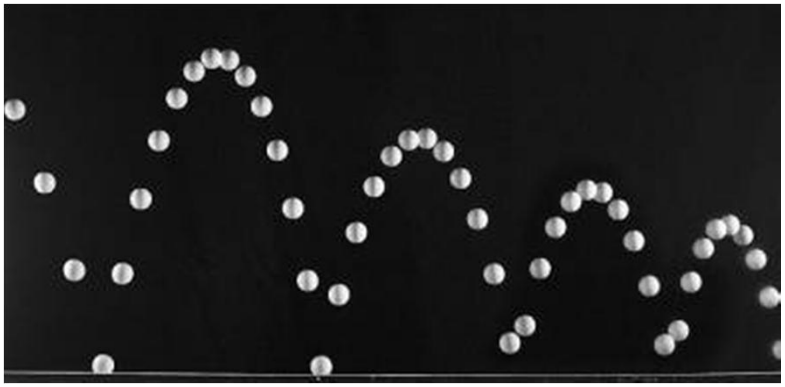
- How can we see “inside” materials and devices at nanoscale?
- Intermittent Processes – phase transitions, fluctuations, stochastic, irreversible
- Can we couple to strain, spin textures, charge, orbital order, ions, lattice defects/disorder?

Synchrotrons:

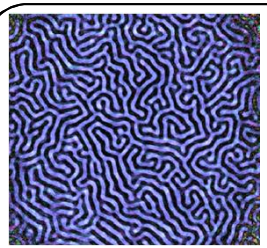


XFEL-O:

XFELs:

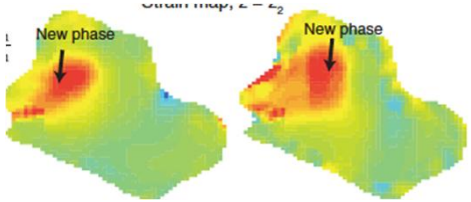


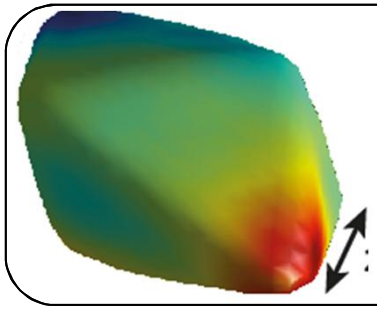
Coherent Diffractive Imaging today:



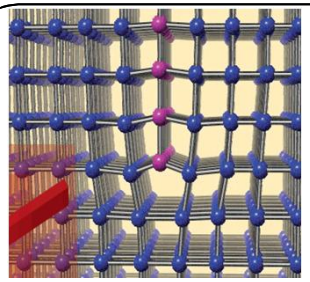
Spin Structure/Dynamics
+non-resonant magnetic scattering?

Phase Transitions:

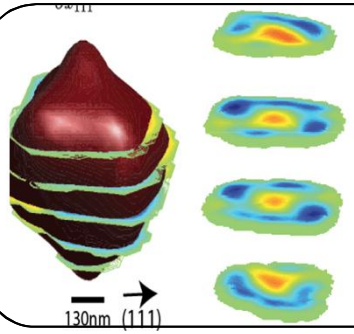




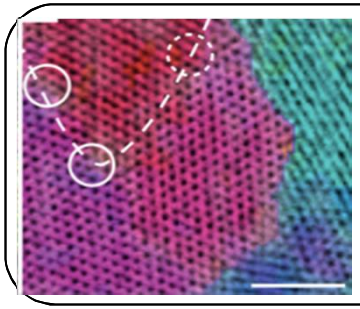
Lattice Strain



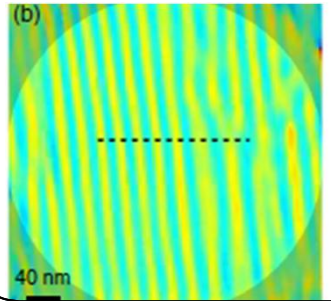
Crystalline Defects / Disorder



Ionic Diffusion



(Bio)Photonic Crystals



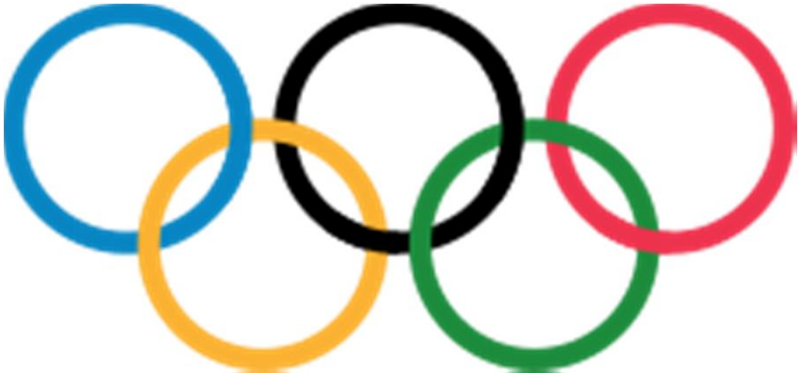
Ferroelectric Domains

?

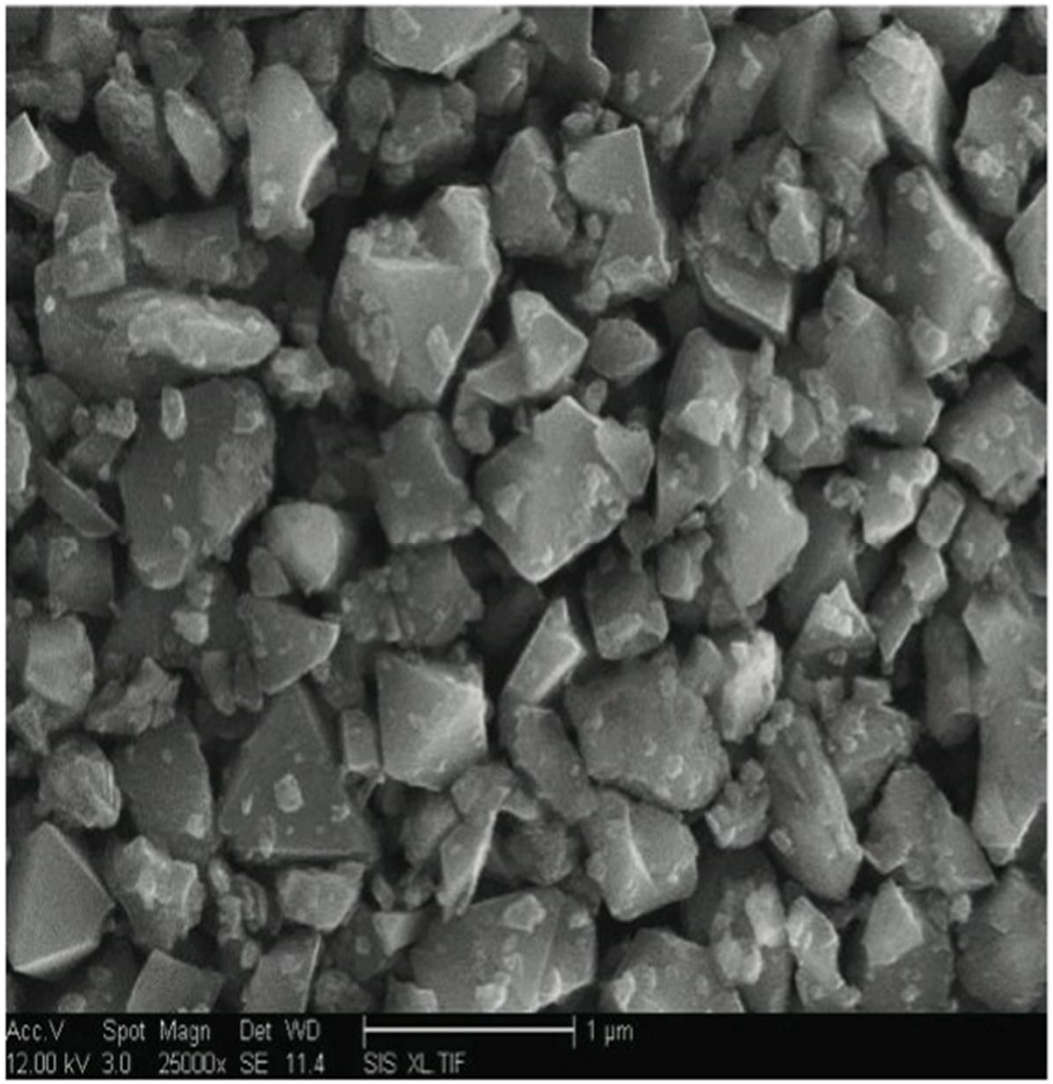
Charge-
Orbital- order?
Spin currents?
Resonances

