# Matter in Extreme Conditions

**A. Gleason, SLAC/Stanford University**

**UXSS 2019, Lecture 6**
**June 19, 2019**

U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

# Outline

- Motivation: What is meant by 'extreme' matter and why do we care?
- Tools: What are the type of experiments we can perform?
- Equations of State & Shock Physics
- Temporal revolution: How XFELs are revolutionizing our understanding of matter at extreme conditions.
- Earth / Planetary Science case studies in the ultrafast
- Outlook

# Motivations: What is an extreme state of matter?

SLAC

| | Earth's surface | |
|---|---|---|
| High Pressure | 1 atm | ........Earth's core |
| High Pressure & Temp. | 1atm, 16 $^{o}$C | .......Earth's core |
| High Temperature | -89.2 – 66.8 $^{o}$C | .........Sun's core |
| High Magnetic Field | 45 uT | ..Superconducting magnet |
| High Strain rate | 0 – $10^{-14}$ / sec | .........Shock wave |

……
High Electric fields
High Radiation environments

# Motivations: What is an extreme state of matter?

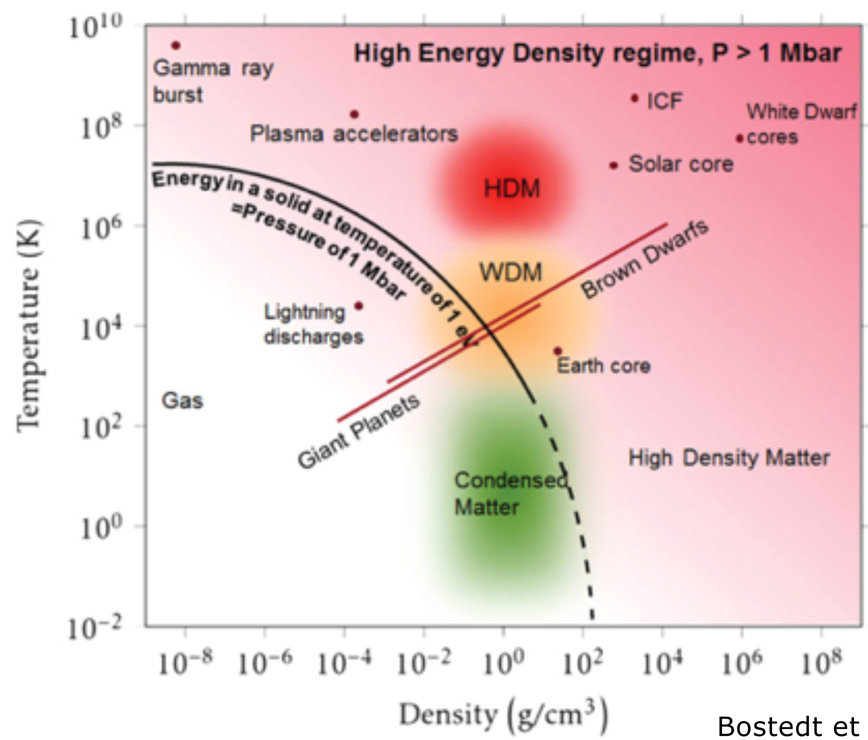
SLAC

| | Earth's surface | |
|---|---|---|
| High Pressure | 1 atm | 3.6 million x....................Earth's core |
| High Pressure & Temp. | 1atm, 16 $^{o}$C | 3.6 million x + 6k x……....Earth's core |
| High Temperature | -89.2 – 66.8 $^{o}$C | 15 million x......................Sun's core |
| High Magnetic Field | 45 uT | 1 million x ................Superconducting magnet |
| High Strain rate | 0 – $10^{-14}$ / sec | 1 billion x .......................Shock wave |

……

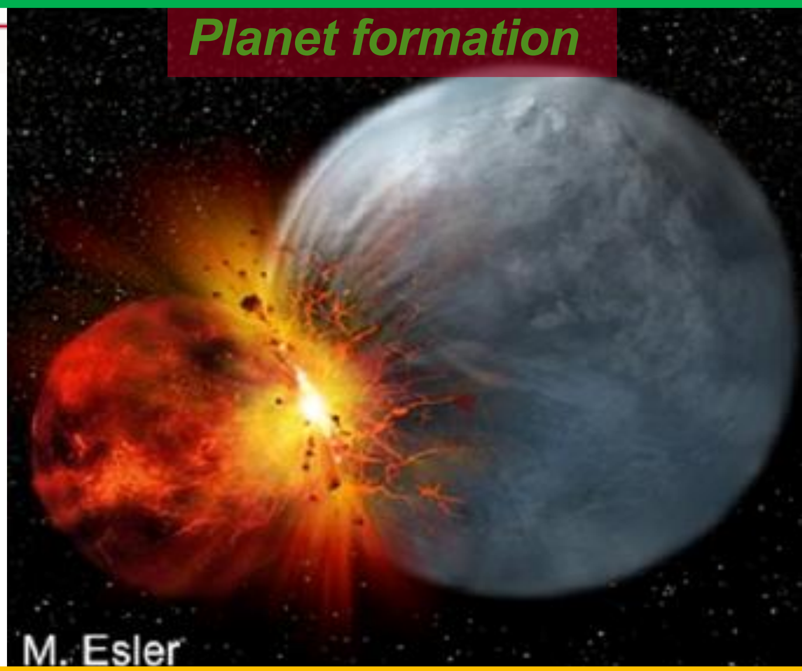
High Electric fields

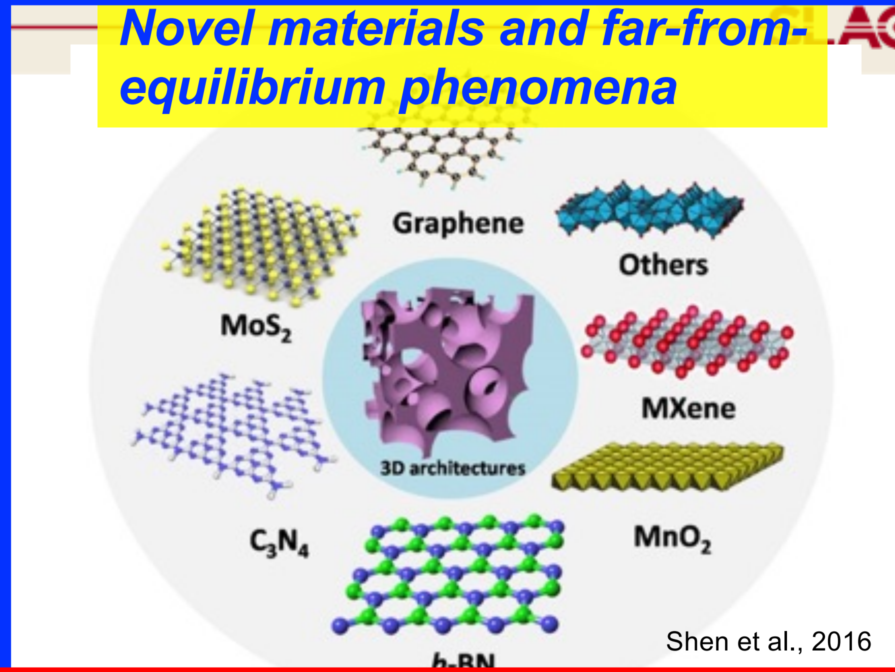
High Radiation environments

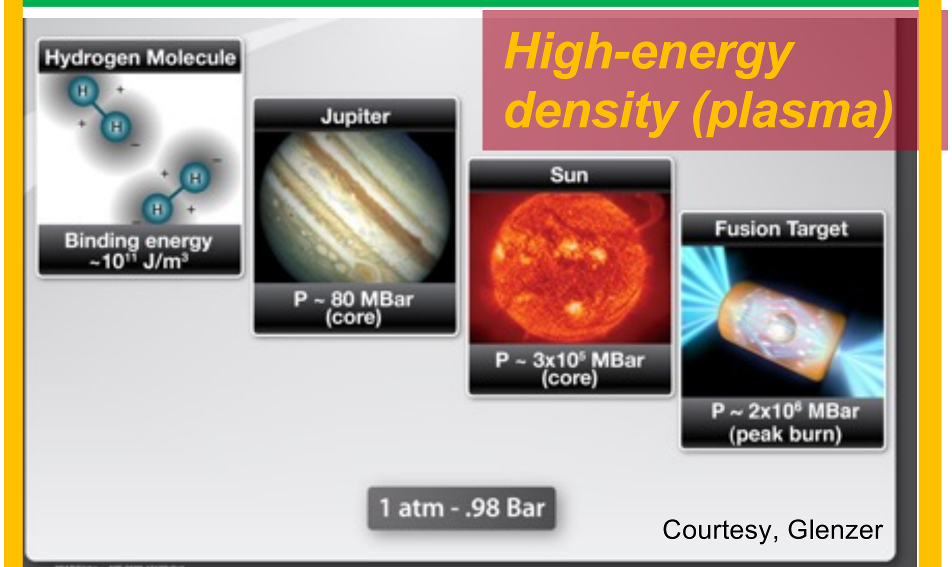


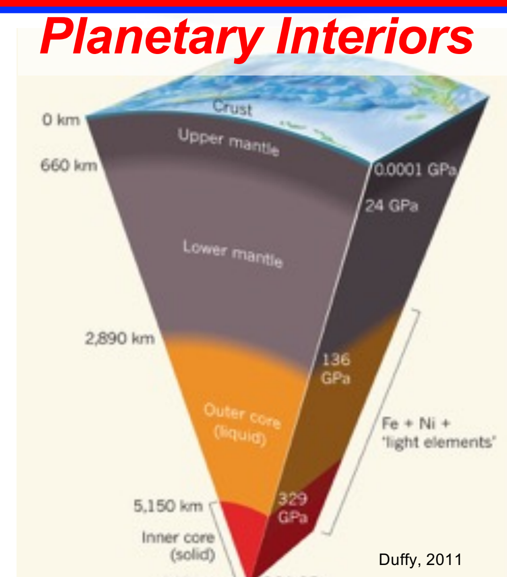

Bostedt et al., 2016

# Motivations: Why should we care about extreme states....application?



# Motivations: What is an extreme state of matter?

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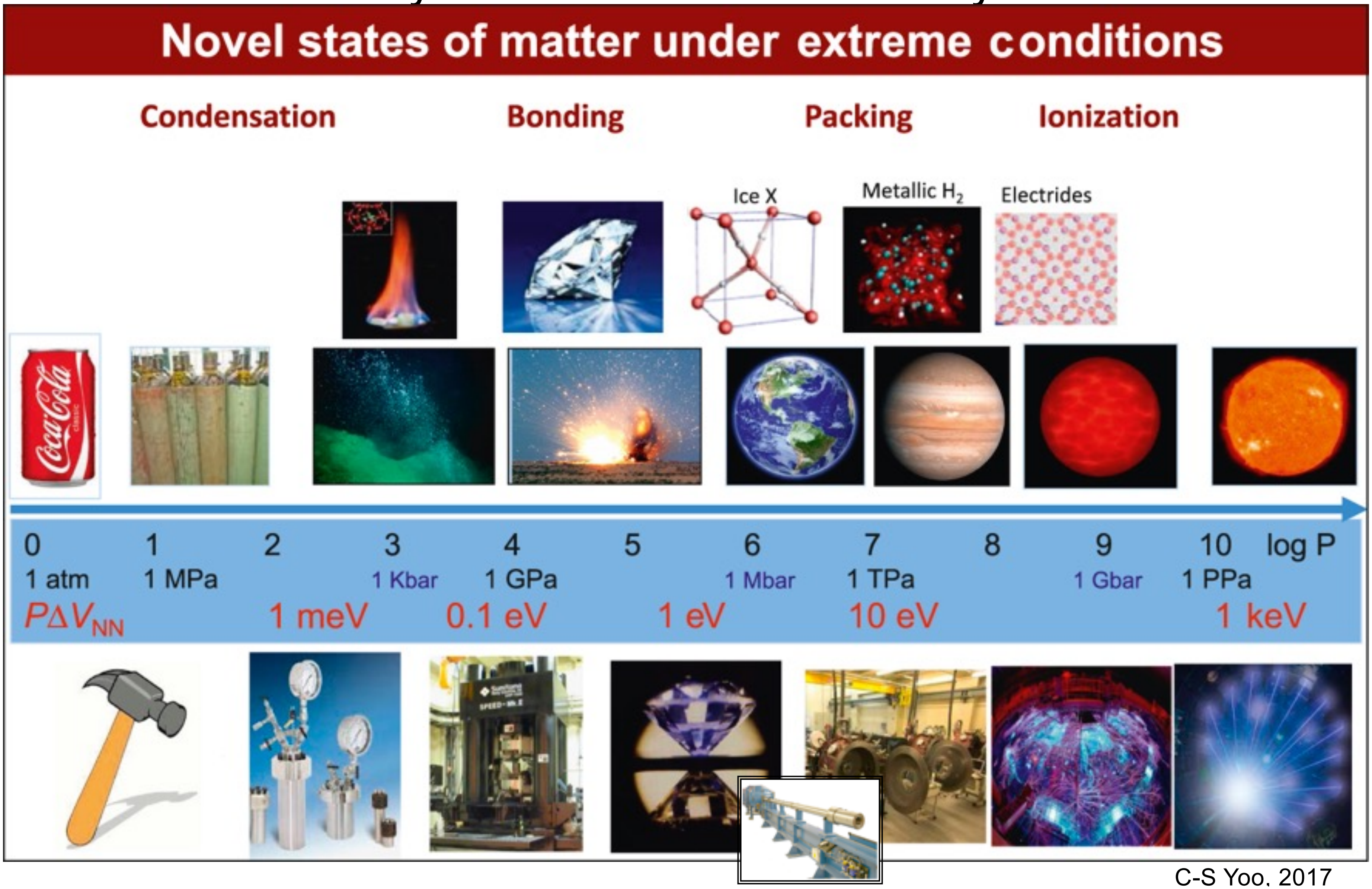
What is meant by ‘extreme’ matter and why do we care?




