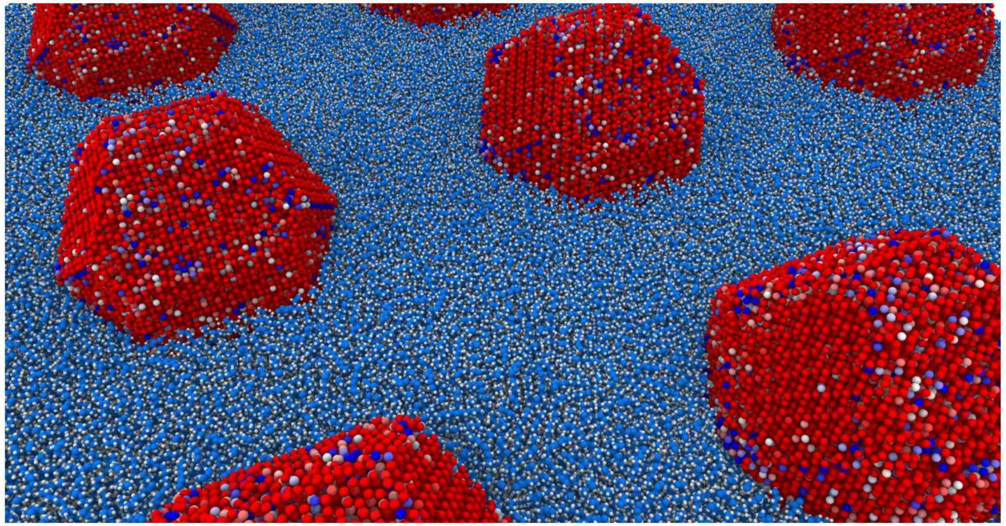
SAND2019-10440C

APS Shock Compression of Condensed Matter
June 20th 2019

Scale and rate dependence of phase transition pressure in CdS nanoparticles

J. Matthew D. Lane,
Jason P. Koski, Aidan P. Thompson, Ishan Srivastava, Gary S. Grest, Tommy Ao, Brian Stoltzfus, Kevin Austin, Hongyou Fan, Dane Morgan*, and Marcus D. Knudson

Sandia National Laboratories, Albuquerque, NM
*MSTS, Los Alamos, NM



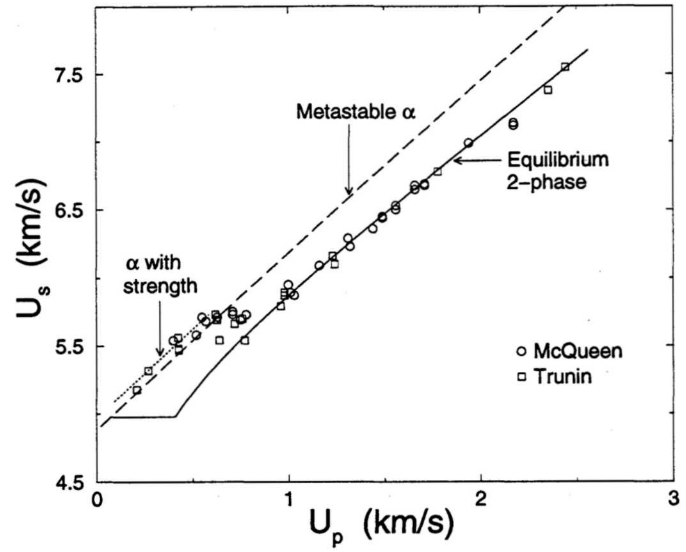
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

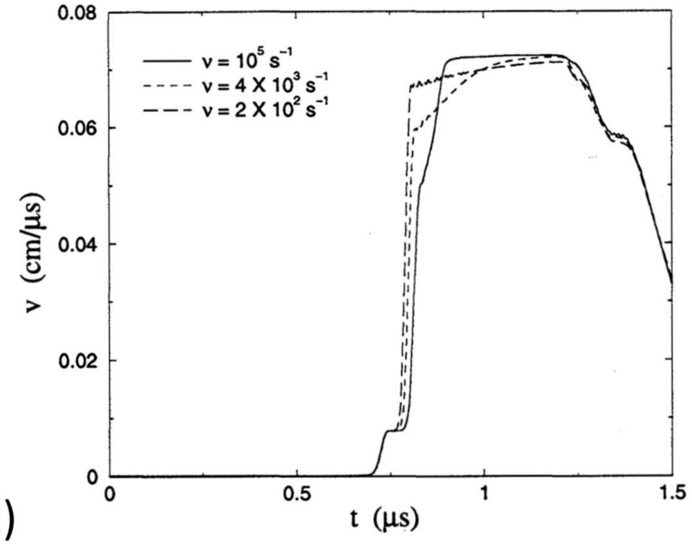
Motivation for transition kinetics

- Depends on materials and nature of transitions
  - Materials microstructure
  - Orientation

- Improved understanding of the interplay between time and length scale in phase transitions.
- Our aim is to improve the fundamental understanding of phase transition kinetics with a model system

Titanium



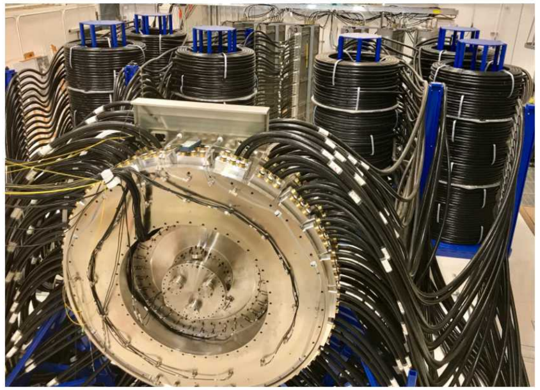


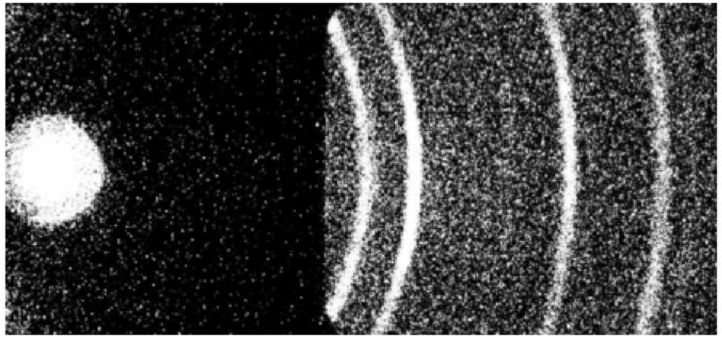
C. W. Greeff, D. R. Trinkle and R. C. Albers, SCCM (2002)

Matt Lane – jlane@sandia.gov

Broad project goals

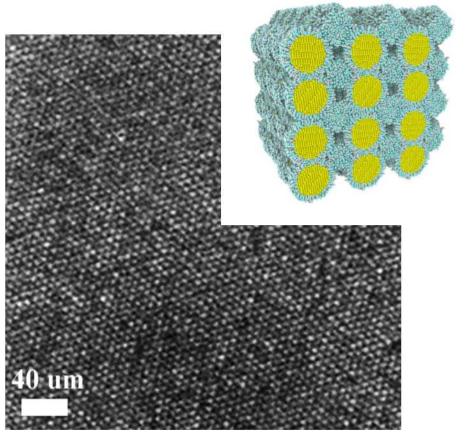
1. Careful control of loading and ramp profile: Thor pulsed power driver at Sandia.





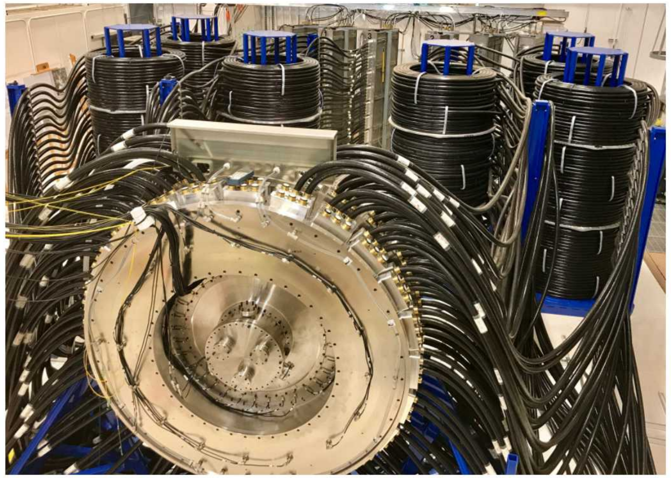
2. Diagnostics for phase transition identification: Implement a platform-independent X-ray diffraction (XRD) diagnostic capable of analysis in a variety of materials, VISAR and PDV.