“Citius, Altius, Fortius”, rephrased:

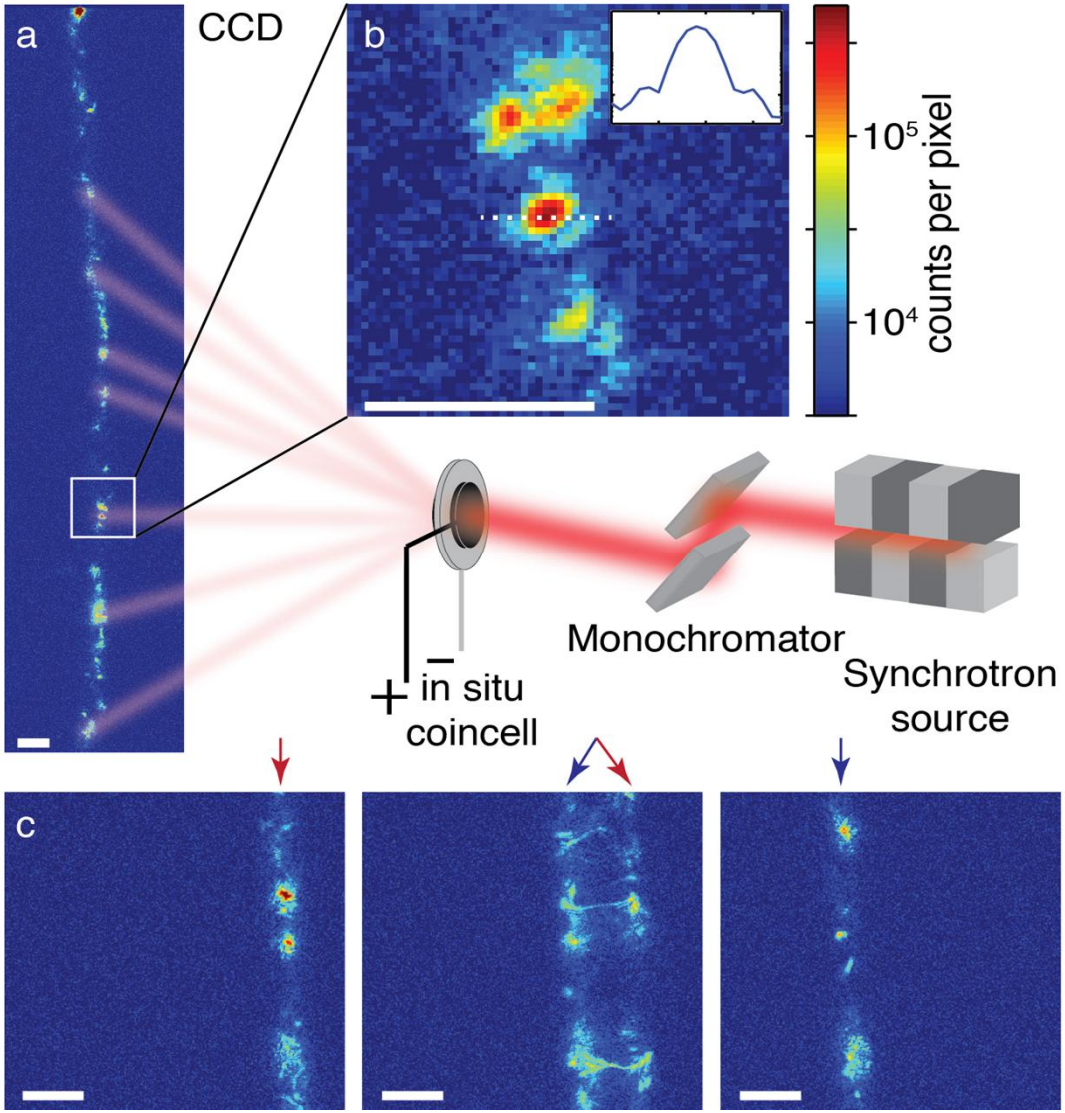
- Faster & Slower
- Smaller
- Weaker (weakly-scattering)

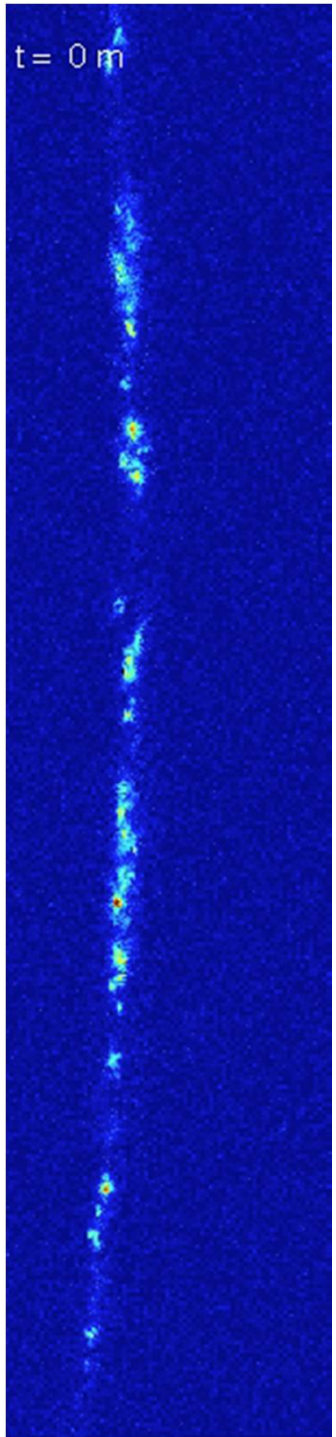


$LiNi_{0.5}Mn_{1.5}O_4$ disordered spinel 400-700 nm particles



In-Operando CXDI of Li diffusion in $LiNi_{0.5}Mn_{1.5}O_4$





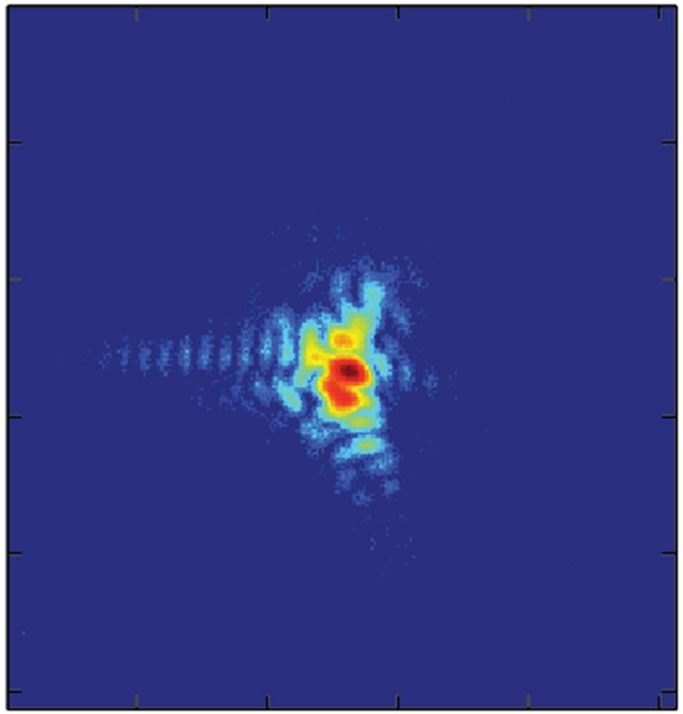
$LiNi_{0.5}Mn_{1.5}O_4$

- Full charge and full discharge in 10 hours
- 100 s per image, 600 images
- Single nano particle transformations