C-S Yoo, 2017

# Question 1

What are some ways we generate extreme conditions in the laboratory?

a. Gas-gun or explosively driven
   + impact flyer plate

b. diamond-anvil cell

c. via laser ablation at 10^12 Watts/cm2

d. all of the above

# Question 1



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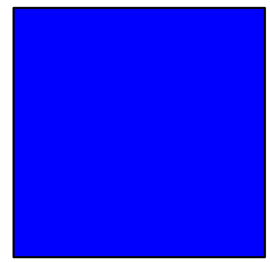
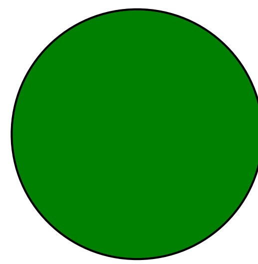
## Question 2

Of the high-pressure platforms listed below, which one generates the *highest* strain rate $[(\Delta L/L_0)$ / time ]?

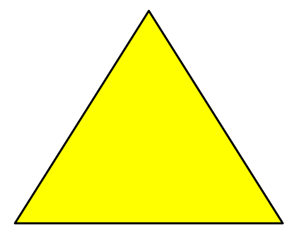
a. Gas-gun + impact flyer plate



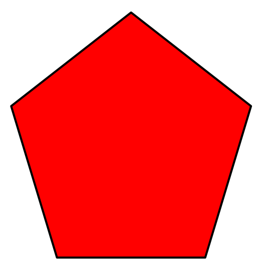
b. diamond-anvil cell



c. via laser ablation at 10^12 Watts/cm2



d. all of the above



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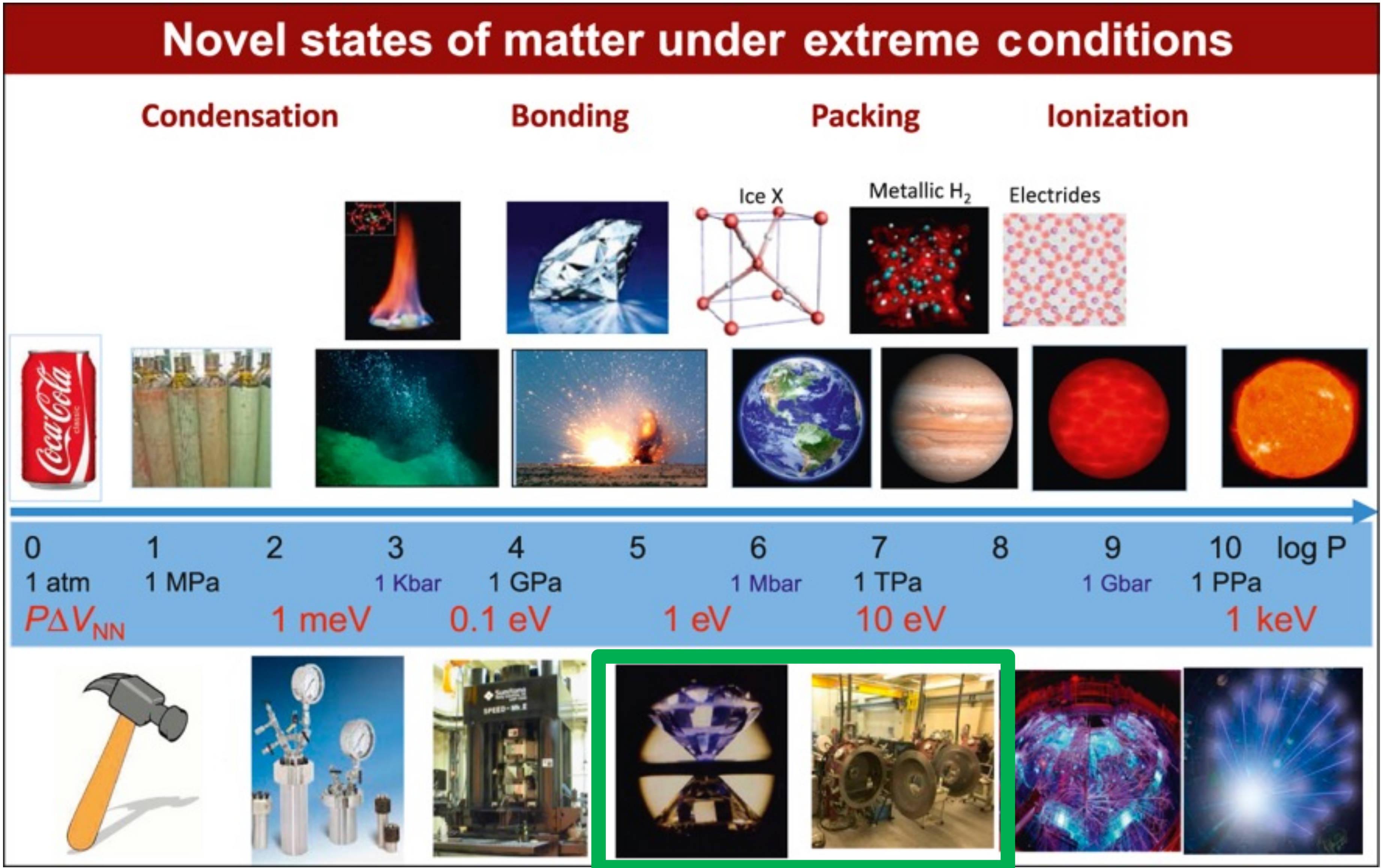
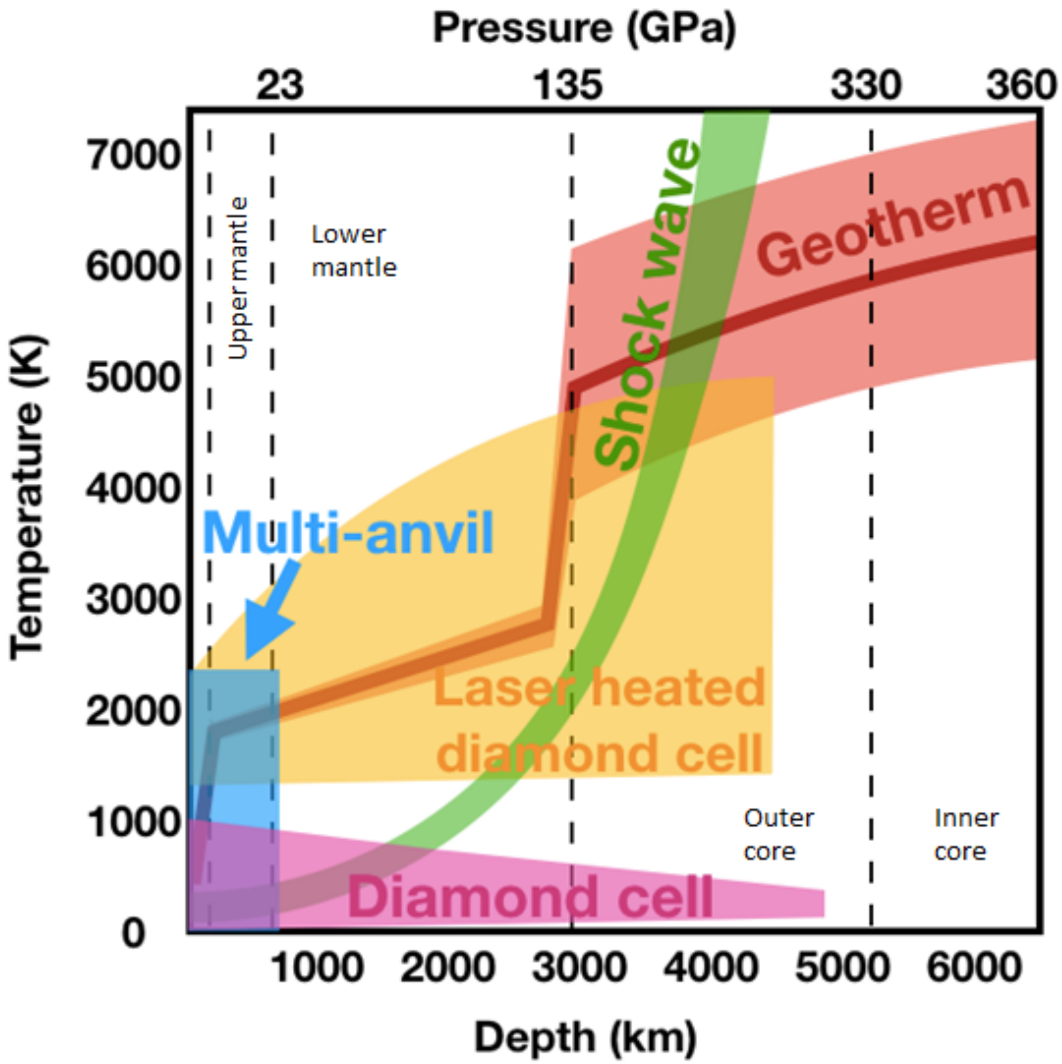
# Tools: how do we generate extreme conditions in the laboratory?




C-S Yoo, 2017

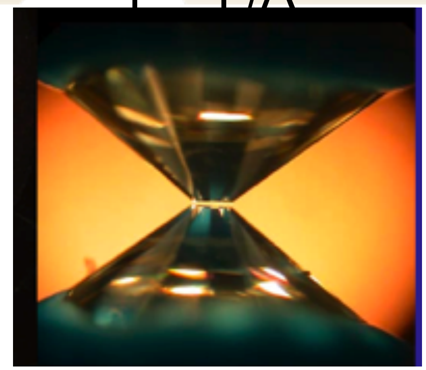
# Tools: how do we generate extreme conditions in the laboratory?



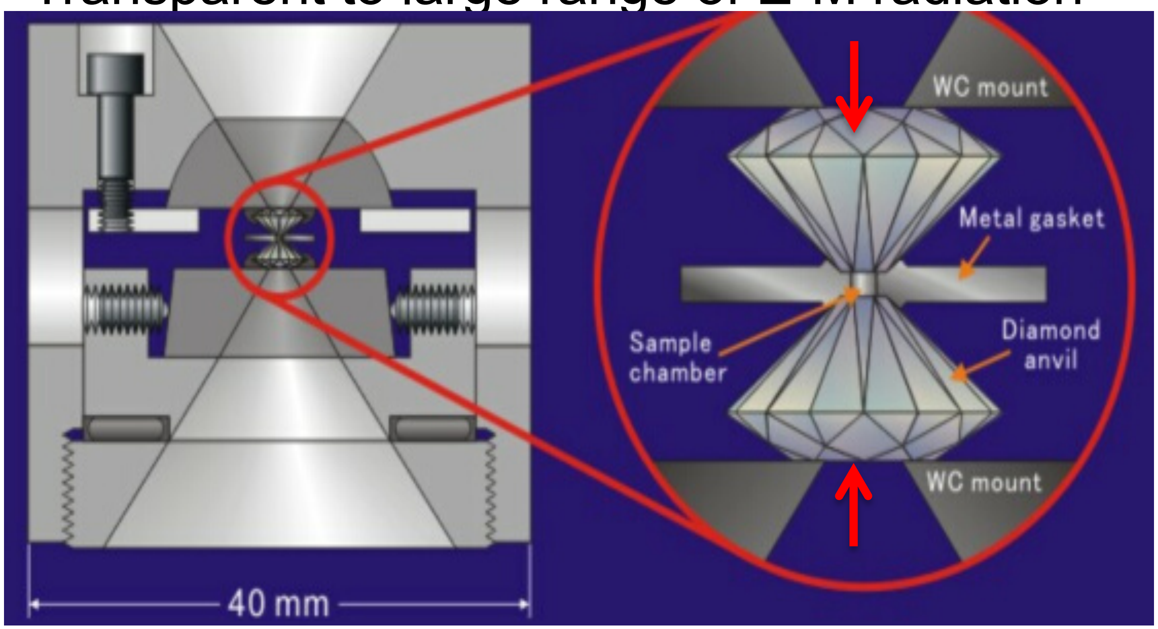

By courtesy of Z. Geballe

# Static compression: Diamond-anvil cells (DACs)

P = F/A

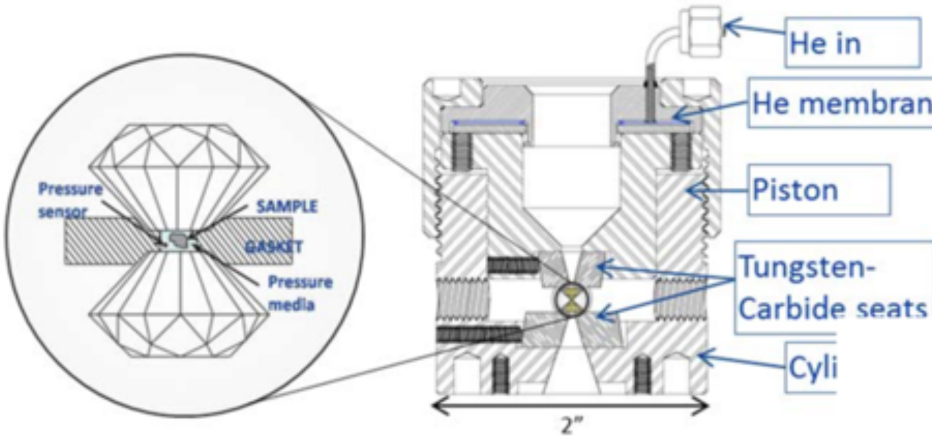


- Pressure: ambient to 300 GPa
  (1 GPa = 10,000 bar)
- Temperature:
  resistive heating up to 1500 K
  laser heating up to 5000 K
- Sample size: < 0.001 $mm^3$
- Transparent to large range of E-M radiation