3. Careful control of length scale: Introduce a “synthetic material target” which allows for the careful control of length scale to study the combined effect of rate and scale on transition kinetics



Matt Lane – jlane@sandia.gov

Control of rate: Thor driver, new diagnostic



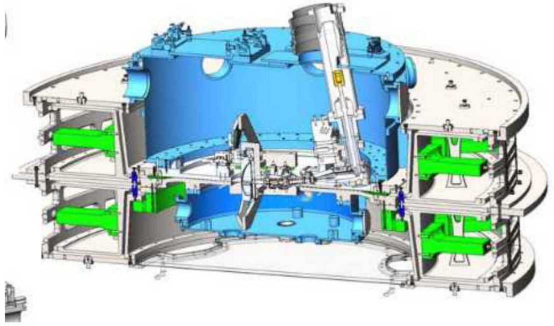
Thor is a pulsed-power accelerator similar to Z, which can drive ramp waves to **pressures of approximately 25 GPa** in its current 64 brick configuration.

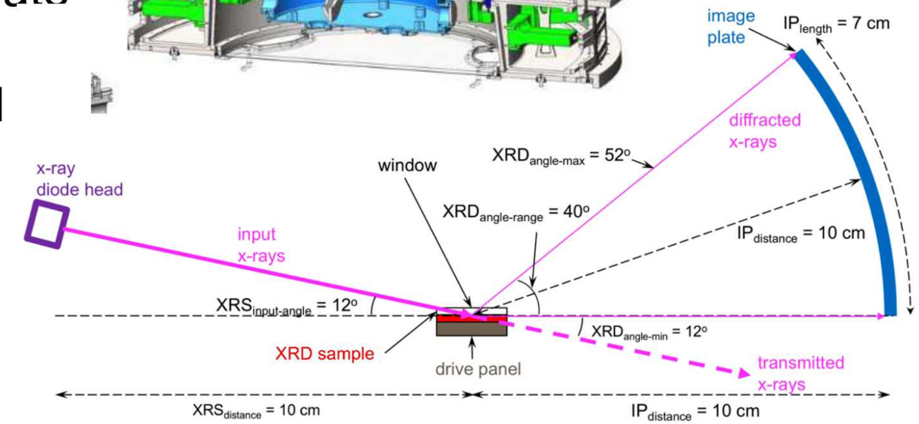
Thor can be configured like Z but with lower peak pressure, but better pulse shaping

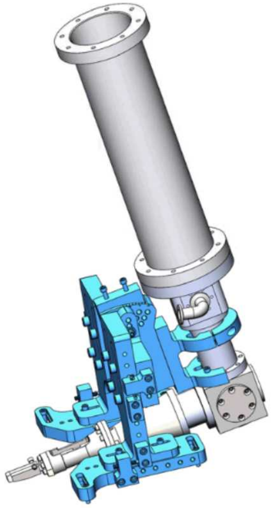
Careful control of ramp profile

- Adding X-ray diffraction diagnostic to existing velocimetry (VISAR & PDV)

- NSTec Supersaver (x-ray diode) to generate line emission from molybdenum metal anodes.







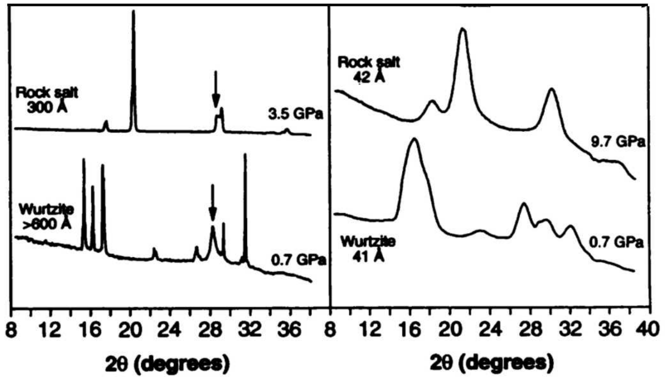
Specifications:

- 17.48 keV from Mo-K-α
- 20 – 30 ns duration flash
- Expect 10^8 to 10^9 photons incident on the diffraction sample
- Good penetration of 20-50 um, allows high-Z targets
- Image plate for most shots, could be replaced with CCD

Matt Lane – jlane@sandia.gov

Control of length scale: “synthetic microstructures”

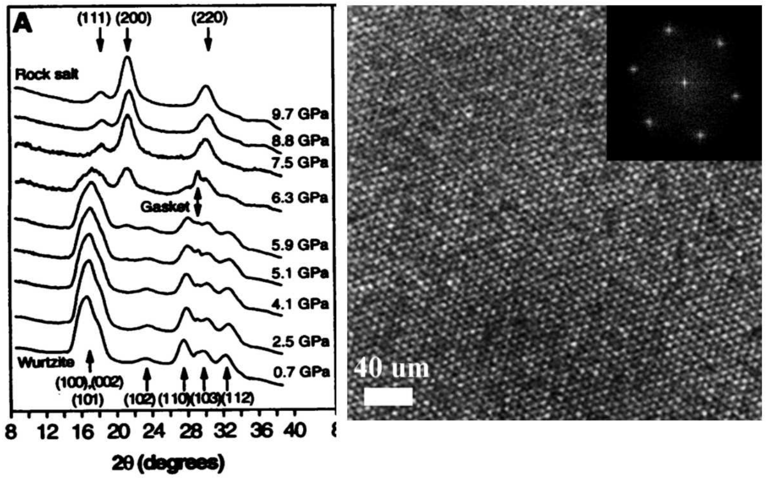
Bulk Nano spheres



XRD data delineates the transition clearly

Tolbert, Alivisatos, Science, 265, 373 (1994)

Wu et al., JACS, 132, 12826 (2010)



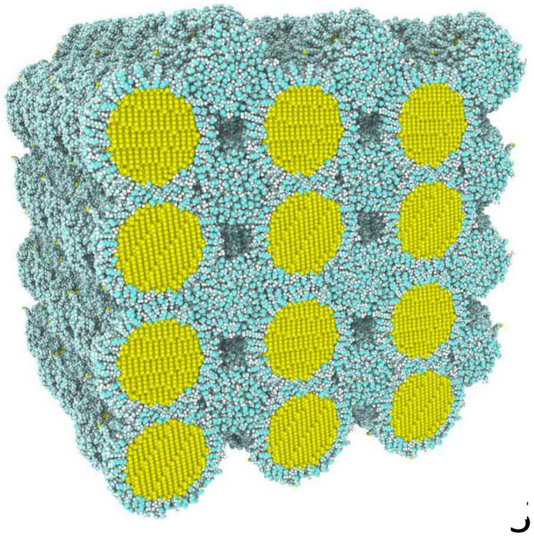
We can create a “synthetic microstructure” by leveraging the synthesis and assembly processes to create well-characterized films.

These nanoparticle films **mimic some aspects of grain structure** microstructure, but with better (monodisperse) size control.

- Coated spherical monodisperse particles
- Particles from 2 to 50 nm in diameter, initially
- Well-ordered fcc super lattice structures

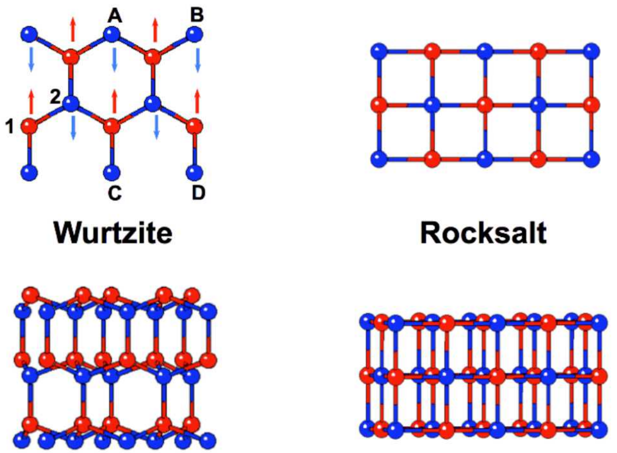
A particle size dependence of the phase transition has been observed for very small particles

Dynamic compression has been validated with similar arrays of particles (gold), pressures up to 12 GPa were achieved with reasonable pressure ramp profiles. We can do even more on Thor.