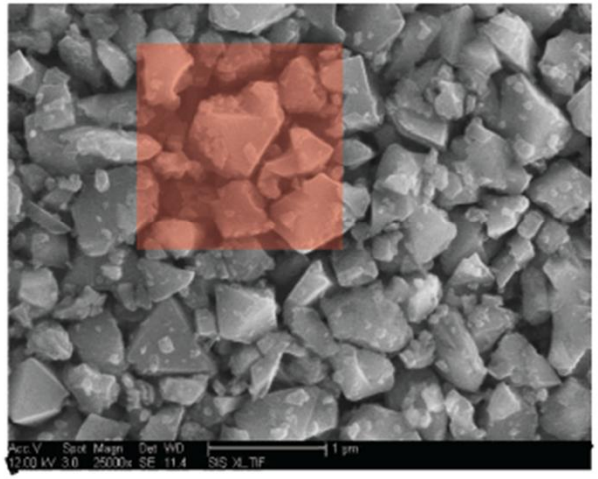
A. Singer, OS et al., Nano Lett. 14, 5295 (2014)

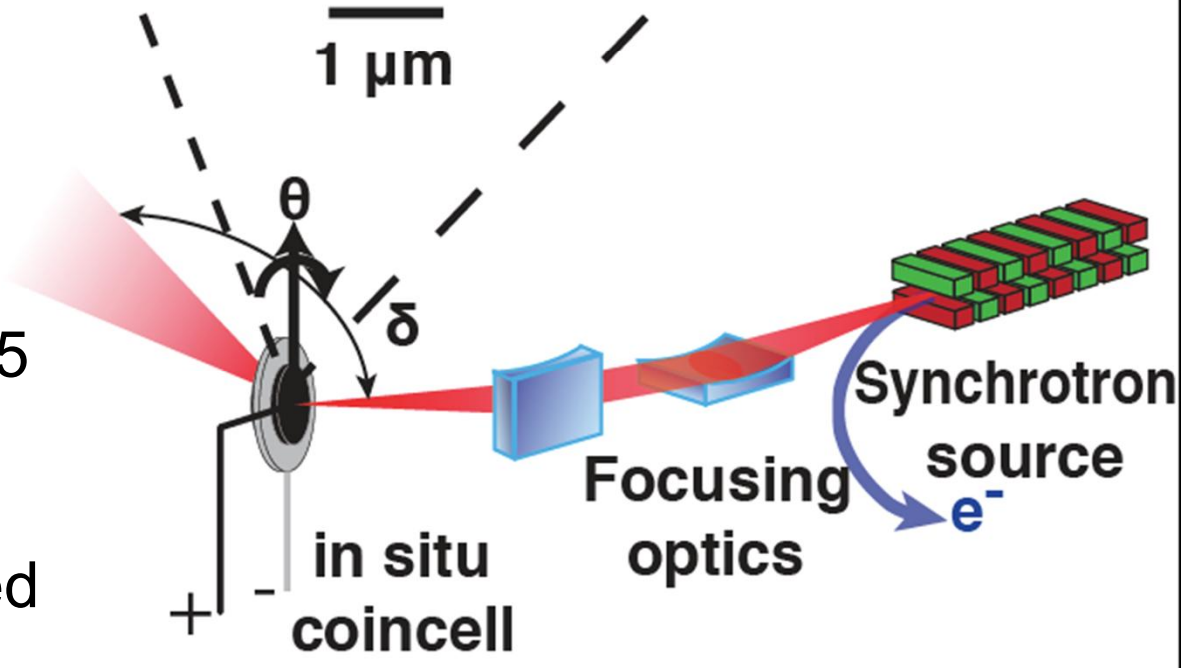
Experimental Method

Area Detector



Cathode SEM

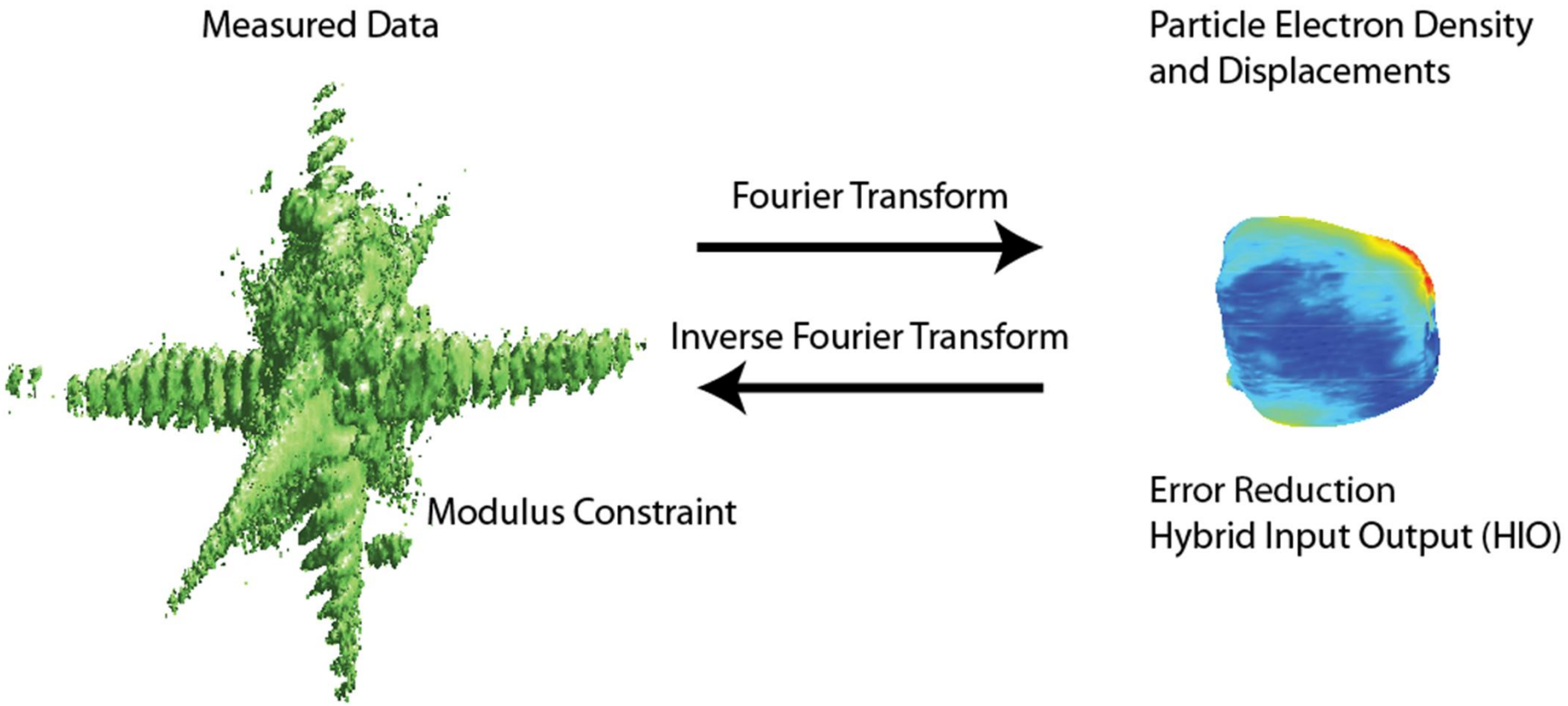




- Focus beam to ~1.5x1.5 micron
- Scan on sample until Bragg condition satisfied

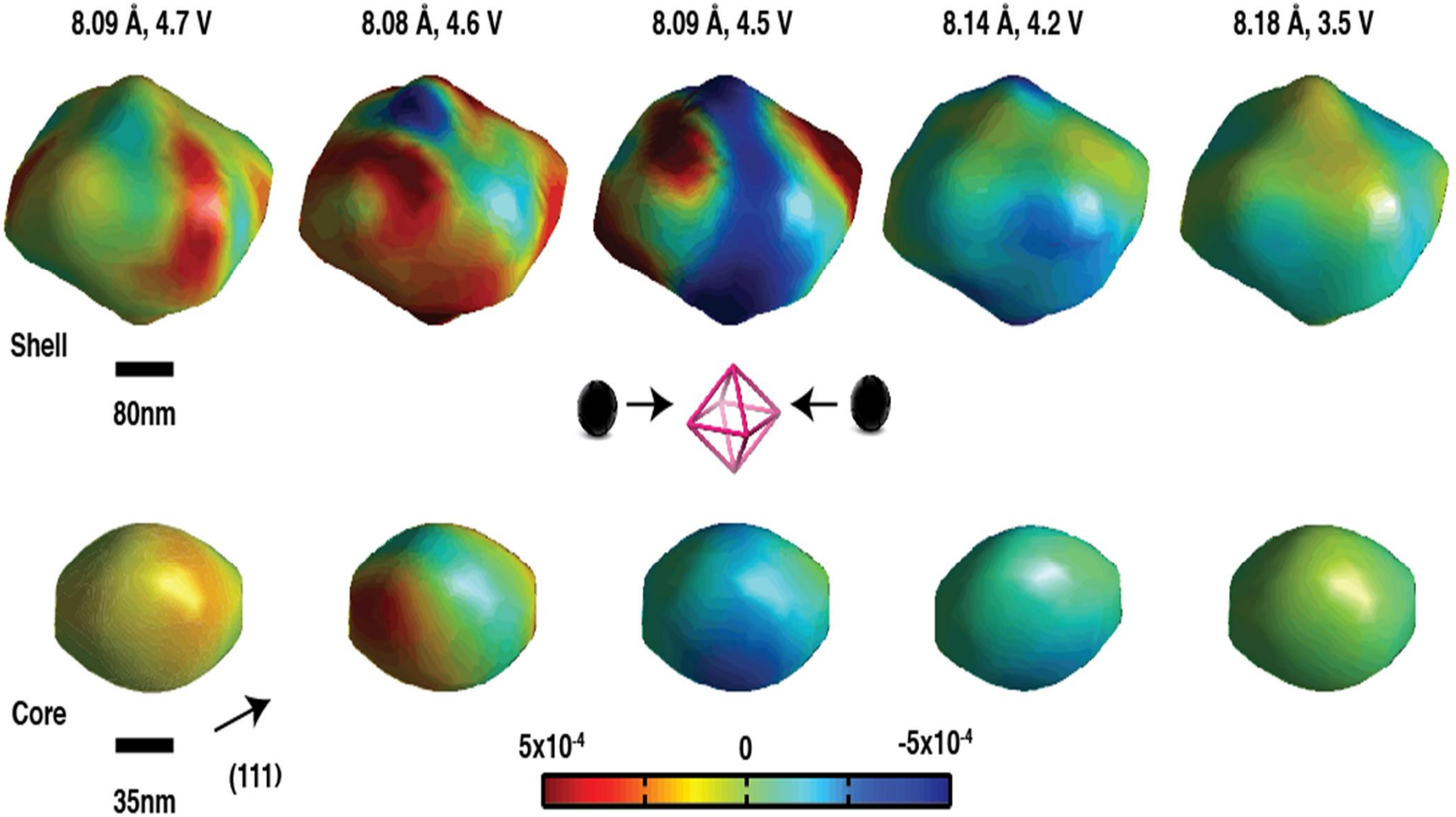
A. Singer, OS et al., Nano Lett. 14, 5295 (2014)