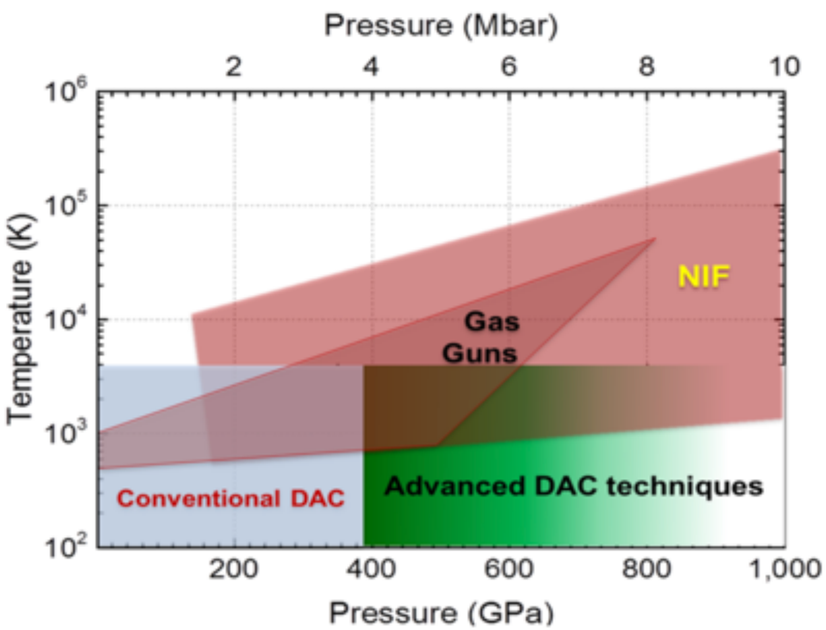


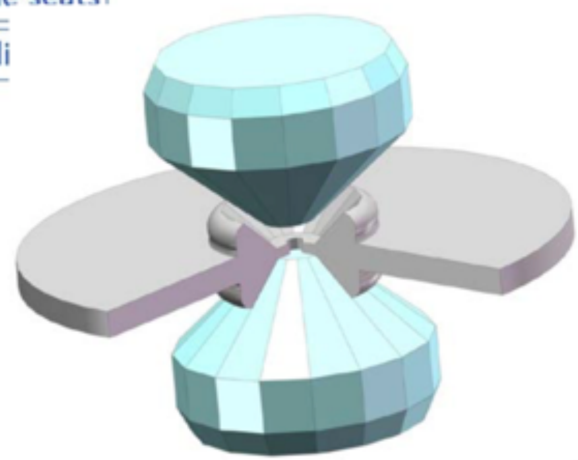

Long compression time (minutes-years)

# Static compression: Diamond-anvil cells (DACs)

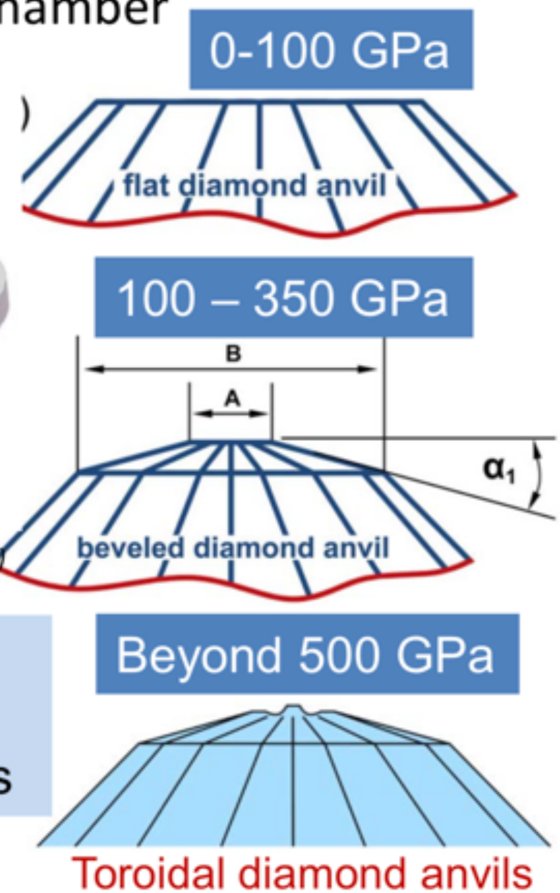



- Piston-cylinder device
- Pressure is generated by decreasing the sample volume by decreasing the height of the sample chamber



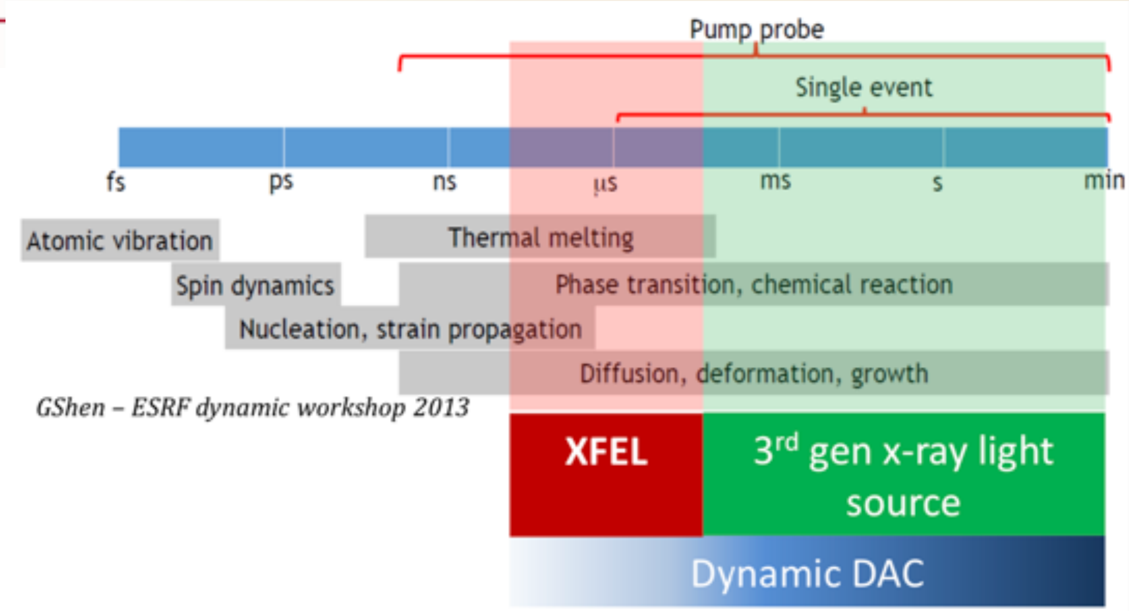
*3D model from Rev. Mod. Phys 90,015007 (2018)*

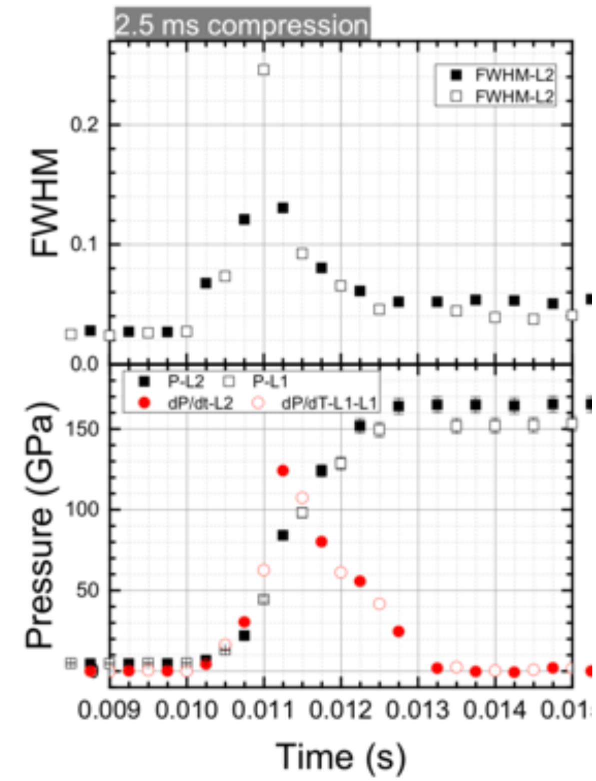


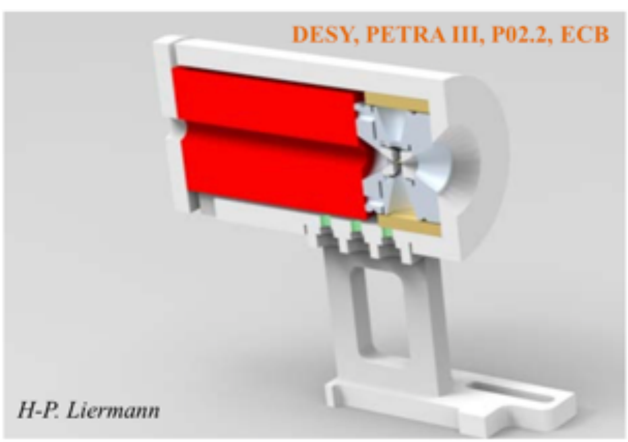

Different type of anvil geometries used for different pressure ranges

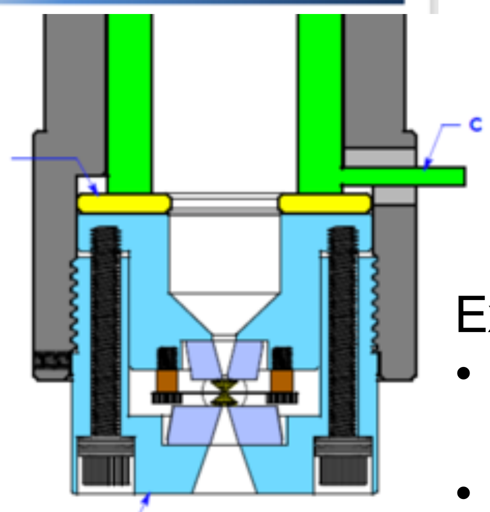
courtesy: Z. Jenei

# Dynamic-DACs



Experiments at:

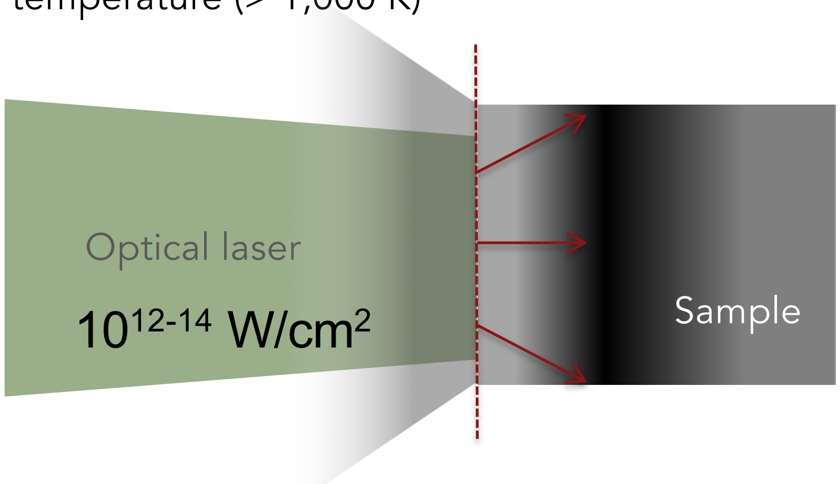
- P02.2 – Extreme conditions Beamline/Petra-III/DESY
- APS Sector 16 – HPCAT/ANL

courtesy: Z. Jenei

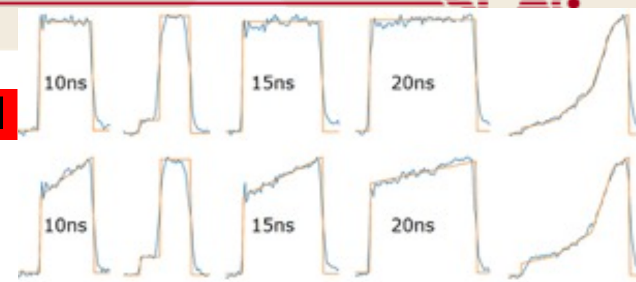
Using 1kV/7A switching amplifier and piezo actuators we achieved peak compression rates of **120 TPa/s** ~ $\dot{\varepsilon} \sim 2.75 \cdot 10^2\ s^{-1}$