Phase transition kinetics in CdS

Pressure-induced Cadmium Sulfide (CdS) phase transition from Wurtzite to Rocksalt at ~2-3 GPa



Highly-coordinated military rearrangement

Transition kinetics depend strongly on the crystal orientation

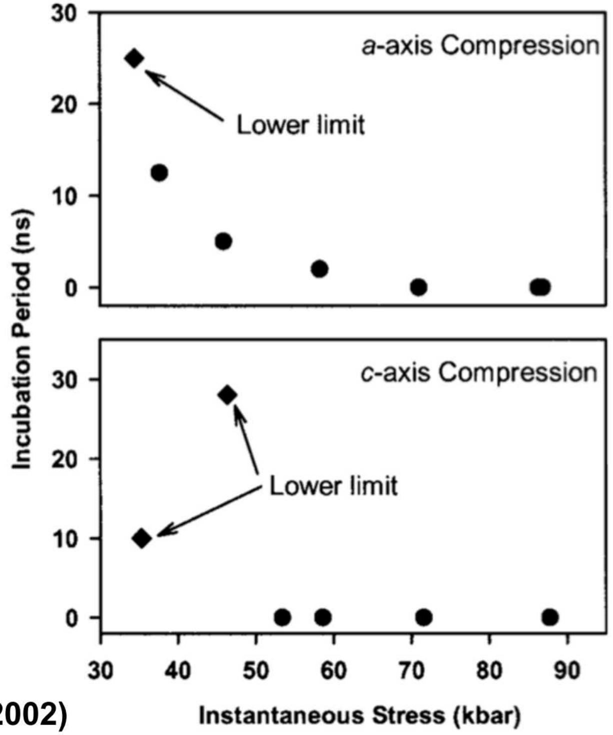
Measurements of the two-step transition, with fast, time-resolved spectroscopy showing the first step is sub-ns

Knudson, Gupta, Kunz. Phys. Rev. B, 59, 11704 (1999)
Knudson, Gupta. Phys. Rev. Lett., 81, 2938 (1998)

At higher pressures transitions are effectively immediate, but at lower pressures there is an “incubation” time for the transition which is different for different orientations.

In a-axis orientation, inelastic deformation is observed before the onset of the phase transition which may influence the mechanism

Second step in transition is delayed depending on peak stress



Knudson, Gupta, J. Appl. Phys. 91, 9561 (2002)

Matt Lane – jlane@sandia.gov

Modeling motivation and methodology

Interatomic Potential for CdS (Rabani et al., 2012)

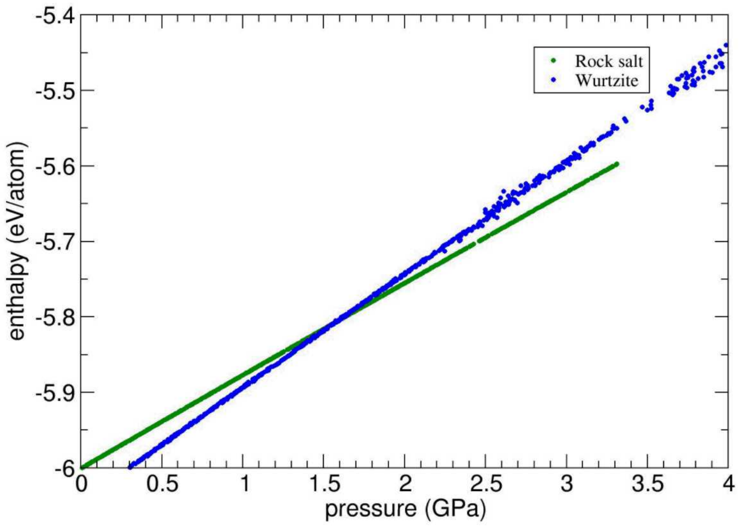
LJ-type with long-range electrostatics, fit to elastic constants

$$V_{ij} = \frac{q_i q_j}{r_{ij}} + 4\epsilon_{ij}\left\{\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right\}$$

	Exp.	MD	Δ
$P_{W\text{->}RS}$ (GPa)	2.5 - 3.2	1.6 - 3 - 11.5	
Wurtzite			
a (Å)	4.13	4.16	1%
c (Å)	6.70	6.59	2%
B (GPa)	65.0	55.2	-15%
Rock salt			
a (Å) P=0	5.44	5.43	0%

- Stable Wurzite and Rocksalt
- Potential predicts both phases and the dynamic transition

- Hugoniostat methodology to allow long-time simulations of shocked states (Ravelo et al., 2004)



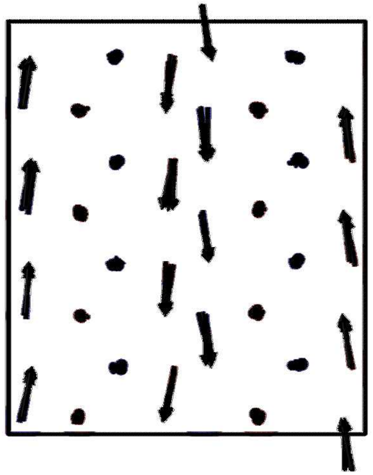
Matt Lane – jlane@sandia.gov

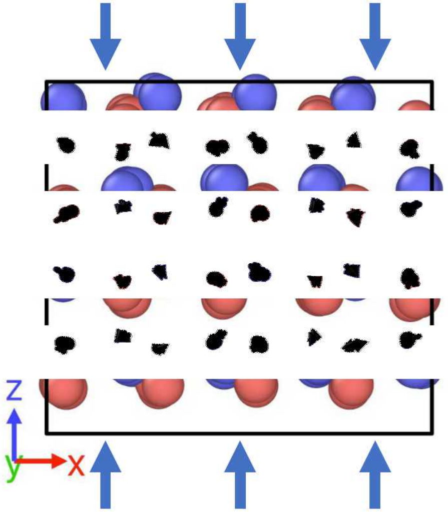
Orientation-dependent mechanisms c-axis

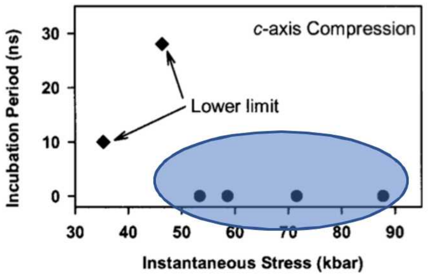
(High-pressure regime – shear activation)

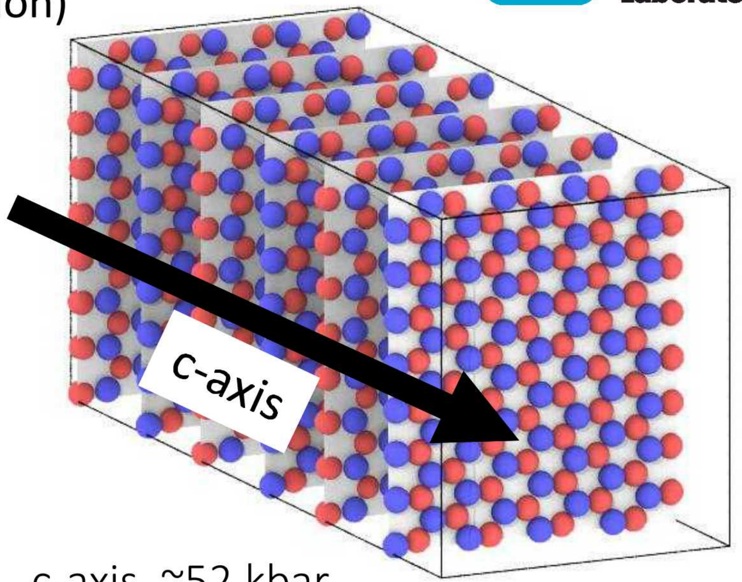
Solid-solid pressure-induced phase transitions have been studied in bulk geometries and for military (Martensitic) transformations in dS.

c-axis compression:



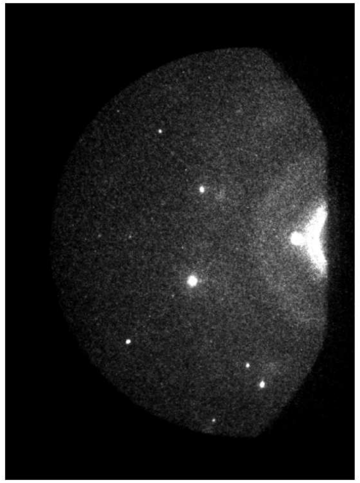




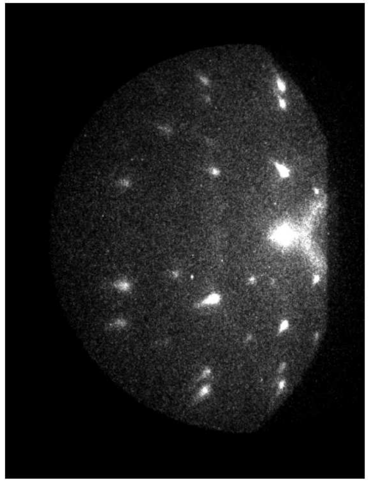


c-axis, ~52 kbar

Ambient phase



High pressure phase



Knudson, DCS exps.