Phase retrieval: No measured phases



- Basic idea: apply modulus constraints in real and Fourier space, keep phases
- Fourier space constraint: what you measure
- Real space constraint: finite nanocrystal

3D-Mapping of Li distribution:



A. Ulvestad, OS et al., *Nano Lett. 14, 5123 (*2014)

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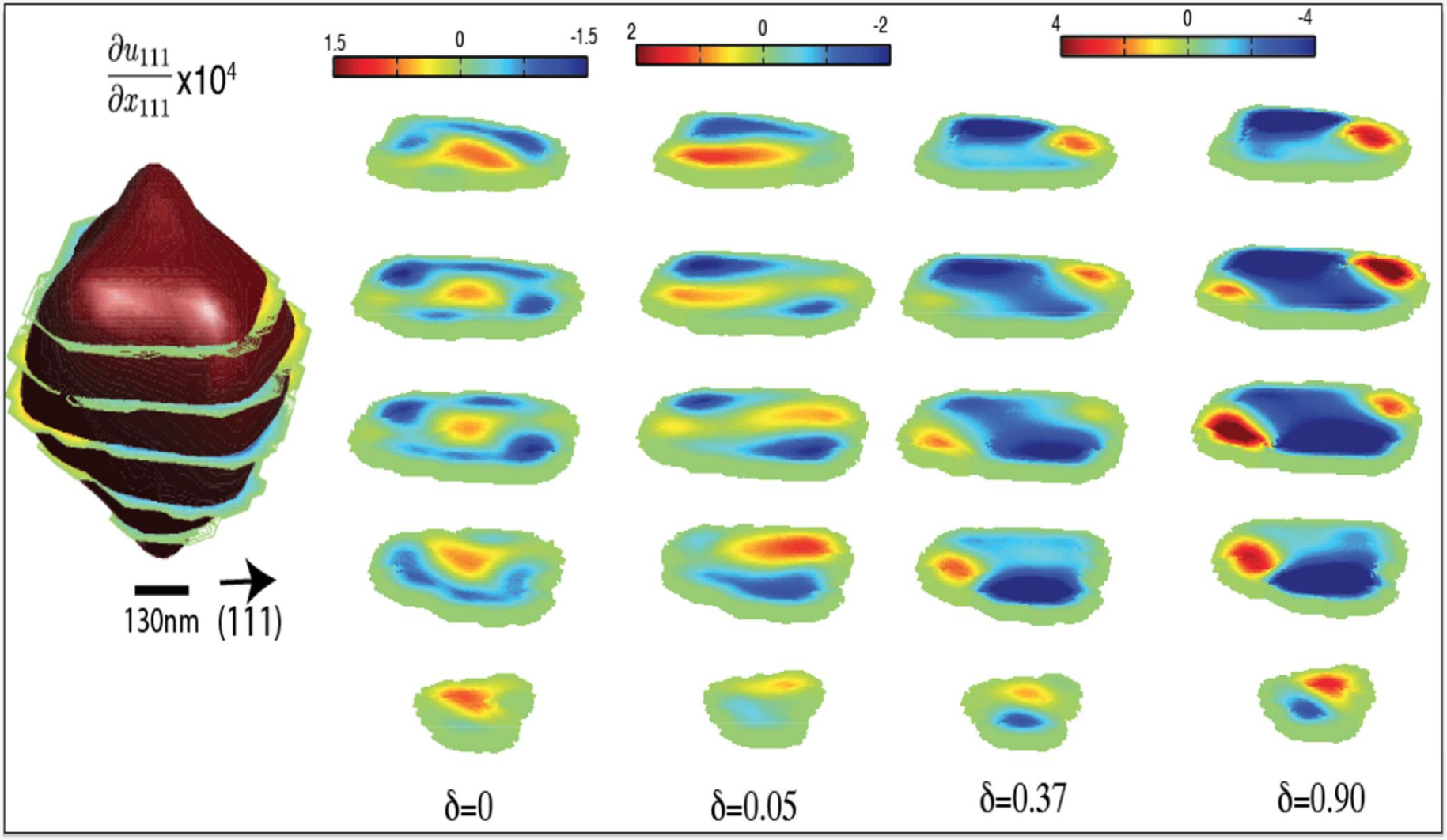
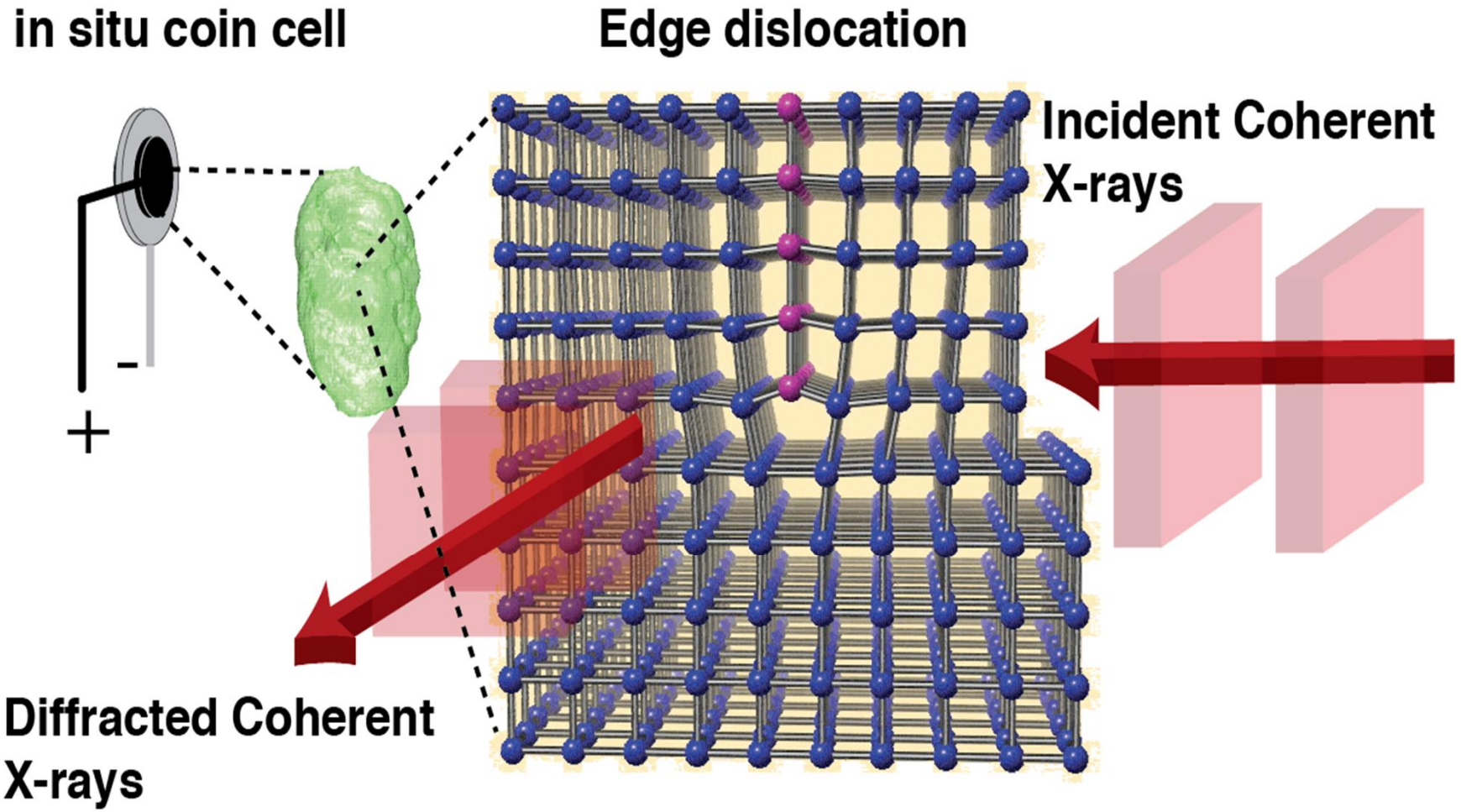