# Dynamic compression: laser driven shock waves

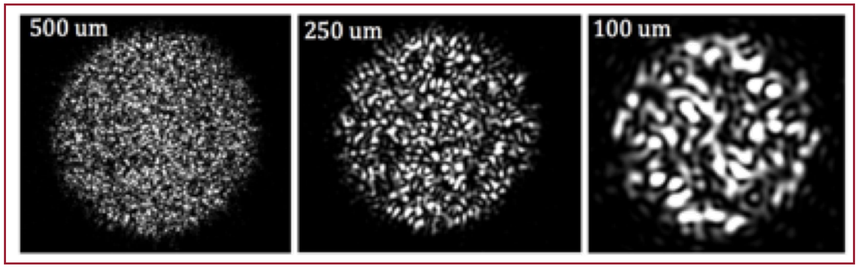
Short compression time (100s ps to 10s ns) and short lived
High temperature (> 1,000 K)

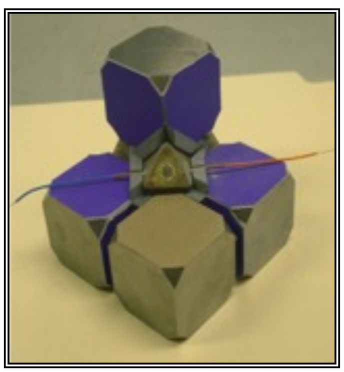


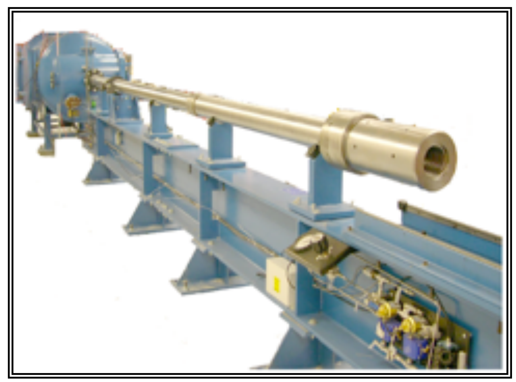

temporal profile

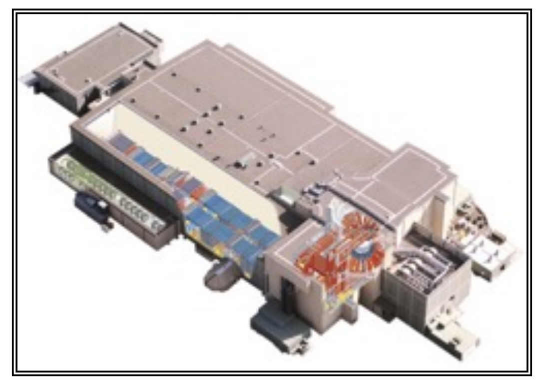


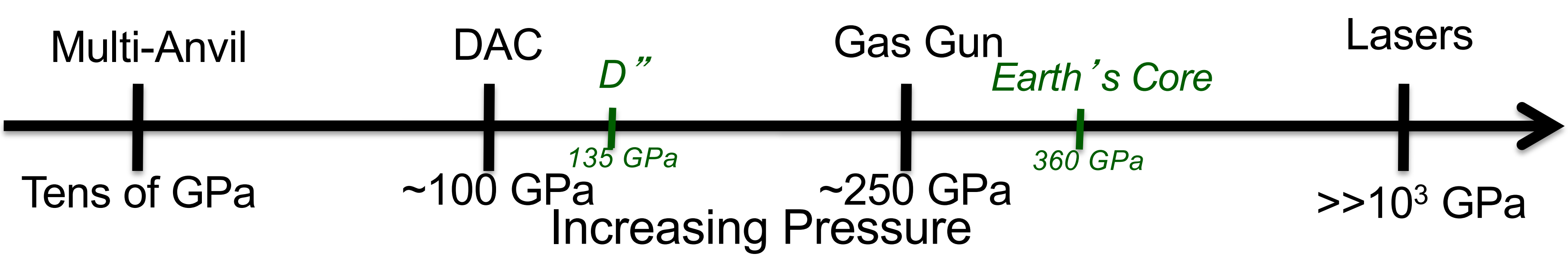

spatial profile









## Question 3

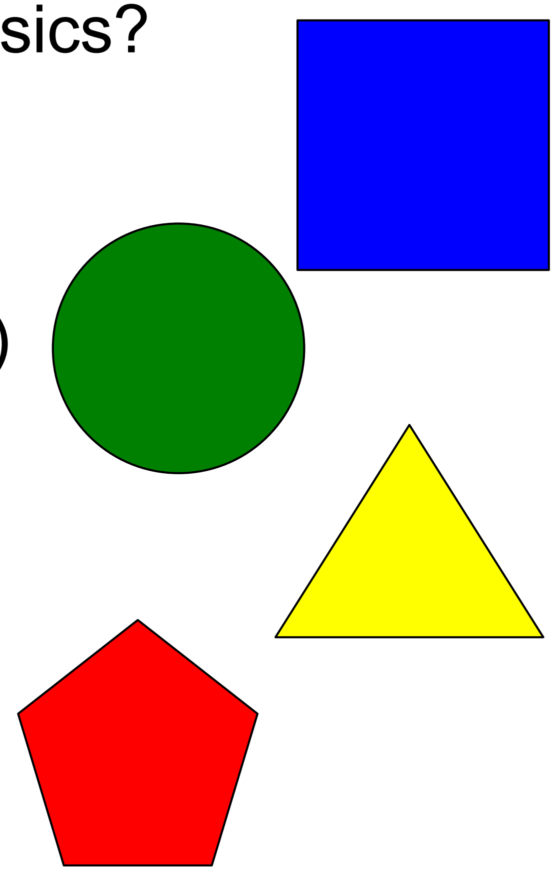
What is the simplest equation of state you've likely already heard of/encountered in physics?

a. Galileo's Law

b. Ideal gas law (PV = nRT)

c. Law of big strain

d. none of the above



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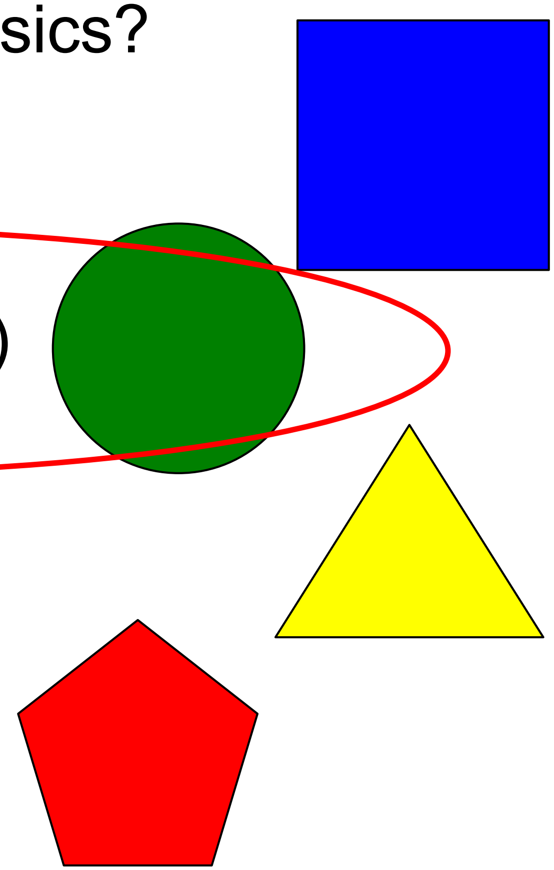

# Equations of State

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**Pressure-Volume Equations of State**

***What is the function that describes reduction in volume for an increase in pressure?*** **<u>V(P) = ?</u>**

*<u>constant compressibility</u> (F=k*x)*

$\Delta V/V_0 = -1/K * \Delta P$

$K = -V_0 * \delta P/\delta V$ (bulk modulus)

*Integrate*: $P = -K*\ln(V/V_0)$ =>

$$\mathbf{V = V_0 \exp(-P/K)}$$

*<u>linear compressiblity</u> (Murnaghan EOS), pressure-induced stiffening*

$K = K_0 + K' * P$

$K_0 + K'*P = -V_0*dP/dV$ => $dP/(K_0 + K'P) = -dV/V_0$

$\ln(K_0 + K'*P)^{1/K'} = \ln V/V_0$ => $(K_0 + K'*P)^{1/K'} = V/V_0$

$$\mathbf{V = V0\ (K_0 + K'*P)^{1/K'}}$$

# Equations of State

SLAC

**Pressure-Volume Equations of State**

***What is the function that describes reduction in volume for an increase in pressure?*** **V(P) = ?**

*polynomial expansion of K =>*

$$K = K_0 + K'P + K''P + \ldots$$

*this has the problem that K -> 0 at high compression, which is physically non-sensical*

*semi-emprical (physically reasonable, not from first principles, agrees with data)*

*carefully choose variables:*

Eulerian finite strain measure:

$$f = \tfrac{1}{2}\left[(V_0/V)^{2/3} - 1\right]$$

# Equations of State

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**Pressure-Volume Equations of State**

***What is the function that describes reduction in volume for an increase in pressure?*** **$V(P) = ?$**

Birch-Murnaghan EOS:

*expand strain energy in Taylor series*:

$F = a + bf + cf^2 + df^3 + \ldots$

*apply boundary conditions and use derivative relations*

*$P = -dF/dV$ & $K = -V(dP/dV)$ to solve for coefficients*

*(just like in 2nd order B-M EOS)*

*get another term, a lot more algebra & K' not constrained to 4*

$$P = 3K_0/2 * [(V_0/V)^{7/3} - (V_0/V)^{5/3}]*[1 + 3/4*(K_0'-4) *((V/V_0)^{-2/3} - 1)]$$

$$= 3K_0f(1+2f)^{5/2} * [1 + 3/4*(K_0'-4) *((V/V_0)^{-2/3} - 1)]$$

*(this is the 3rd order B-M EOS)*

*and, in general,*

$$P = 3K_0f(1+2f)^{5/2} * [1 + x_1f + x_2f^2 + \ldots]$$

# Equations of State

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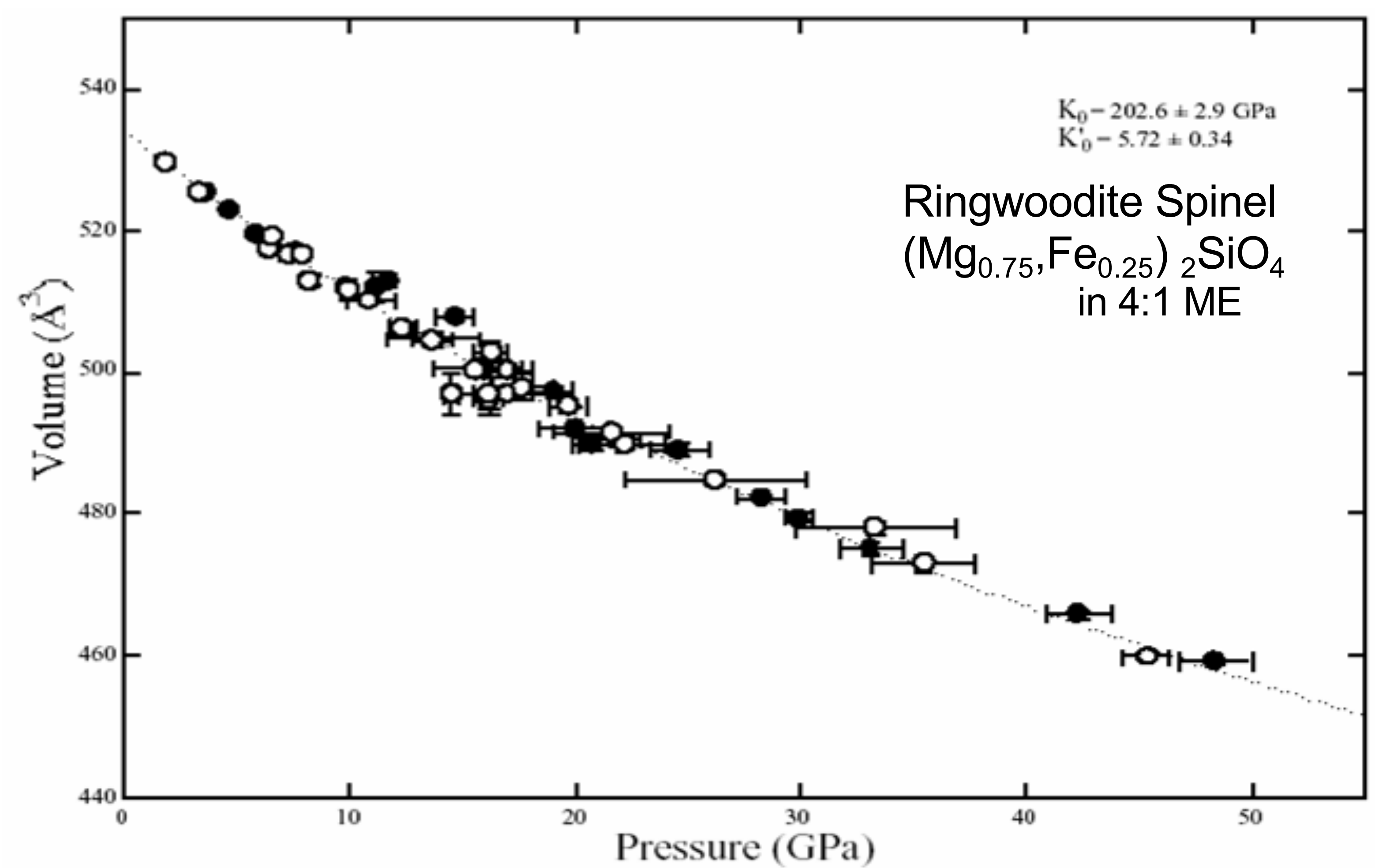
## Pressure-Volume Equations of State