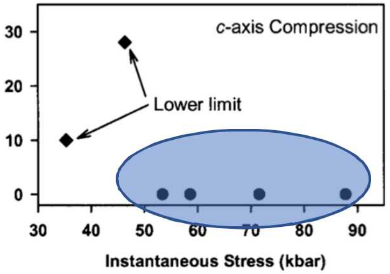
c-axis:

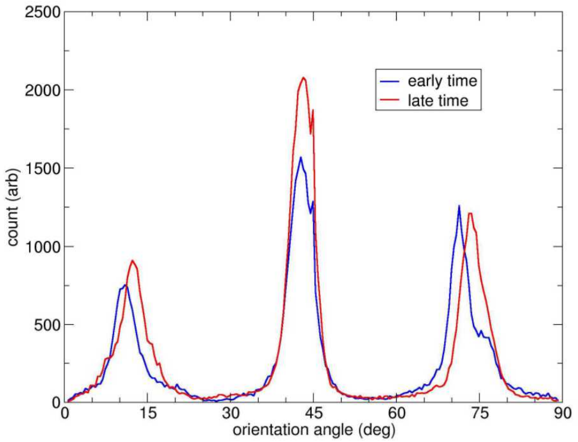
- alternating plane shift along y when compressed along z.
- no observed rate dependence
- final state rocksalt rotated 45 in x-y plane

Displacement vectors show non-affine displacement

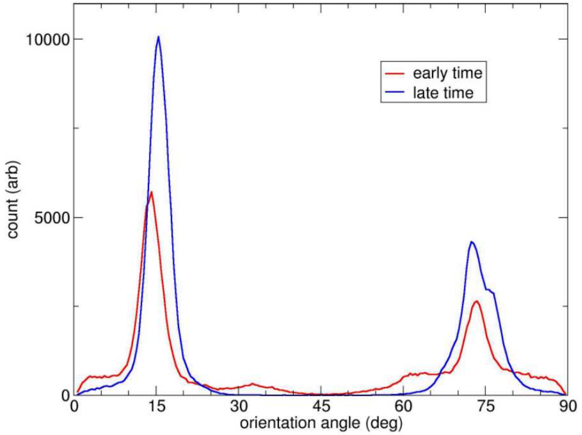
Matt Lane – jlane@sandia.gov

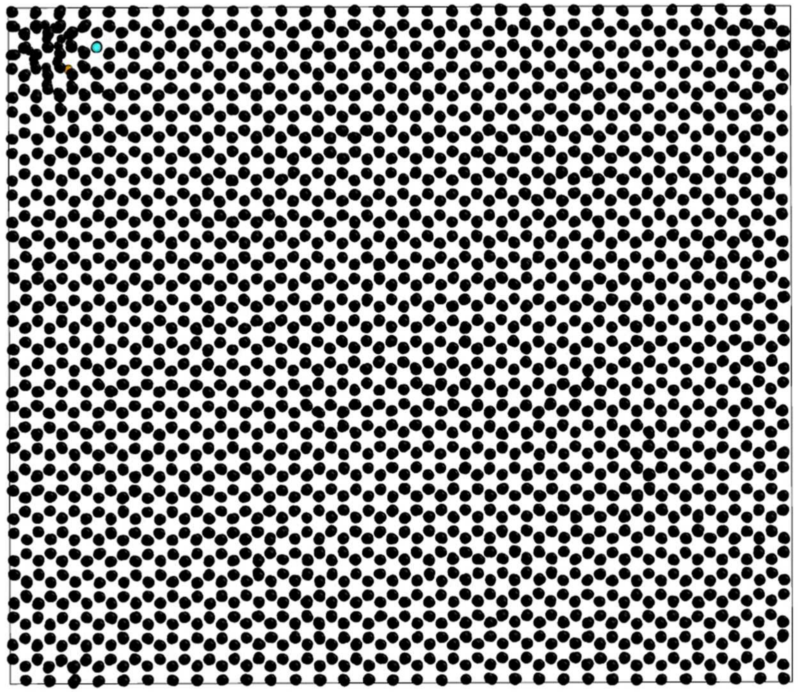
Orientation-dependent mechanisms c-axis



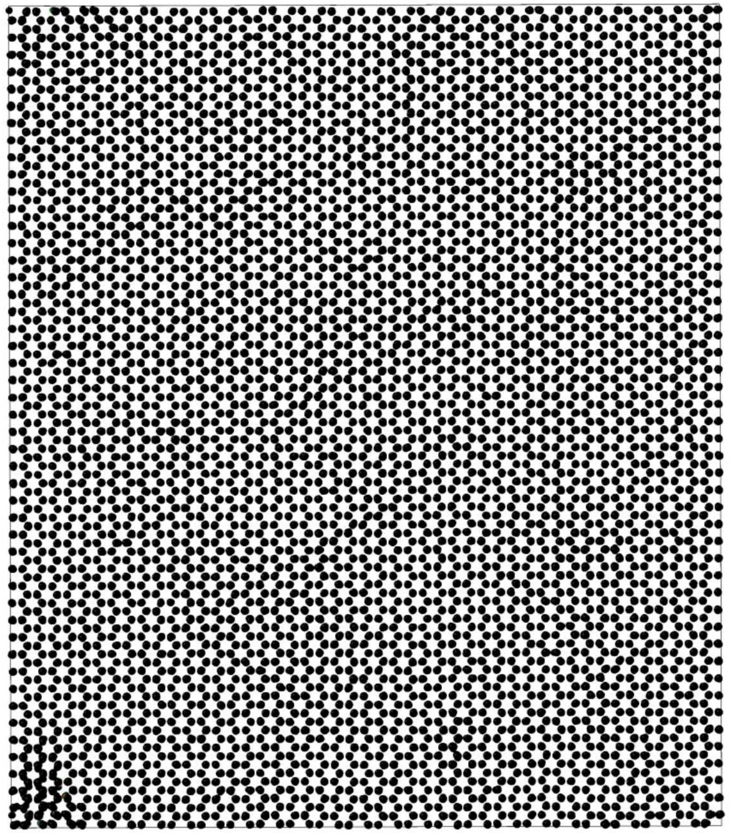


High-pressure regime – shear activation





Three orientations Identified and confirmed with experiment.