A. Ulvestad, OS et al., *Nano Lett. 14, 5123 (*2014)

Can we image a single defect (e.g. dislocation)?



A. Ulvestad, et al., Science 348 (6241), 1344 (2015)

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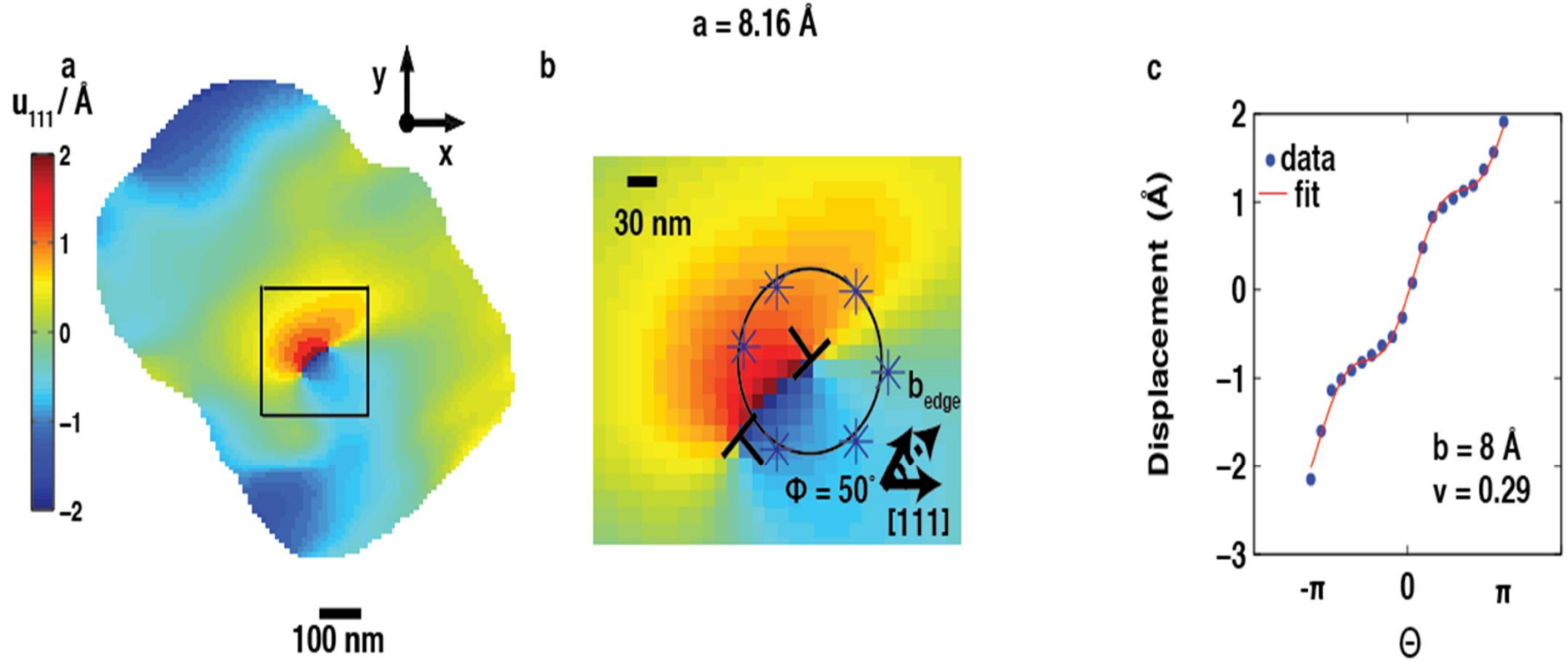
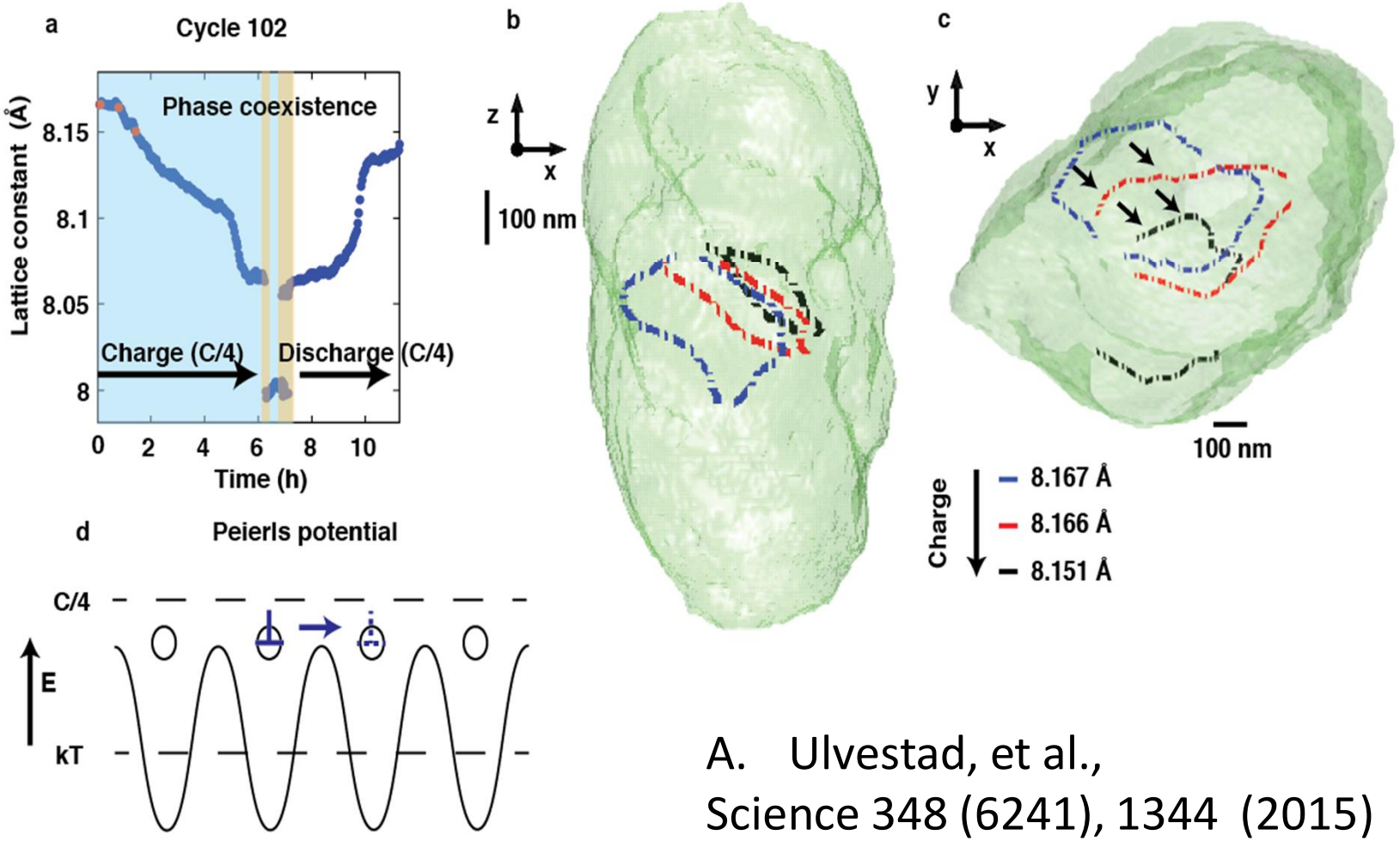
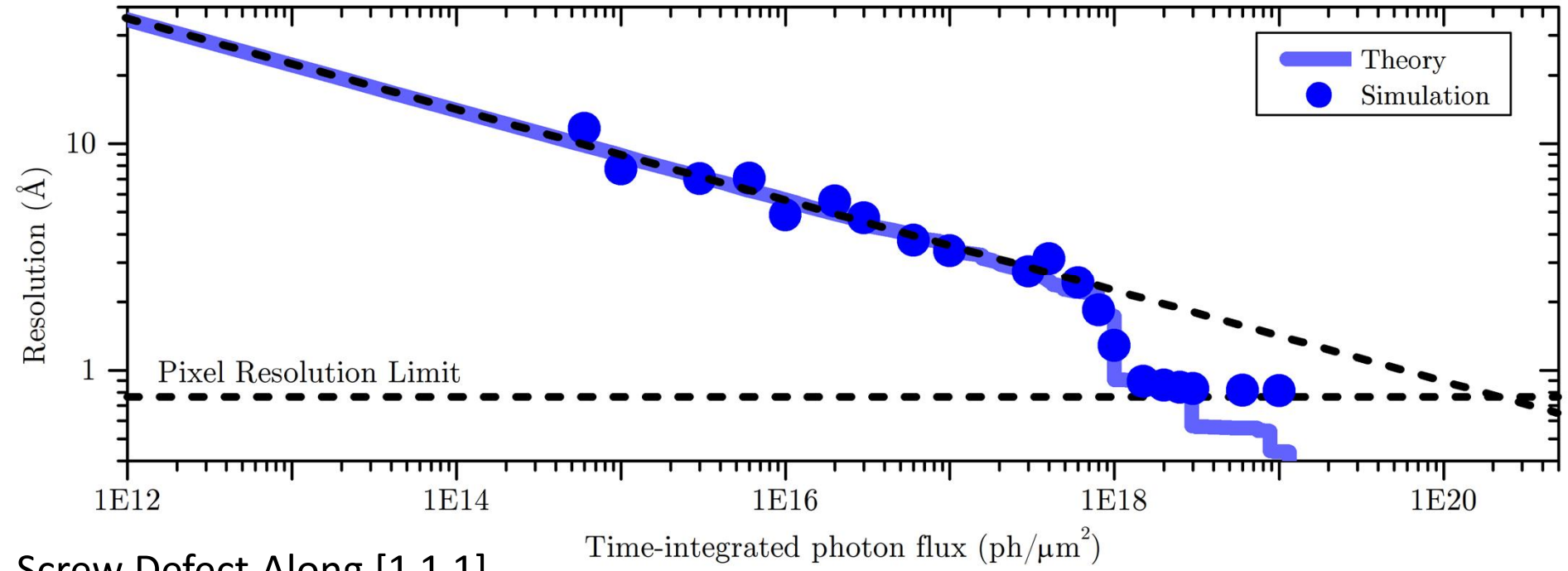