***What is the function that describes reduction in volume for an increase in pressure?*** **V(P) = ?**



# Rankine-Hugoniot equations

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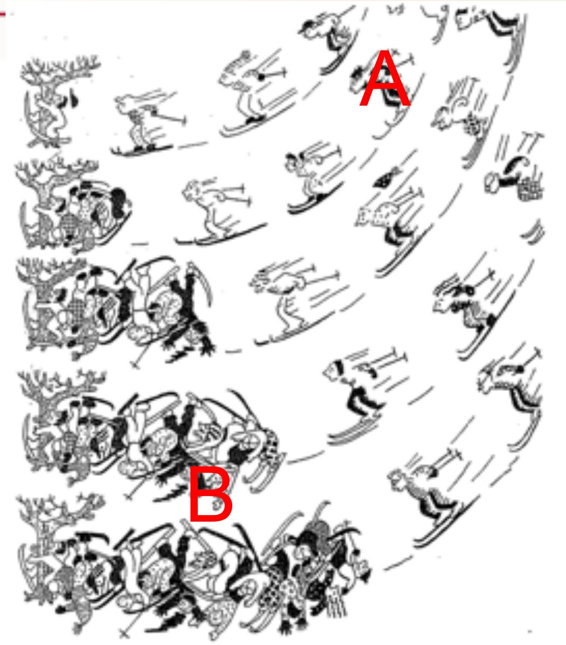
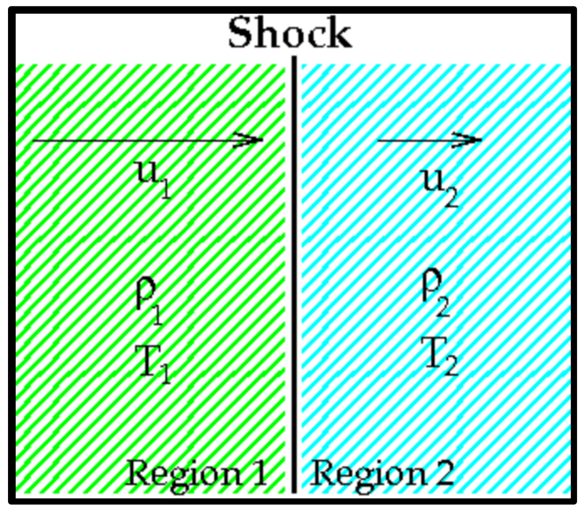



FIG. 3. Receding shock wave.
(Reproduced with permission from Courant and Friedrichs, 1948.)

Duvall and Fowles, 1963



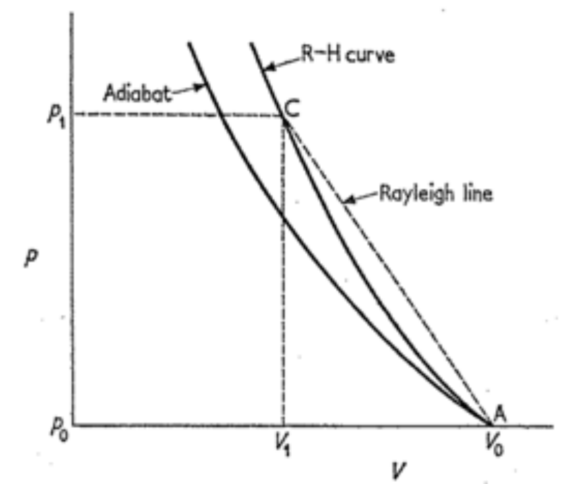
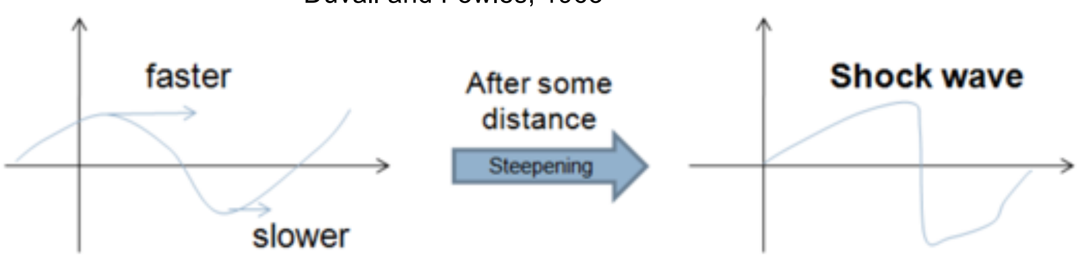




FIG. 5. Comparison of R-H curve and adiabat.




Shock Hugoniot → $(P_1 - P_0) = \rho_0 U_s \cdot u_p$

$$P_1 = \rho_0\left[\left(C\ u_p\right) + \left(S u_p^2\right)\right]$$

Conservation of Mass

$$\rho_0 U_s = \rho_1\left(U_s - u_p\right)$$

Conservation of Momentum

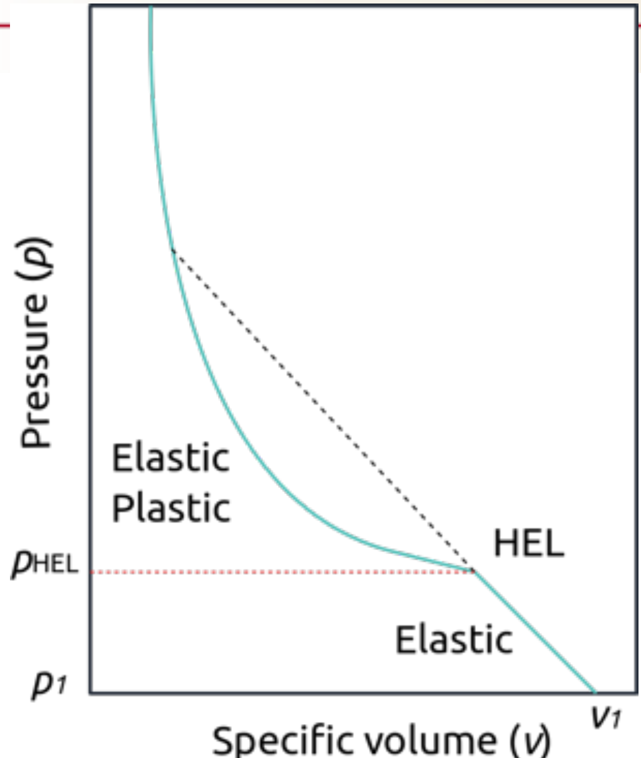
$$\left(P_1 - P_0\right) = \rho_0 U_s \cdot u_p$$

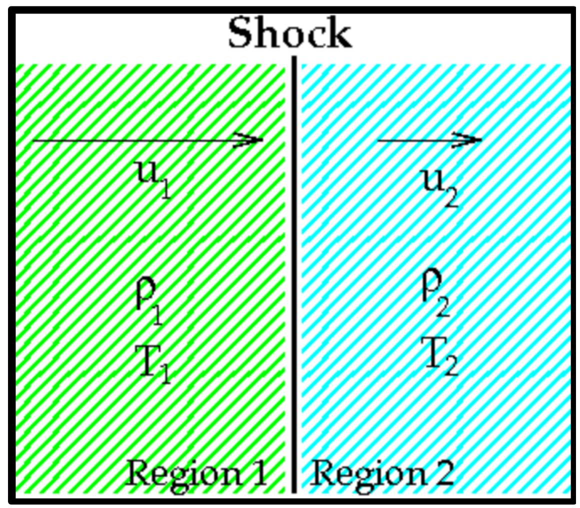
Conservation of Energy

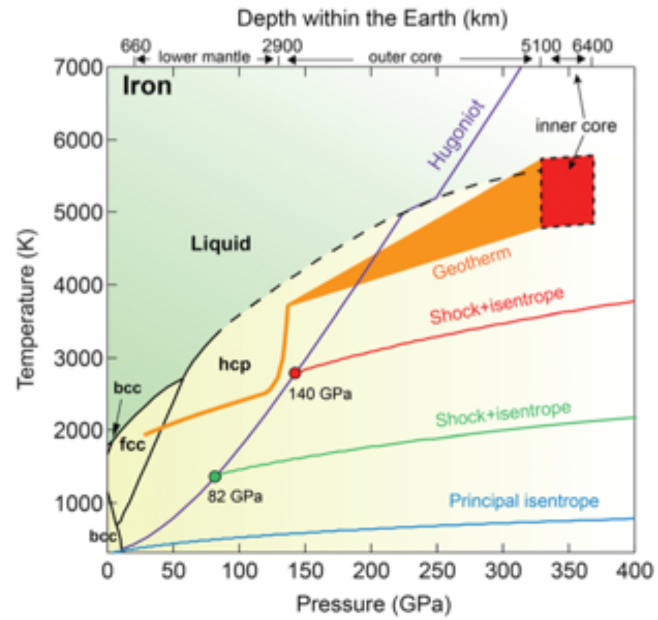
$$P_2 u_p = \rho_1 U_s\left(\frac{1}{2}u_0^2 + \varepsilon_1 - \varepsilon_0\right)$$

# Rankine-Hugoniot equations

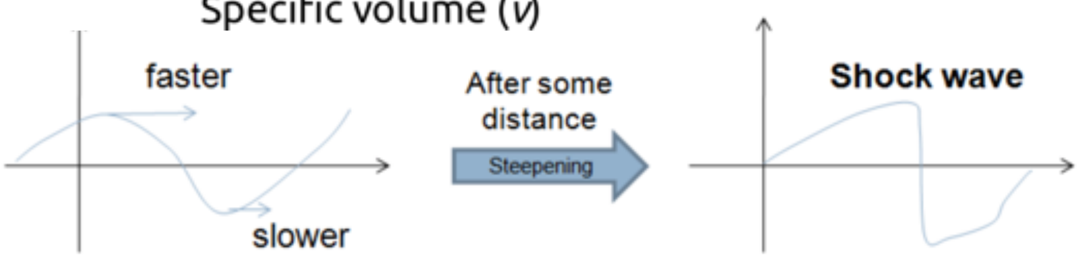





Wang et al., 2013




$$\rho_1\, u_s = \rho_2 (u_s - u_2)$$ Conservation of mass

$$p_2 - p_1 = \rho_2\, u_2\, (u_s - u_2) = \rho_1\, u_s\, u_2$$ Conservation of momentum

$$p_2\, u_2 = \rho_1\, u_s\, \left(\tfrac{1}{2}\, u_2^2 + e_2 - e_1\right)$$ Conservation of energy

# Question 4

What is the shock Hugoniot?

a. Specifically represents the thermodynamic path taken by by a material.

b. Describes the locus of all possible thermodynamic states a material can exist in behind a shock.

c. The combination of conservation of mass, momentum and energy across a shock front.

d. Both b and c

# Question 4

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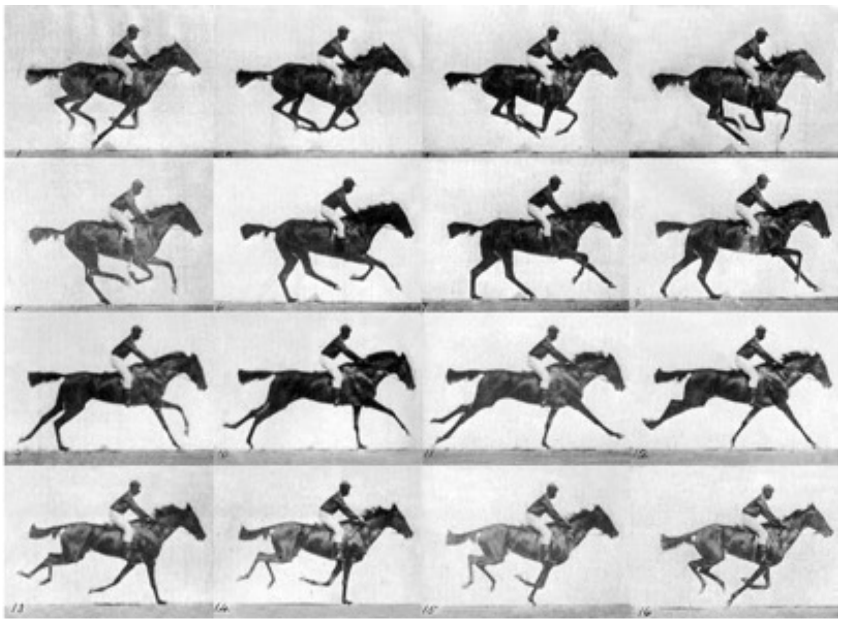
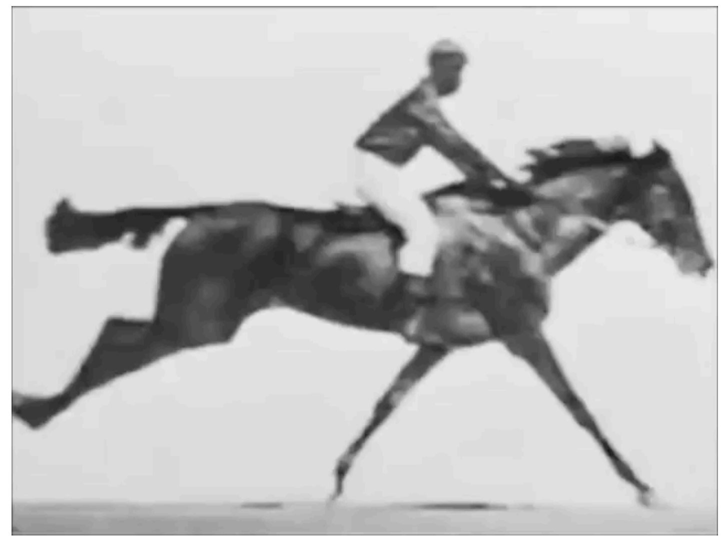
# Temporal Revolution: seeing processes unfold in time