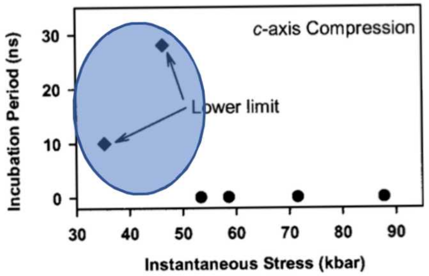


There is a local competition between between the orientations

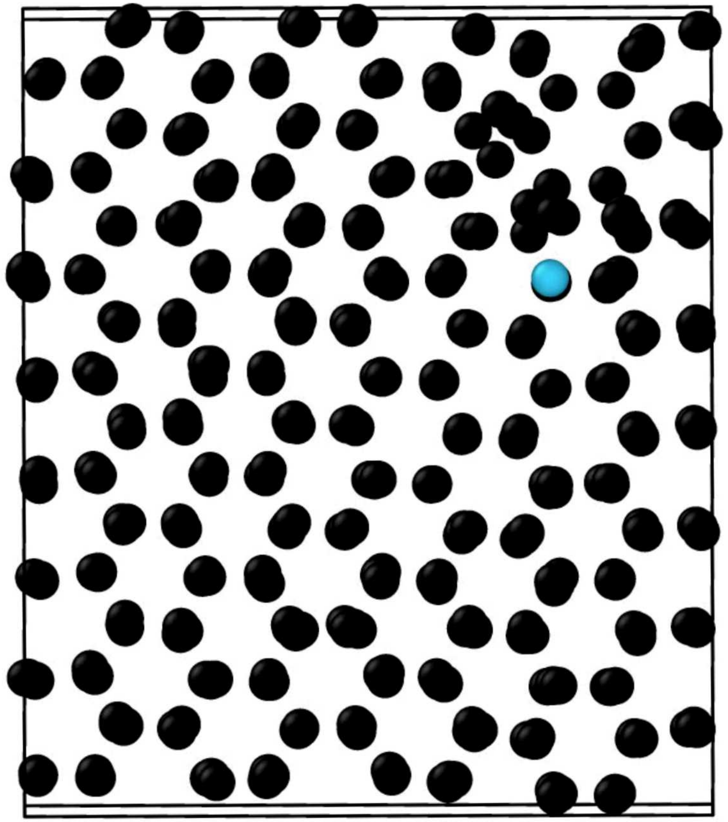
Matt Lane – jlane@sandia.gov

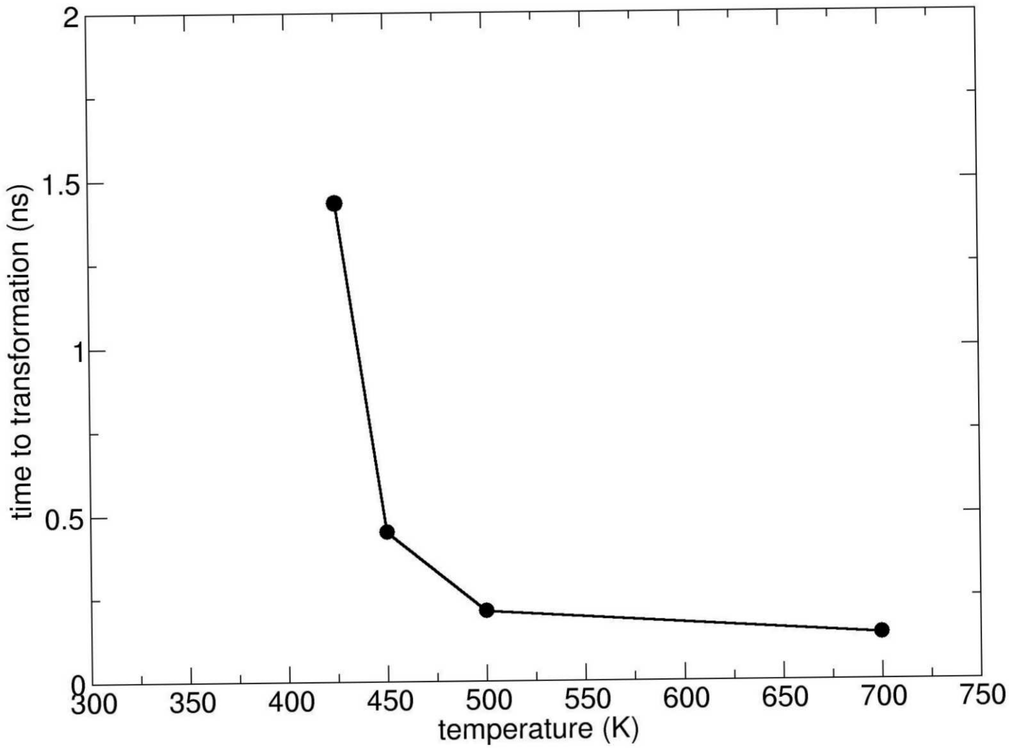
Orientation-dependent mechanism c-axis

Low-pressure regime – thermal activation



Sluggish "incubation" time followed by a rapid transition. Different mechanism and final orientations.



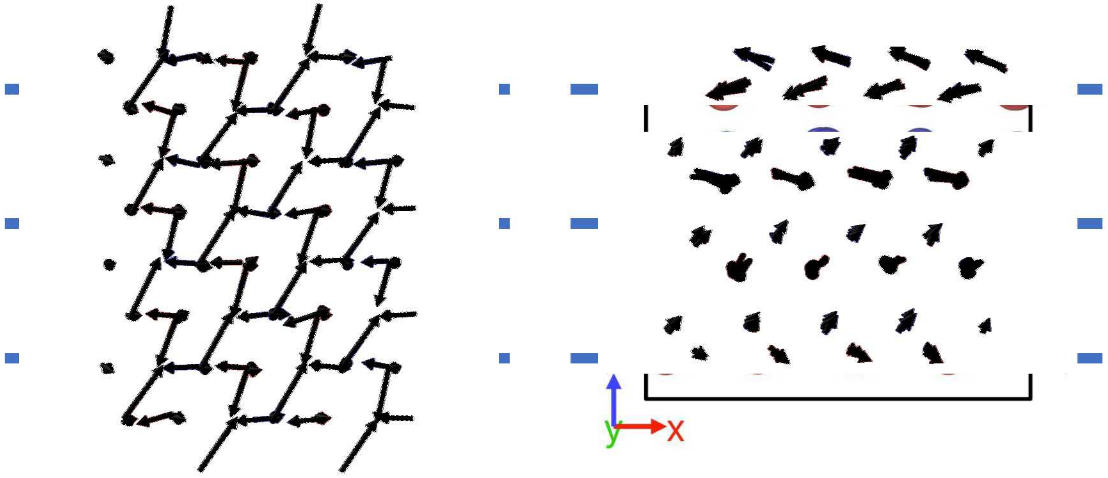


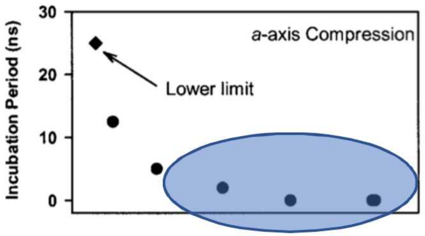
Matt Lane – jlane@sandia.gov

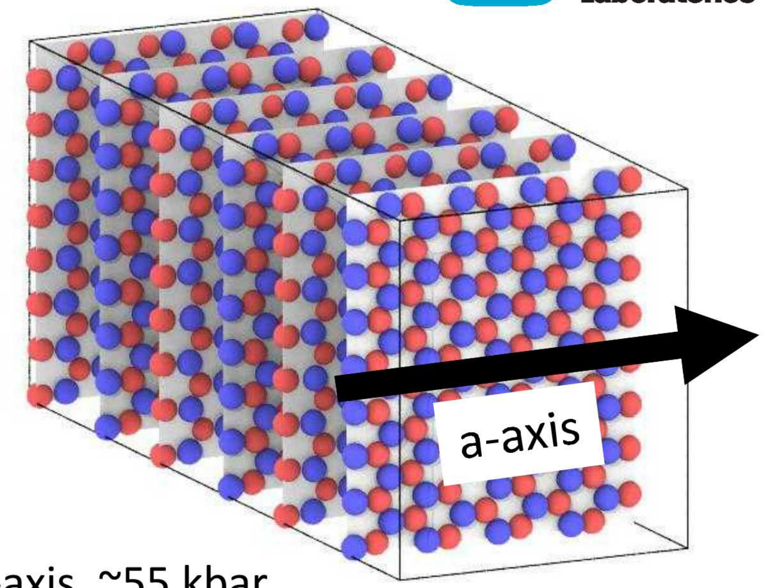
Orientation-dependent mechanisms a-axis

Solid-solid pressure-induced phase transitions have been studied in bulk geometries and for military (Martensitic) transformations in CdS.

a-axis compression:



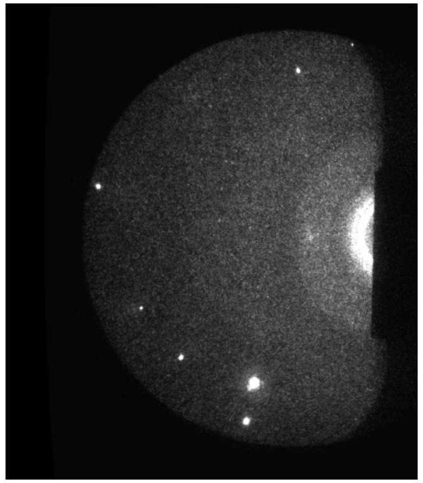




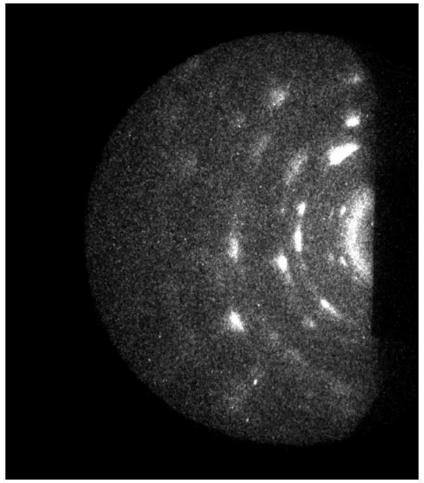
a-axis, ~55 kbar

- Diagonal alternating shifts of individual atoms when compressed along x.
- lower rates lead to lower transition pressure
- final state rocksalt rotated 9 degrees in x-z plane