A. Ulvestad, et al., Science 348 (6241), 1344 (2015)

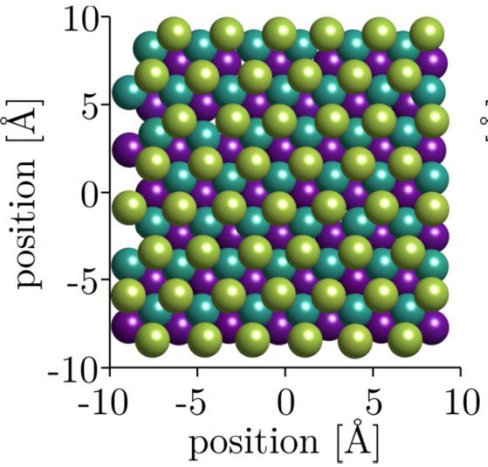
Imaging a single defect (e.g. dislocation)

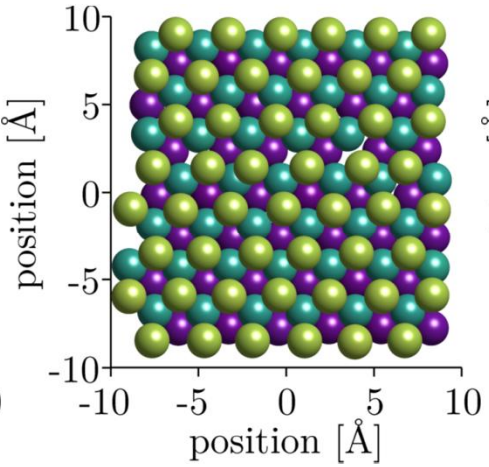


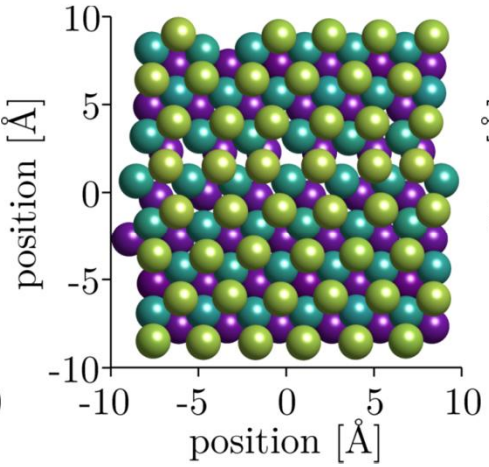
A. Ulvestad, et al.,
Science 348 (6241), 1344 (2015)

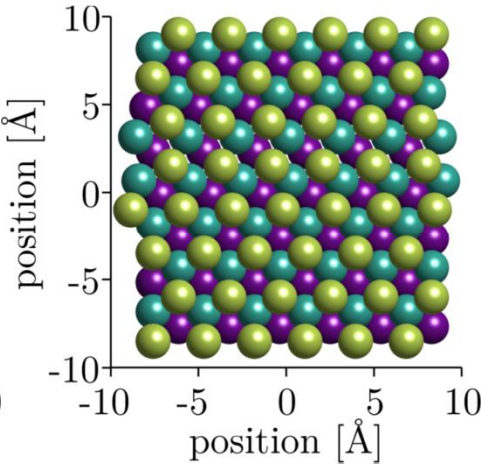


Screw Defect Along [1 1 1]