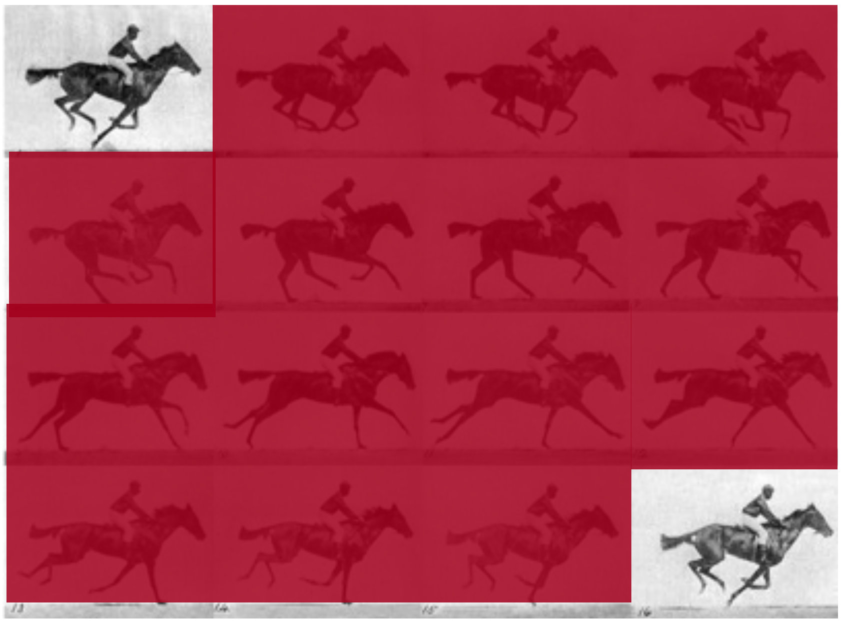
Horse named Sallie Gardner was photographed in time while galloping.





E. Muybridge (1872): Cameras+ tripwires showed that all four hooves do leave the ground at once!

# Temporal Revolution: seeing processes unfold in time



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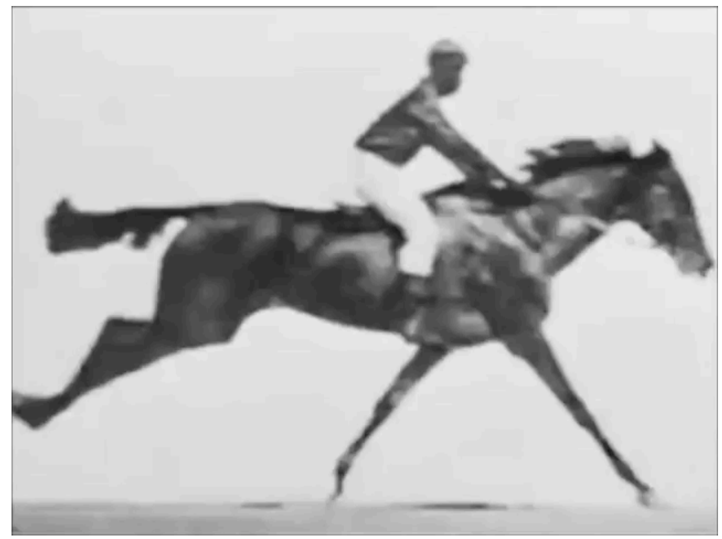
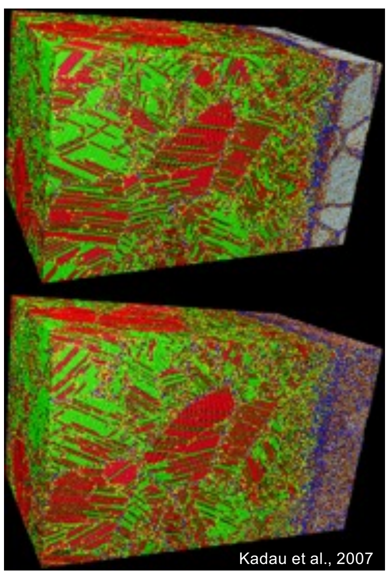


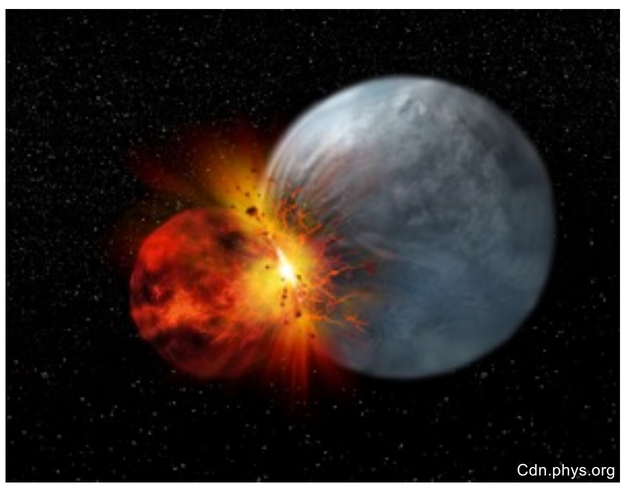
Until the advent of time-resolved X-ray probes combined with dynamic compression platforms we were missing some information about transformation pathway and mechanism.

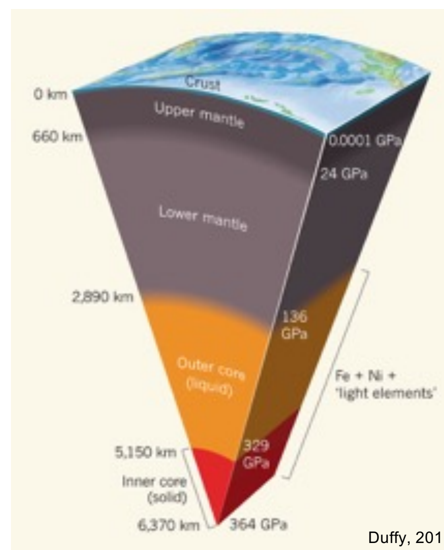
# Frontier Science in condensed matter and plasma physics

To understand the fundamental physics that govern atomic interactions in condensed matter, measurements are required at relevant temporal- and spatial-scales.

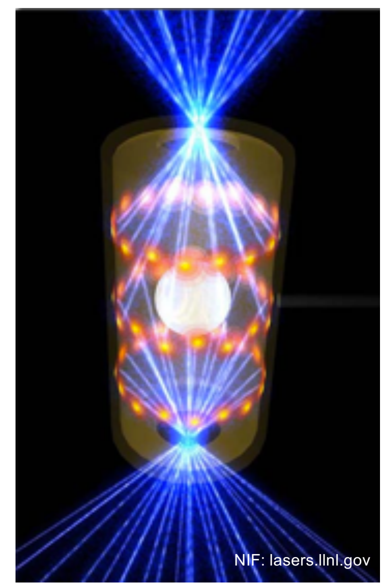
→ shock-loading + ultrafast X-ray techniques

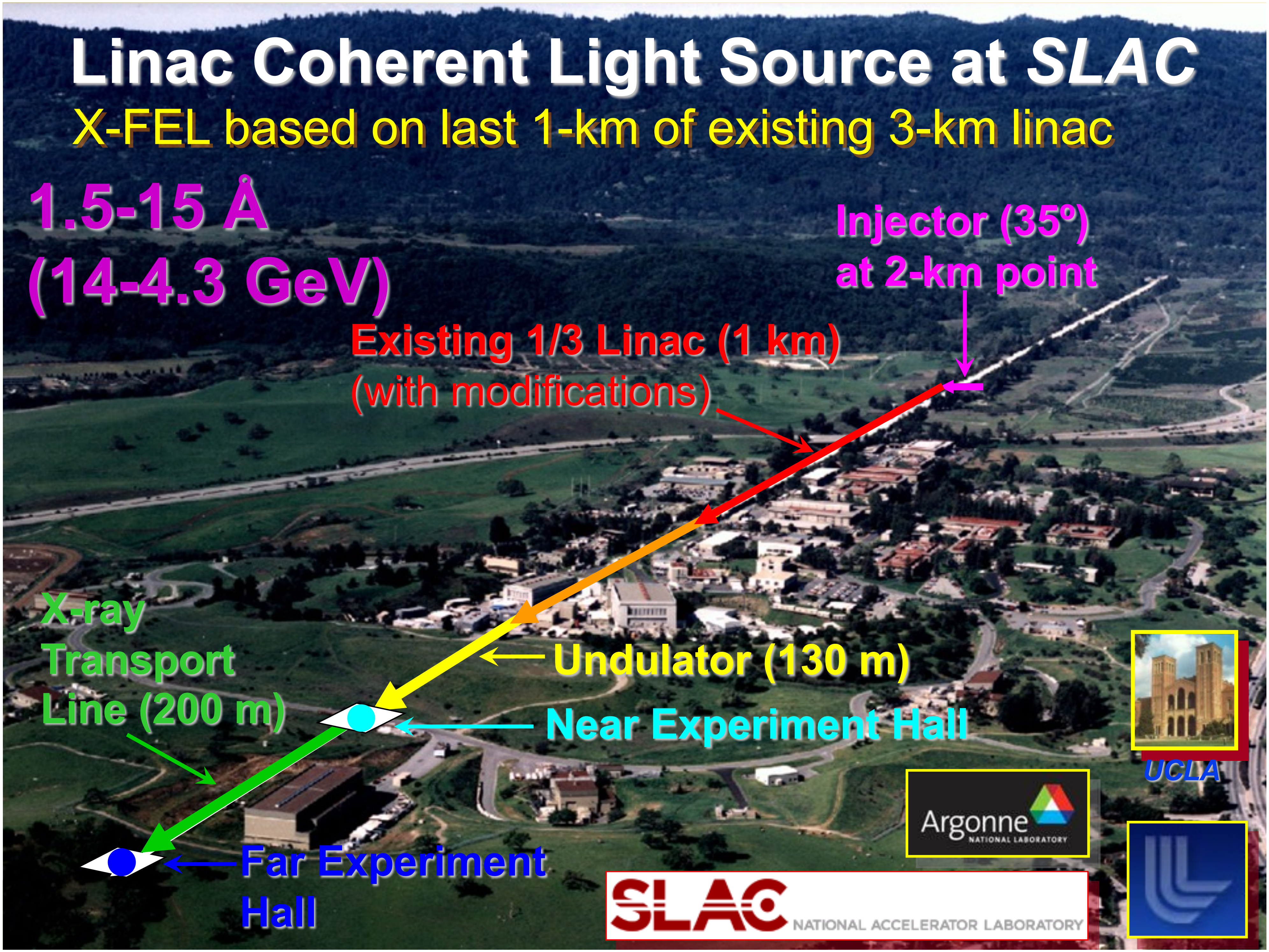

Kadau et al., 2007


Cdn.phys.org



Duffy, 2011


NIF: lasers.llnl.gov



Linac Coherent Light Source at SLAC
X-FEL based on last 1-km of existing 3-km linac
1.5-15 Å
(14-4.3 GeV)
Injector (35º)
at 2-km point
Existing 1/3 Linac (1 km)
(with modifications)
Undulator (130 m)
X-ray
Transport
Line (200 m)
Near Experiment Hall
Far Experiment
Hall
UCLA
Argonne
NATIONAL LABORATORY
SLAC
NATIONAL ACCELERATOR LABORATORY

# Linac Coherent Light Source at SLAC

First hard x-ray free electron laser (FEL)

Short bunch duration
(2~10 fs, 50 - 200 fs)

Full transverse coherence

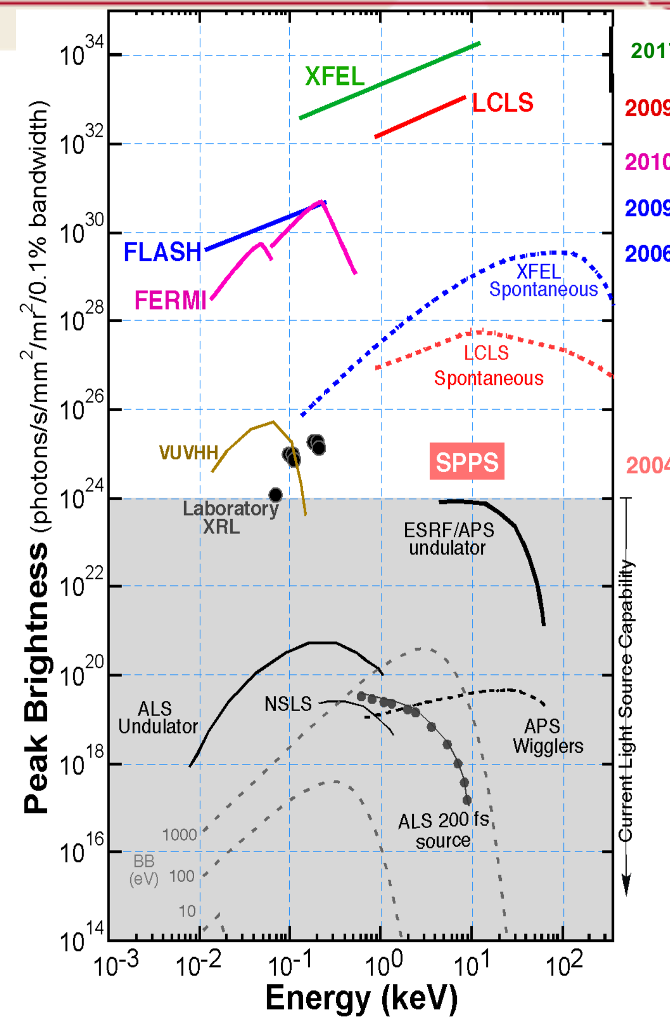
High repetition rate
(~120 Hz)

Tunable from 600 to 9500 eV

- 4-9.5 keV for 1st harmonic at MEC

High # of photons per bunch > $10^{12}$

- 3mJ/pulse




https://portal.slac.stanford.edu/sites/lcls_public

# Question 5

Which is ***not*** a characteristic of XFEL radiation compared to synchrotron radiation?

a. Short pulse duration

b. coherent

c. Large number of photons per pulse (e.g., $10^{12}$)

d. continuous

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Which is ***not*** a characteristic of XFEL radiation compared to synchrotron radiation?