Ambient phase



High pressure phase

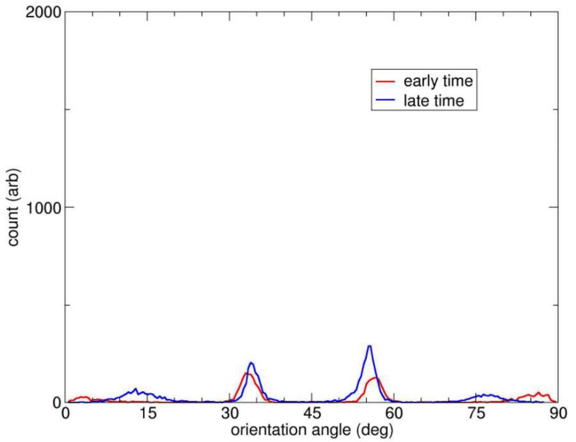


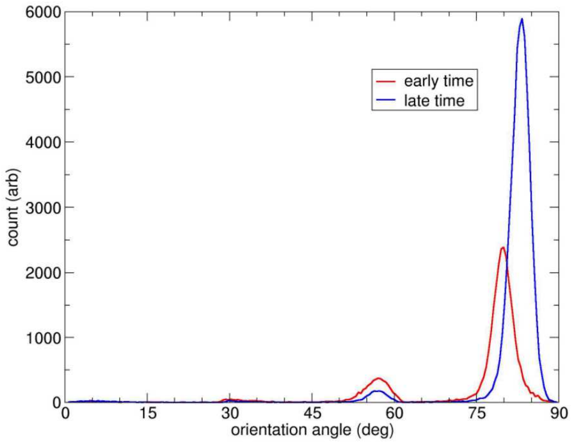
Knudson, DCS exps.

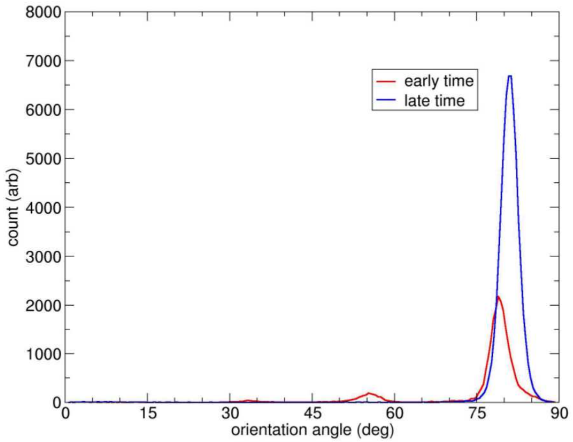
Displacement vectors show non-affine displacement