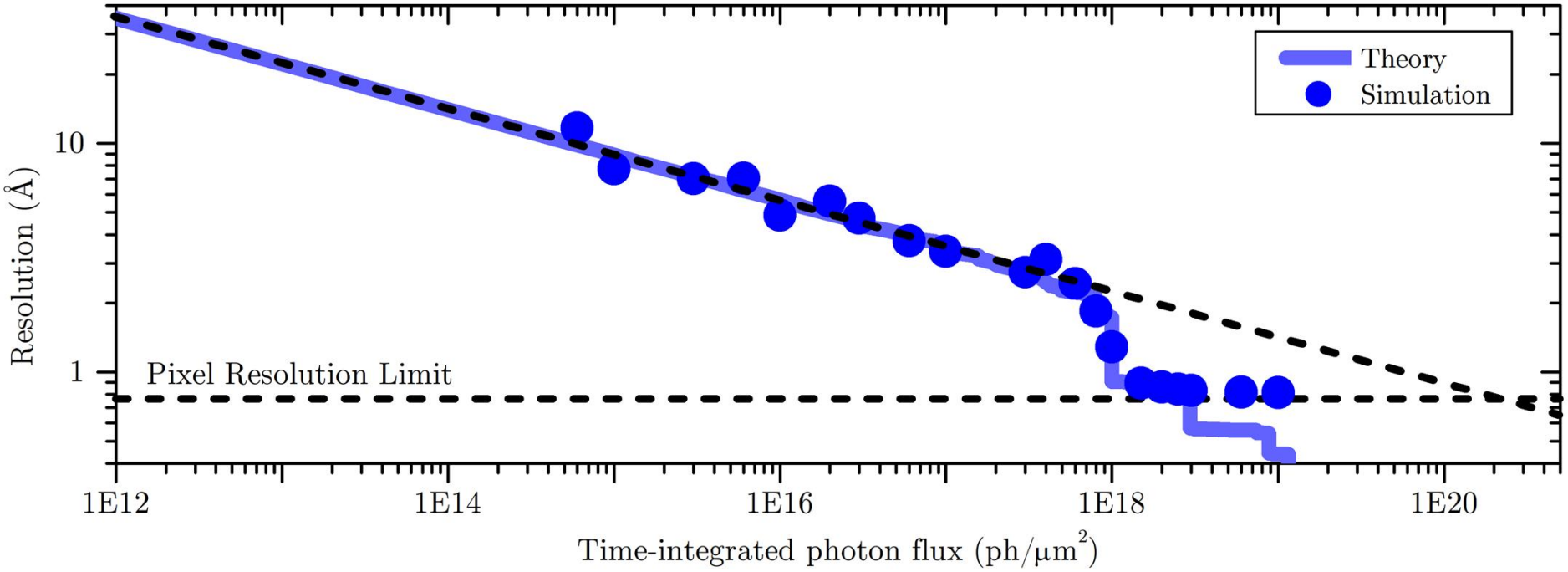


$6x10^{15}$ ph/um^2
MaxE: 1.41 Å
MAE: 0.35 Å

$3x10^{17}$ ph/um^2
MaxE: 1.38 Å
MAE: 0.25 Å

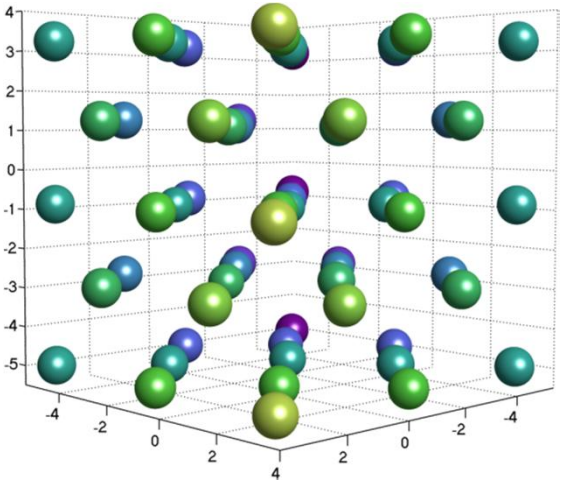
$2.5x10^{18}$ ph/um^2
MaxE: 1.07 Å
MAE: 0.25 Å

Actual

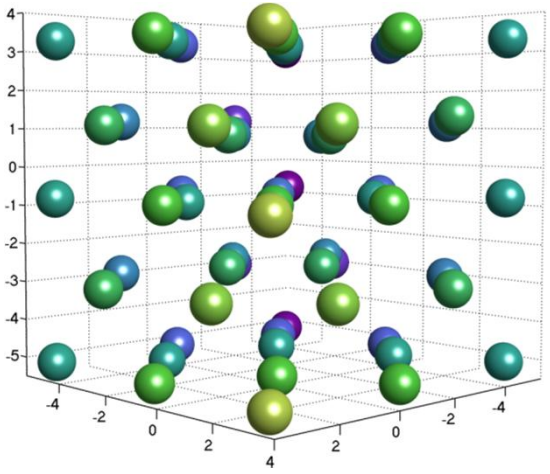


Vacancy

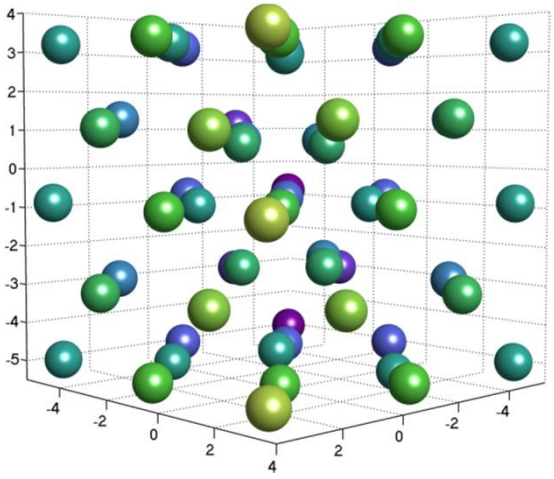
"Coherent diffractive imaging: towards achieving atomic resolution", S. H. Dietze & O. G. Shpyrko, J. Synchrotron Rad., 22, 1498 (2015)