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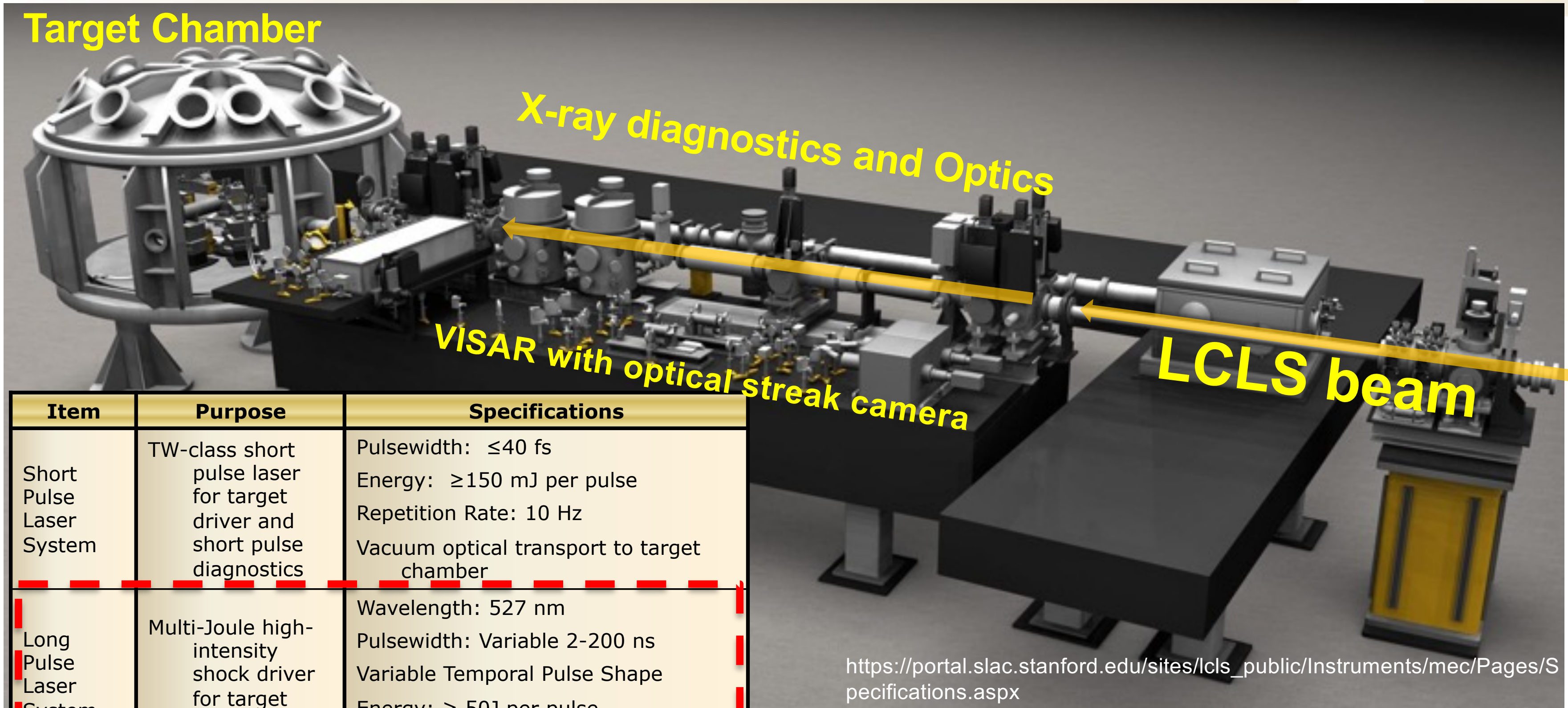
# MEC instrument optics and diagnostics

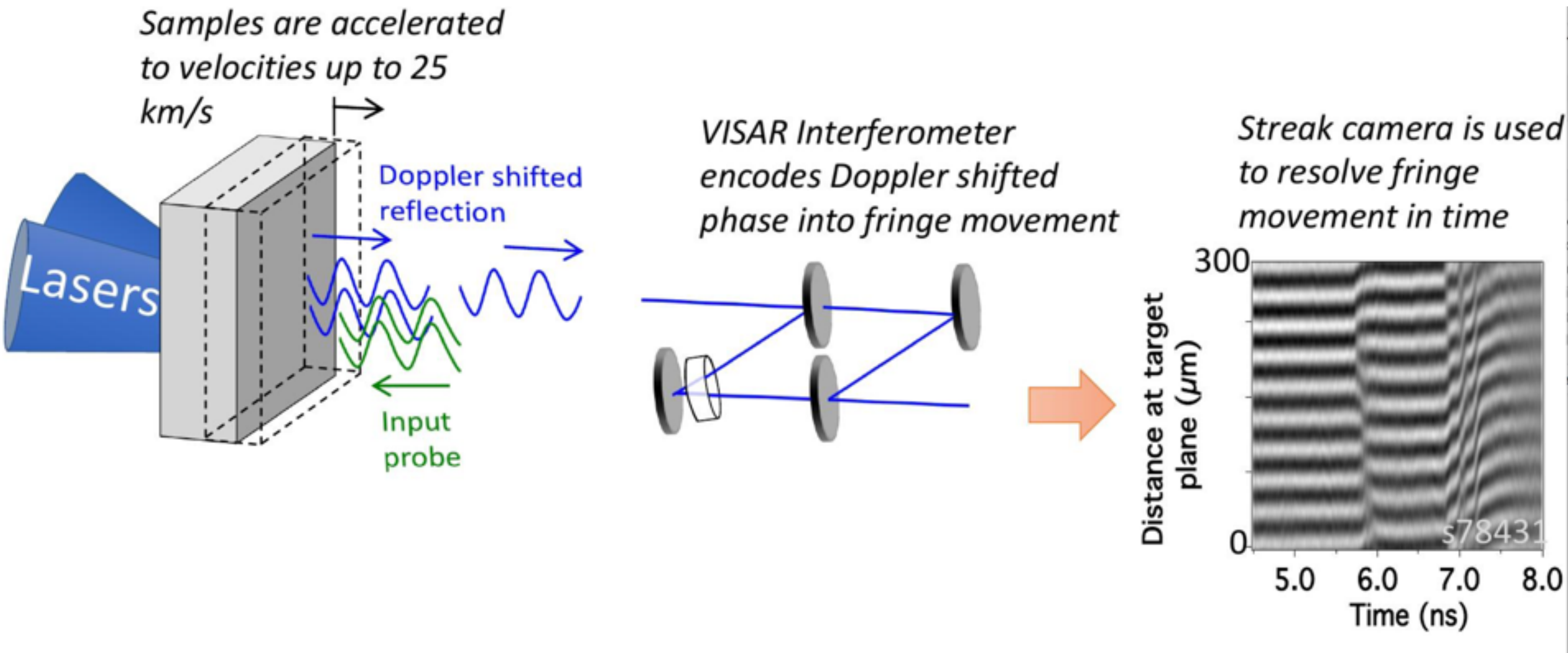



| Item | Purpose | Specifications |
|---|---|---|
| Short Pulse Laser System | TW-class short pulse laser for target driver and short pulse diagnostics | Pulsewidth: ≤40 fs<br>Energy: ≥150 mJ per pulse<br>Repetition Rate: 10 Hz<br>Vacuum optical transport to target chamber |
| Long Pulse Laser System | Multi-Joule high-intensity shock driver for target interactions | Wavelength: 527 nm<br>Pulsewidth: Variable 2-200 ns<br>Variable Temporal Pulse Shape<br>Energy: ≥ 50J per pulse<br>Repetition Rate: 1-shot per 10 min |

The Matter in Extreme Conditions (MEC) instrument combines the unique LCLS beam with high power optical laser beams, and a suite of dedicated diagnostics tailored for the study of Warm Dense Matter, High Pressure Physics, Shock Physics, and High Energy Density Physics.

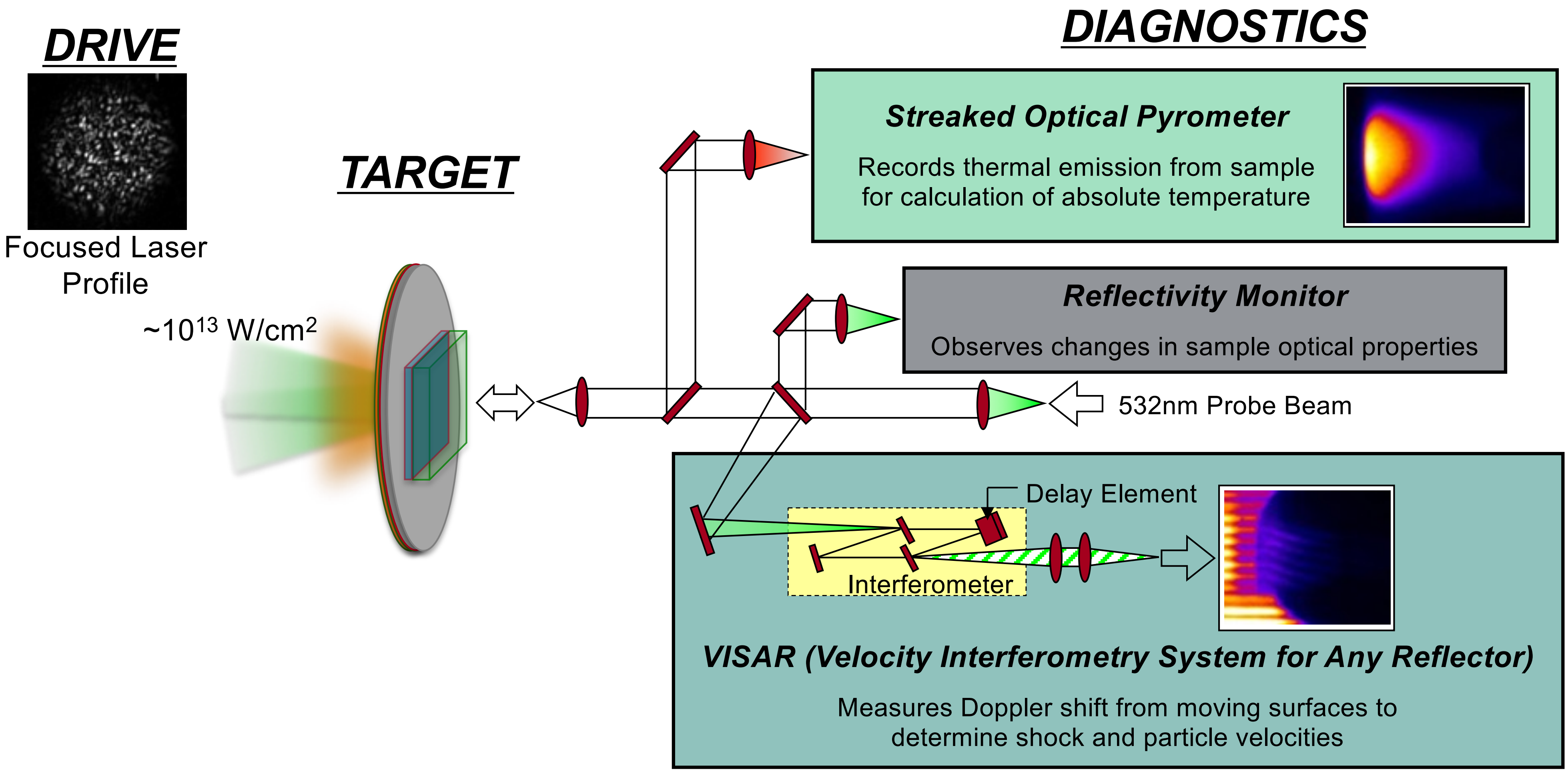
# Velocimetry to deduce time-resolved materials properties