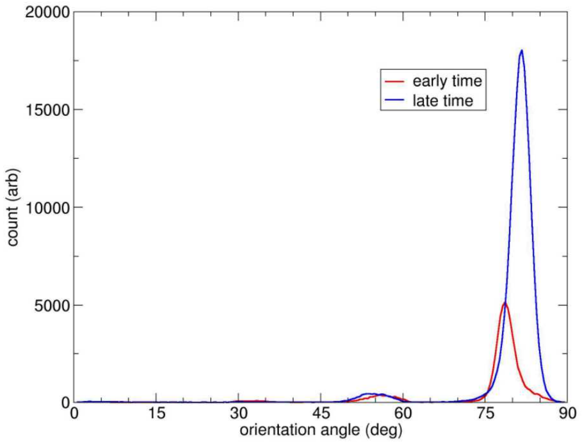
Matt Lane – jlane@sandia.gov

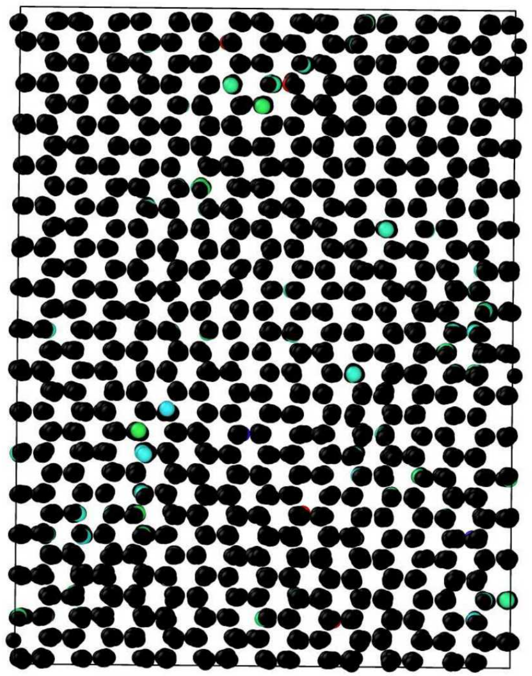
Orientation-dependent mechanisms a-axis

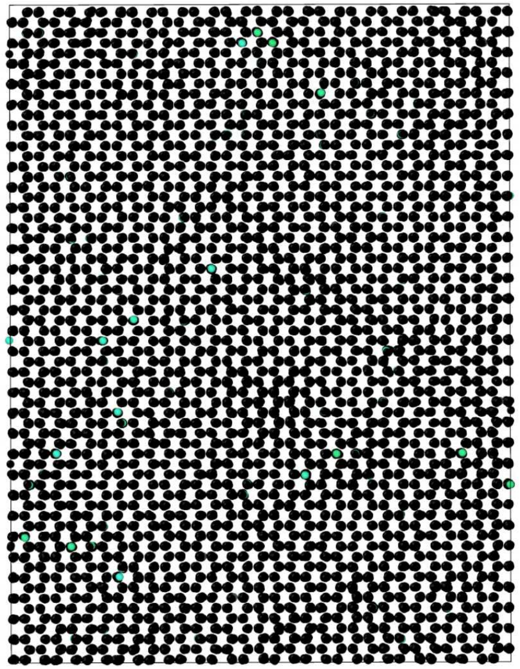


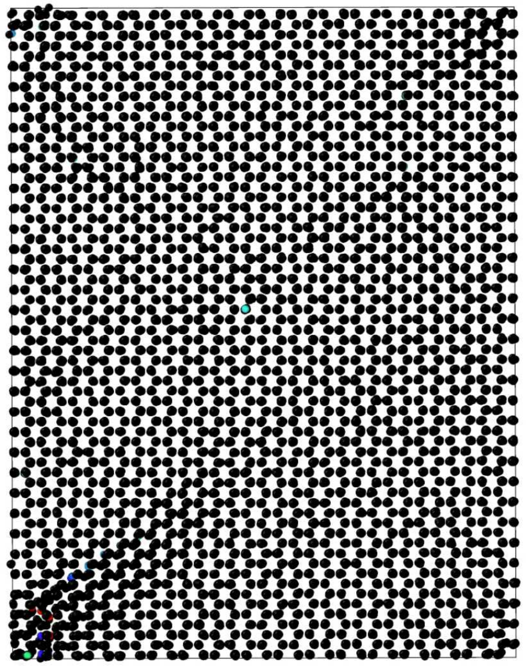


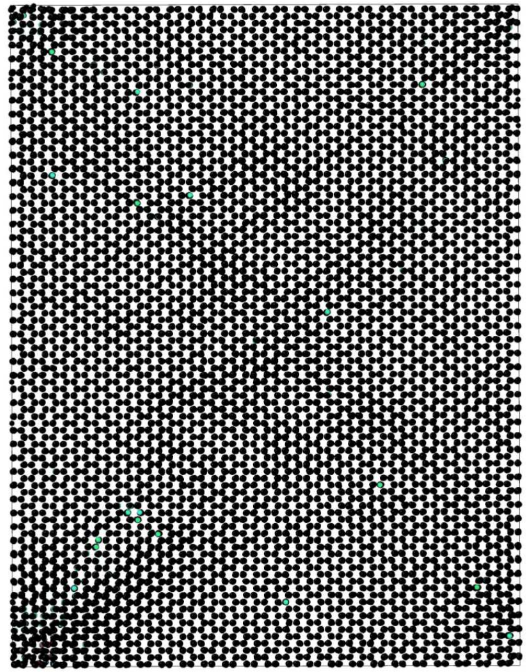




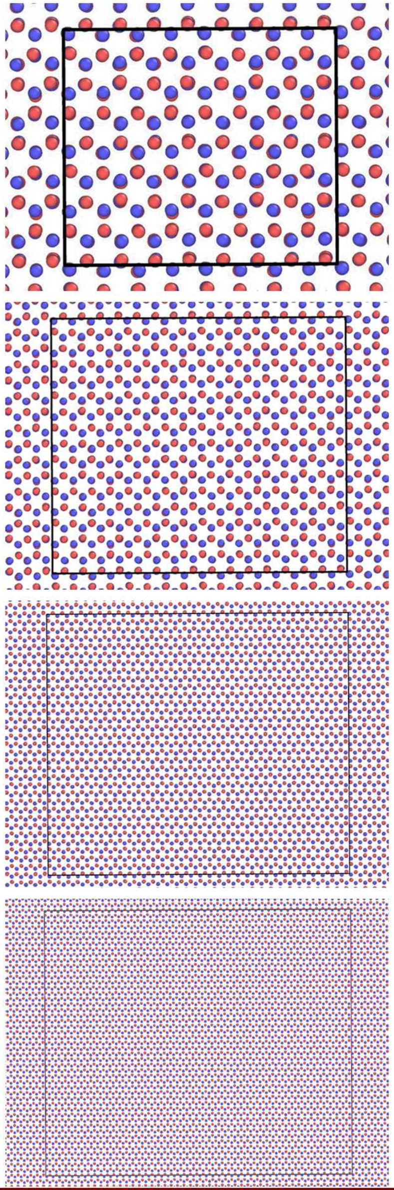


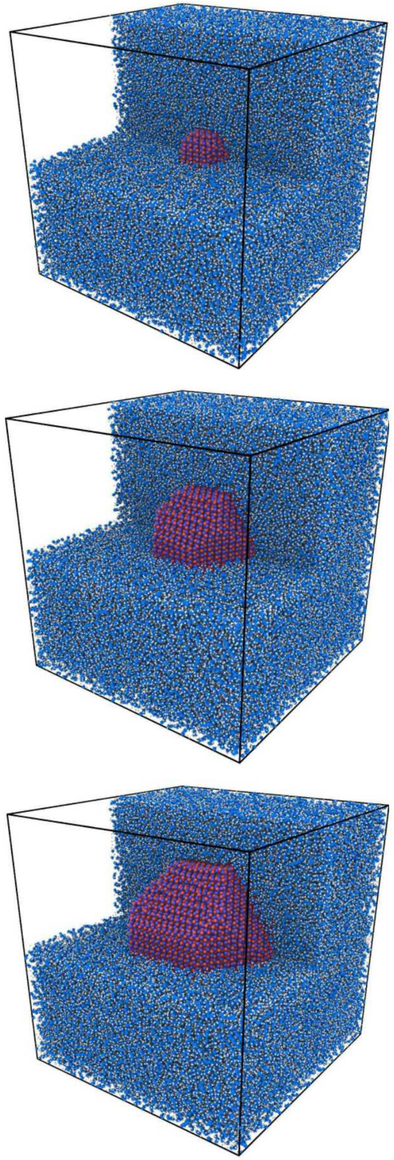




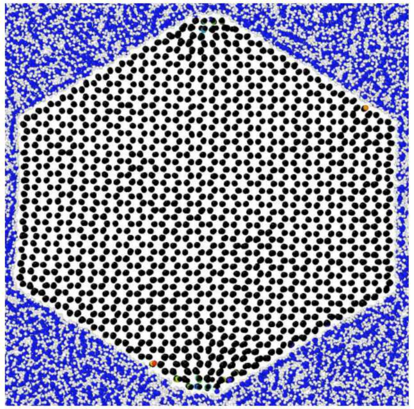


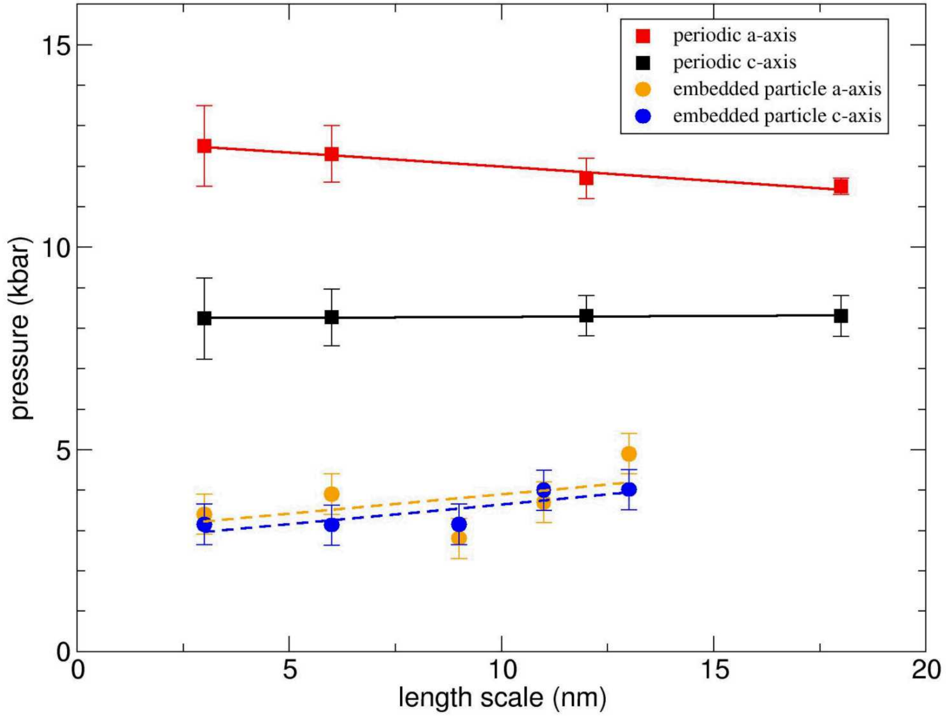
Modeling length scale effects





Length scale can be controlled with and without introducing surface. We see difference trends





Orientation pressure thresholds are reduced for cut nanoparticle which bodes well for randomly oriented films.

Matt Lane – jlane@sandia.gov

Conclusions and direction

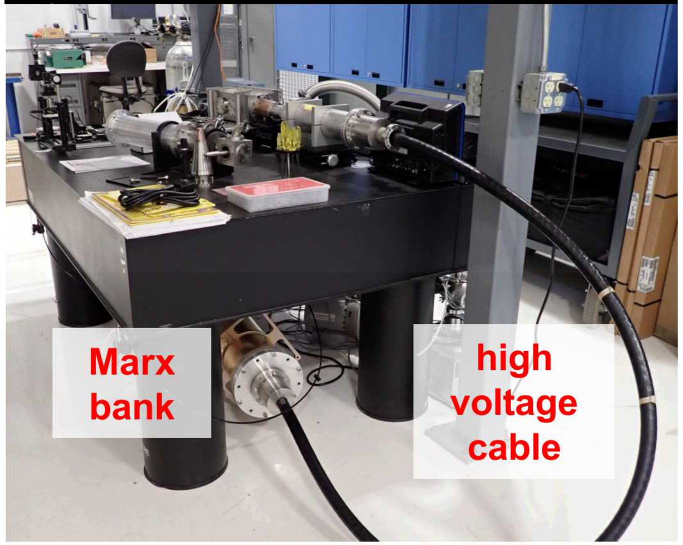
- We are conducting a combined experimental and modeling effort to explore the interplay between length and time scales in phase transitions within a carefully controlled model system
- We've identified transition mechanisms and orientations resulting from c-axis and a-axis compression in CdS
- Modeling results indicate different trends for homogeneous and surface nucleation as a function of length scale
- Future: Integration of experimental results and modeling

Matt Lane – jlane@sandia.gov

Modeling timescales

XRD diagnostic hardware implementation

Future Thor XRD pulser in 961 high

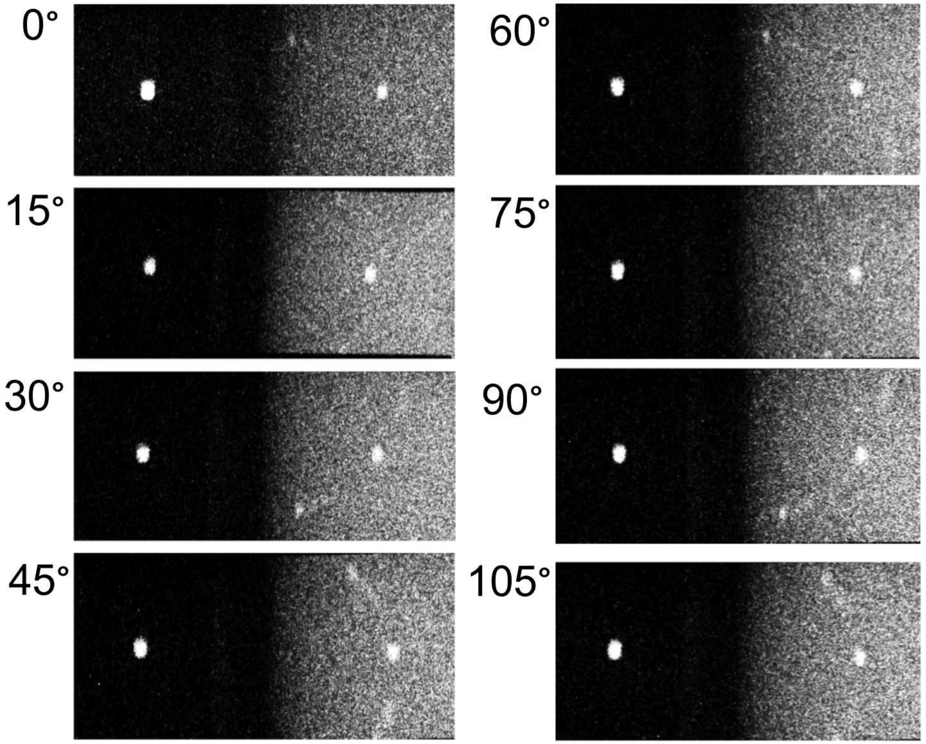


Specifications:

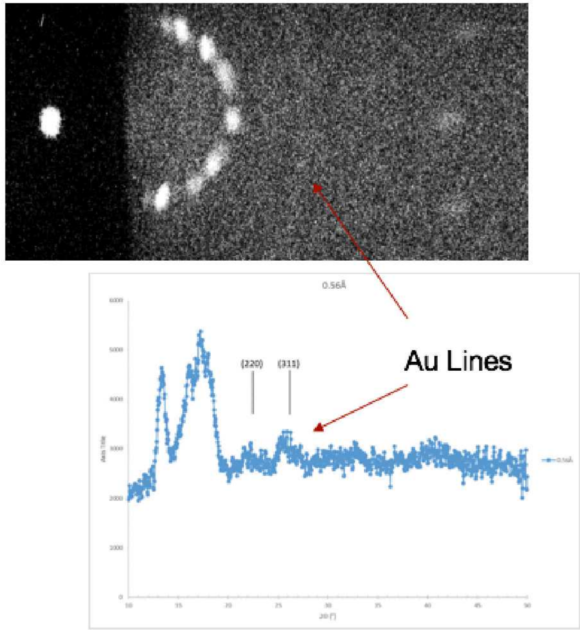
- 17.48 keV from Mo-K-α
- 20 – 30 ns duration flash
- Expect 10^8 to 10^9 photons incident on the diffraction sample
- Good penetration of 20-50 um, allows high-Z targets
- Image plate for most shots, could be replaced with CCD

- NSTec Supersaver (x-ray diode) to generate line emission from molybdenum metal anodes.
- Radiation testing/certification delayed operations in 961 high bay – completed last week.
- Calibration tests on similar X-ray pulser at MSTS for bulk Au and Silicon and Au and CdS nanoparticles films

CdS (0001) single-crystal Laue spots



Gold nanoparticle films on Si

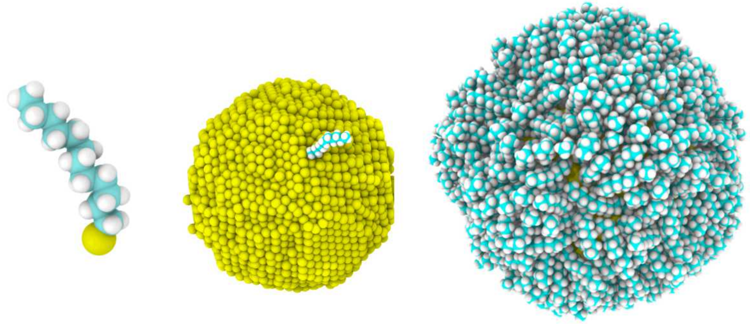


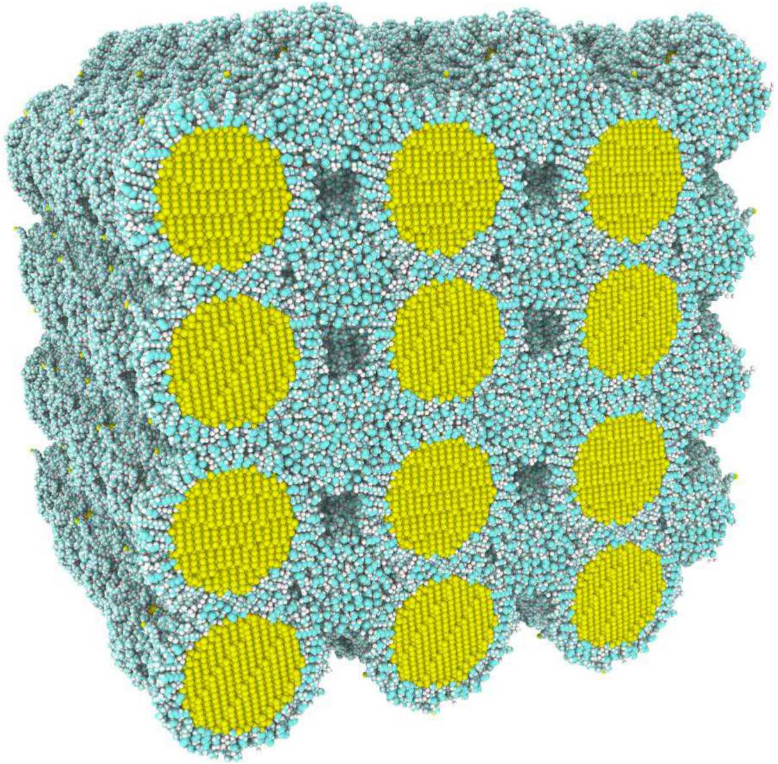
Morgan (MSTS)

Ao (1646)

Matt Lane – jlane@sandia.gov

Modeling of bulk phase transition in MD



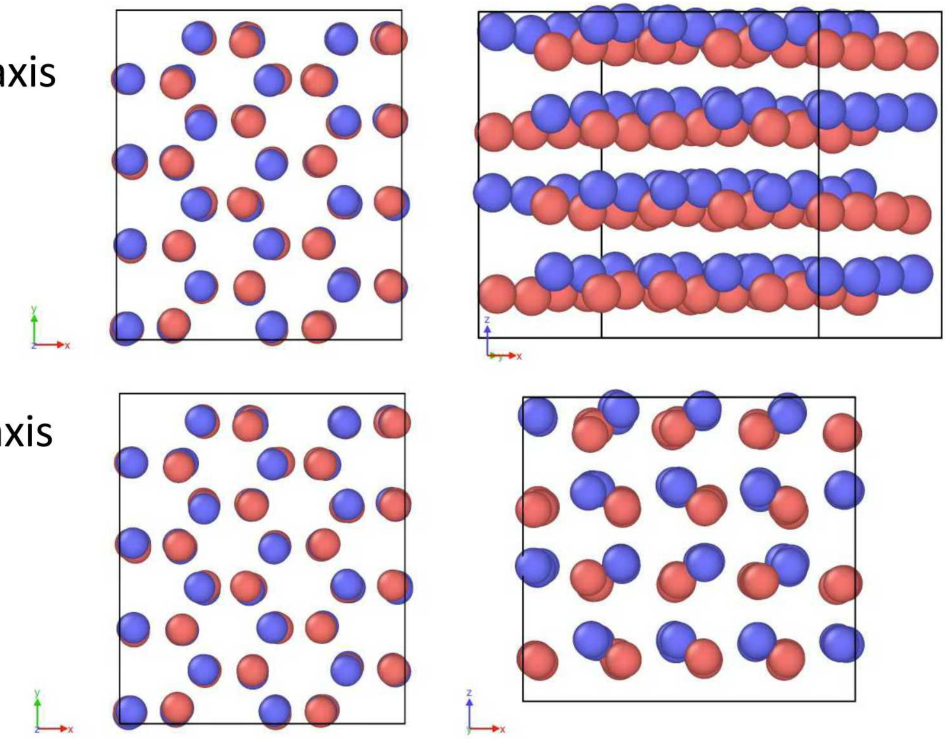


Molecular dynamics studies in dynamic compression of coated particles have been completed. “Synthetic microstructure” showed plastic response in gold.
Li, Bian, Lane, Salerno, Grest, Ao, Hickman, Wise and Fan, Nature Comm., 8, 14778 (2017)

Solid-solid pressure-induced phase transitions have been studied at Sandia in bulk geometries and for military (Martensitic) transformations in CdS.

c-axis

a-axis



Lane (1864)