1.0×10^{18} ph/um^2

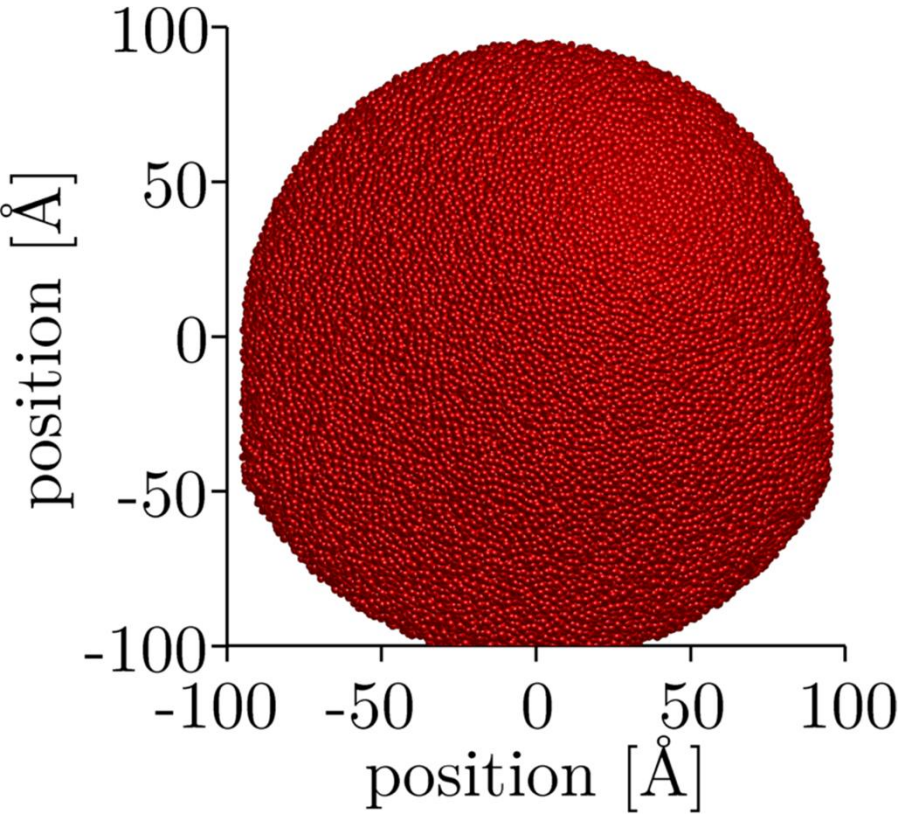


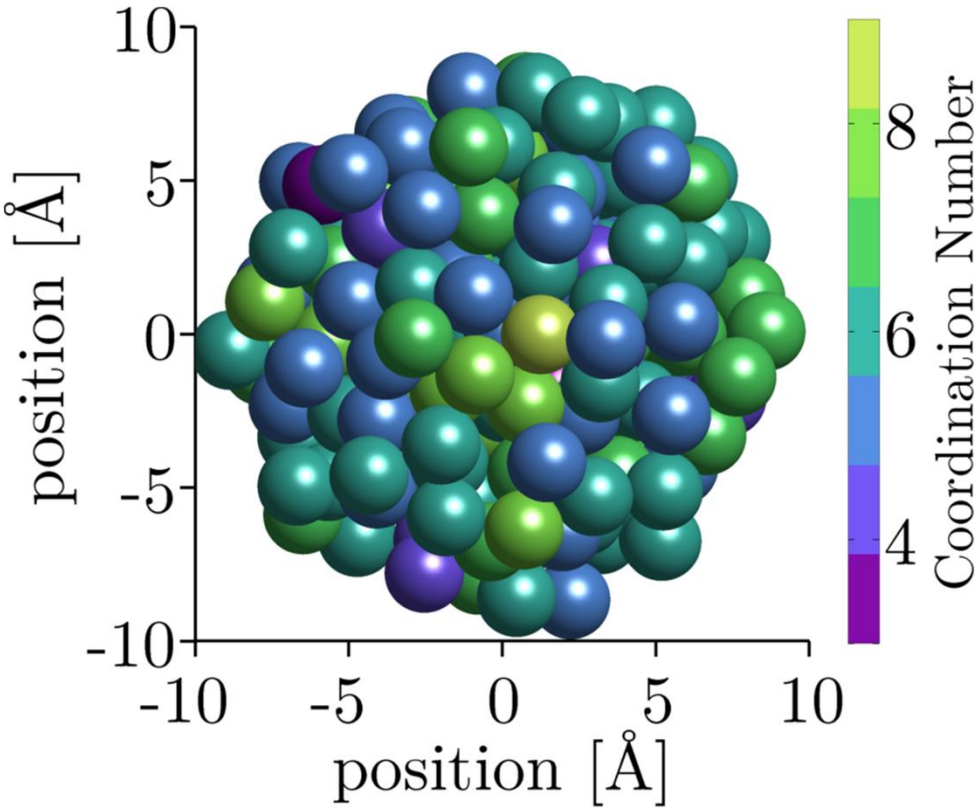
1.5×10^{18} ph/um^2



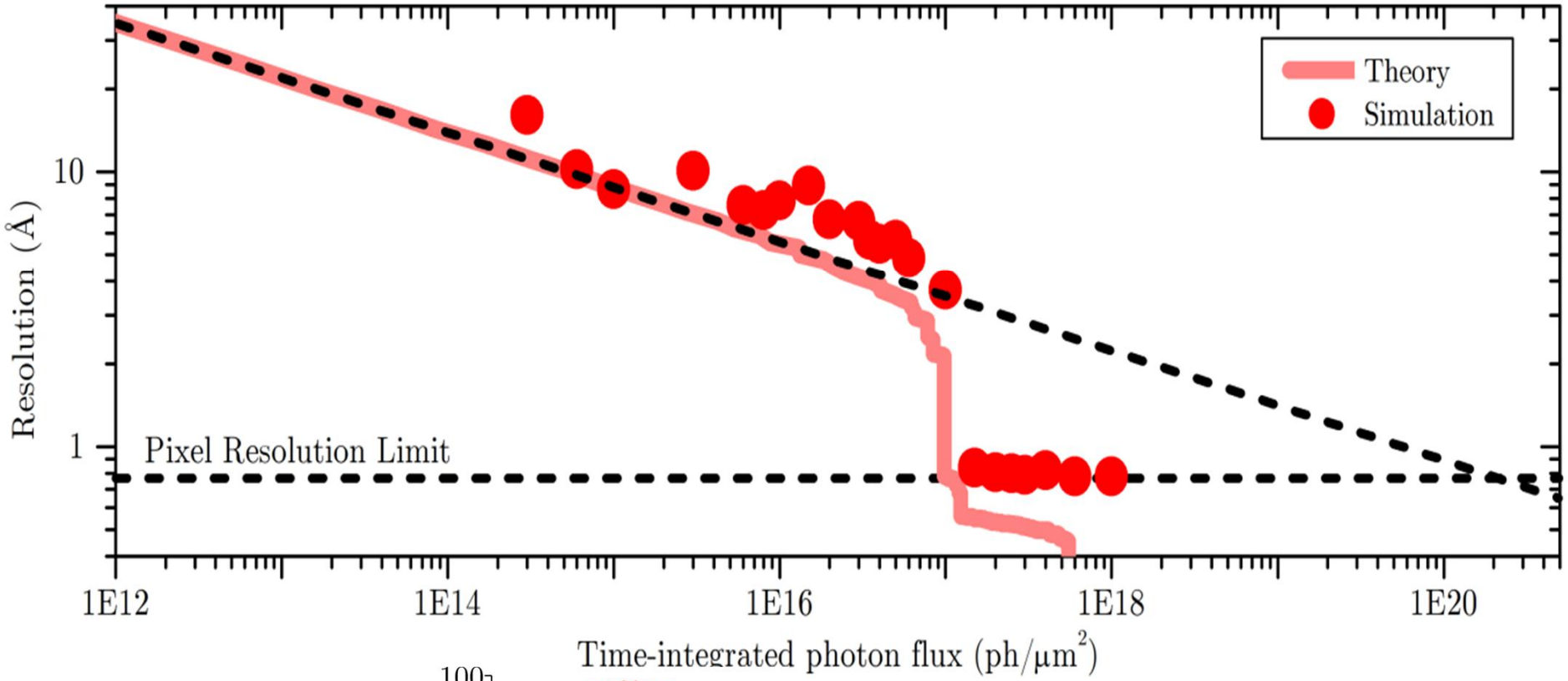
2.0×10^{18} ph/um^2

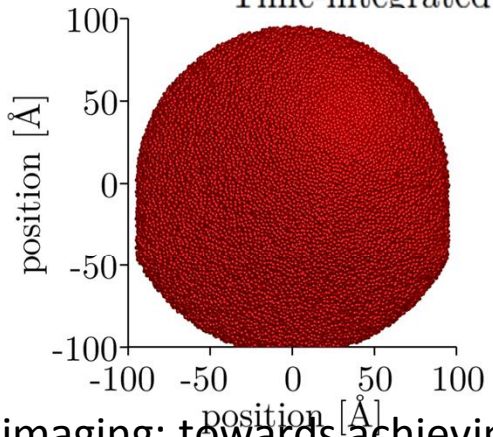
Hard sphere model for amorphous particle

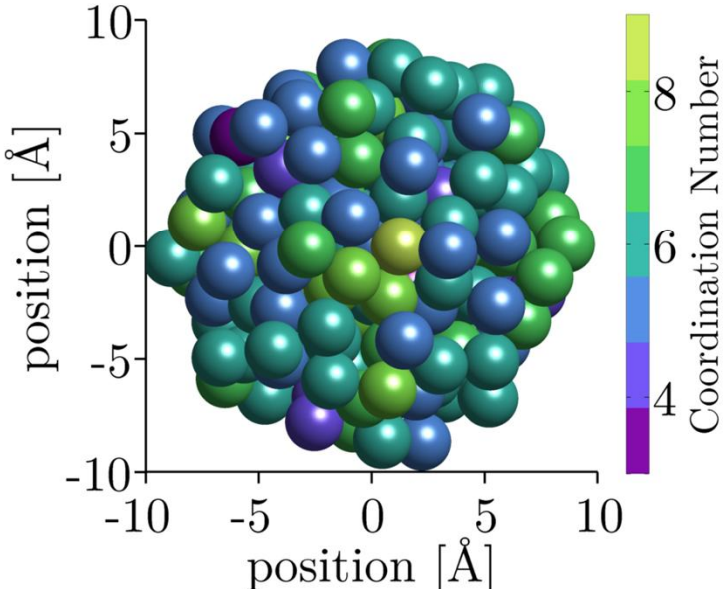




"Coherent diffractive imaging: towards achieving atomic resolution",
S. H. Dietze & O. G. Shpyrko, J. Synchrotron Rad., 22, 1498 (2015)







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