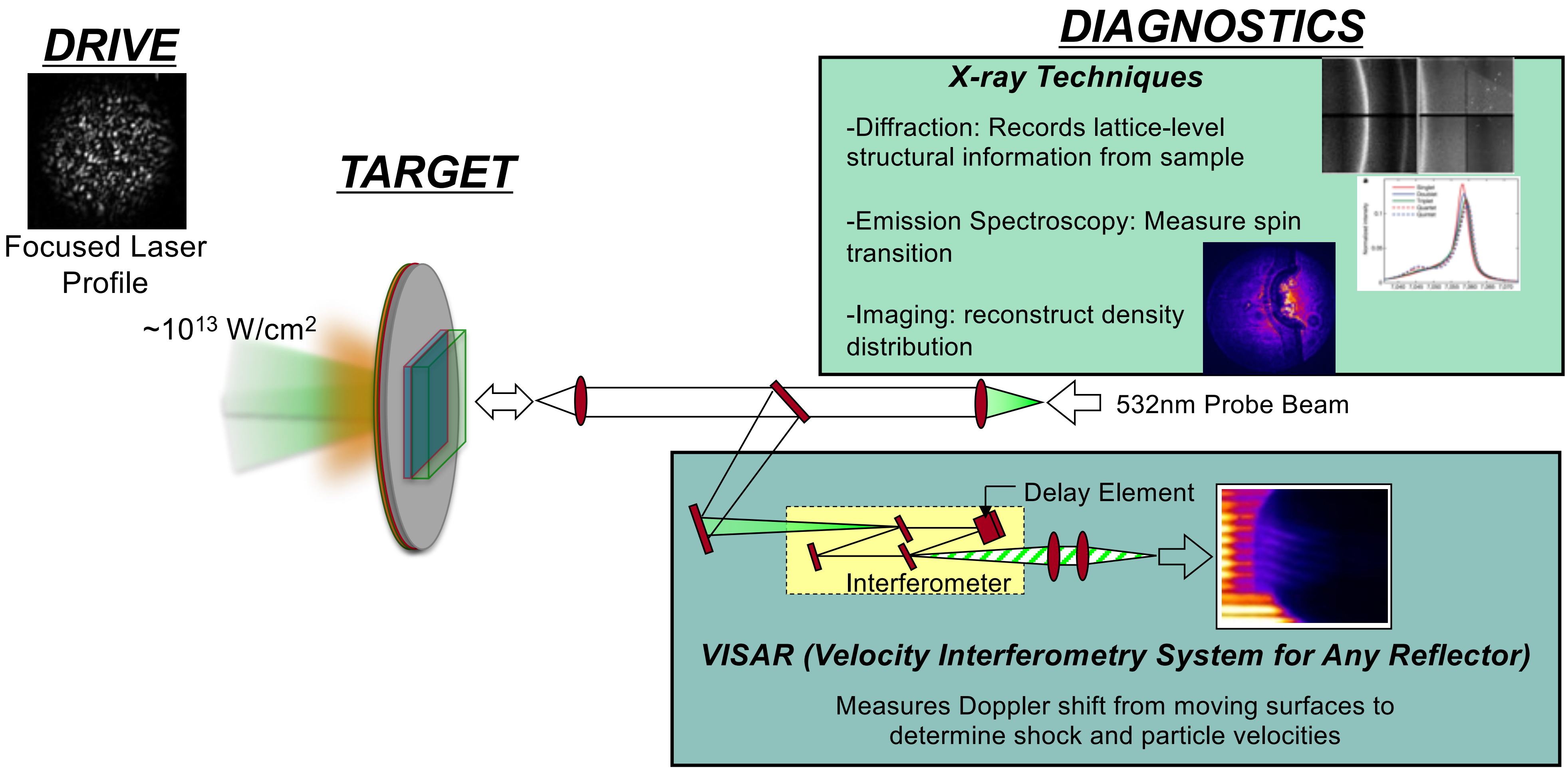



Duffy & Smith, 2019

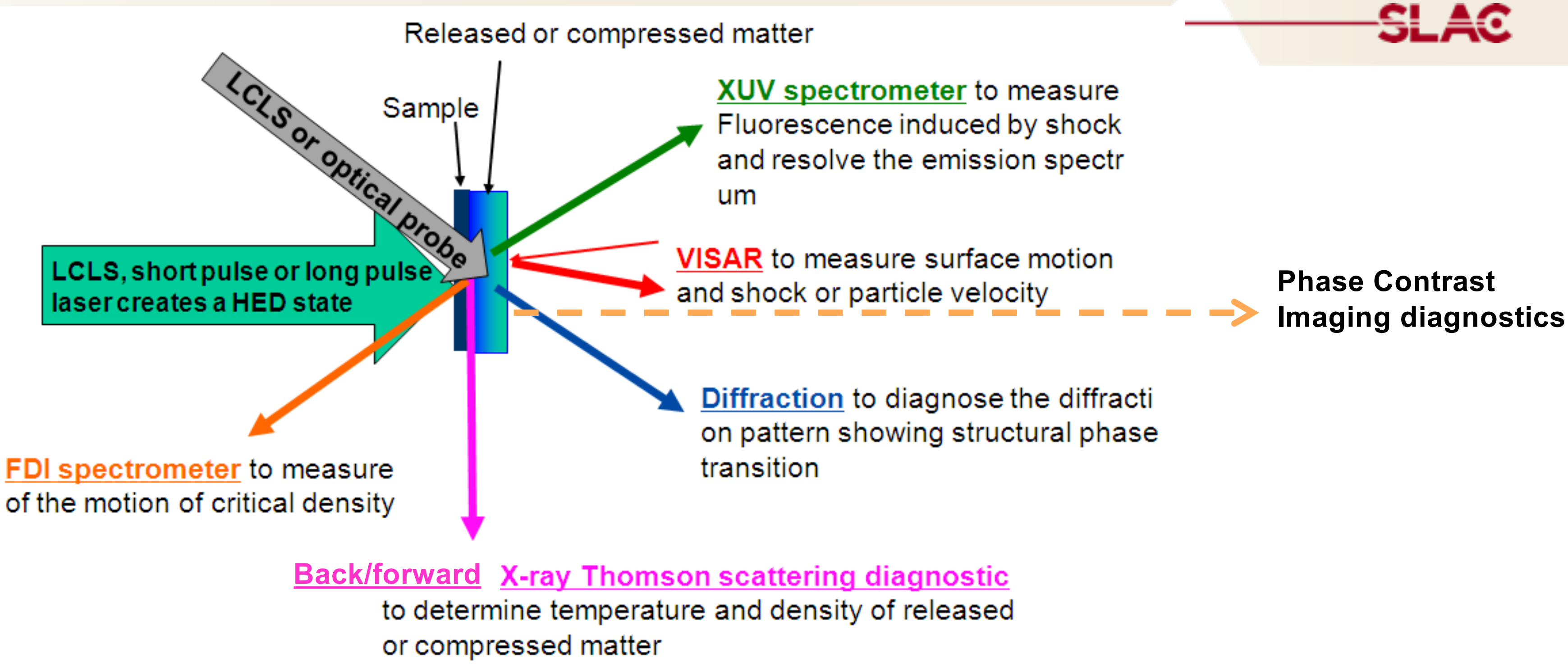
# Laser driven shock compression



# Laser driven shock compression

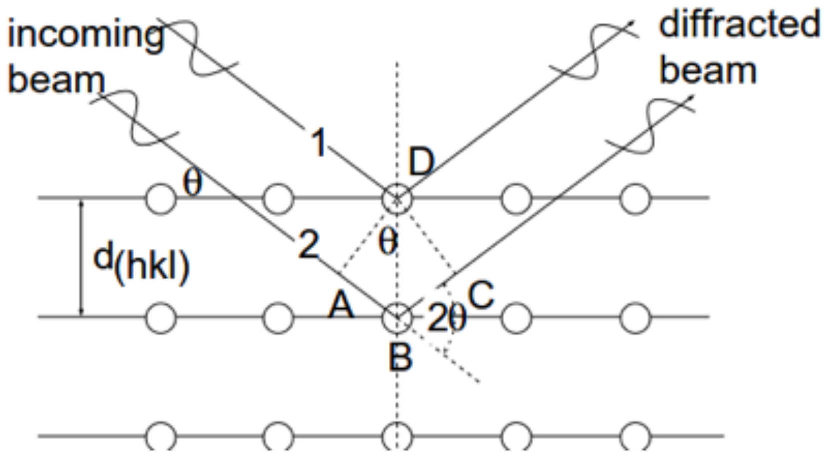


# Typical pump-probe experimental setup

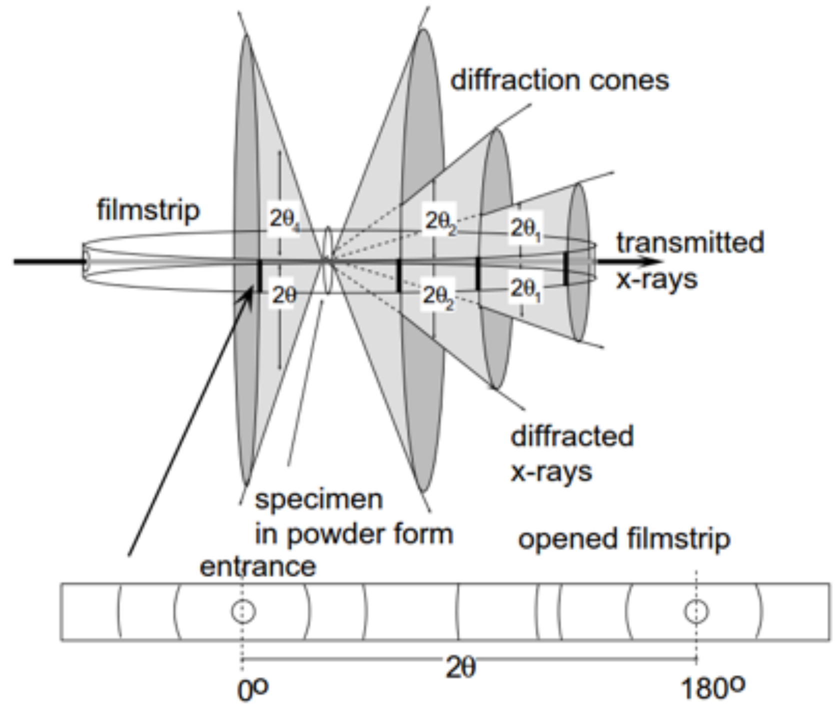



- **LCLS as a pump:**
  - Uniformly and rapidly heat target volumes reaching 100s eV temperature (HDM)
- **LCLS as a probe:**
  - Tunability provides spectroscopic capability for the study of HED
  - High peak brightness provides Thomson scattering capability and Phase contrast imaging capability
  - Short pulse duration can measure WDM in transient phenomena

# X-ray Diffraction (XRD)




$$n\lambda = 2d_{(hkl)} \sin\theta$$ *Bragg*'s Law




Why care about the crystal symmetry?

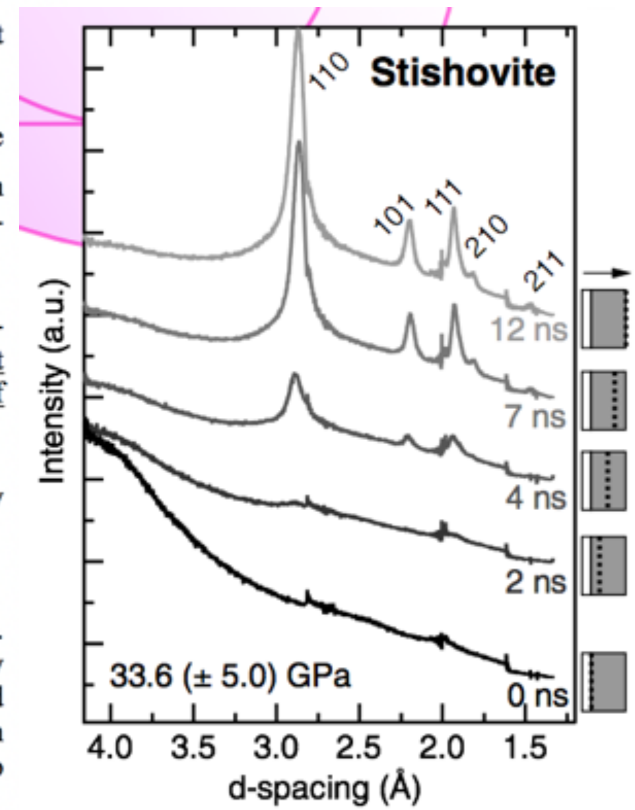
- Mass density (atom locations)
- Electron wave functions, including bonding
- Wave fields for scatted X-ray

# Time-resolved X-ray Diffraction (XRD): transformation kinetics

SLAC

**TRANSFORMATIONS UNDER SHOCK**

| TYPE | ENERGETICS | KINETICS |
|---|---|---|
| I. Mechanical<br>Dynamic Yielding at the HEL | ~0 (defect formation affects thermal state negligibly) | Inertial effect on defect propagation |
| II. Structural<br>a) Solid State<br>1)(Shear-based, martensitic, displacive) | $\Delta E_{tr} \sim -P_{tr}\Delta V_{tr}$ | Rapid kinetics & little impedance at high $\dot{\varepsilon}$; slight orientation dependence caused by shear-enhancement. |
| 2)(diffusion-limited, reconstructive: includes disproportionation reactions | $\Delta E_{tr} \sim -P_{tr}\Delta V_{tr}$ | Slow kinetics due to diffusion-limit: highly T-dependent. Most important equilibrium mode of transformation for minerals. |
| b) Melting | $\Delta E_{tr} \sim T_{tr}\Delta S_{tr}$ | Rapid kinetics but not easily observed. |
| III. Electronic<br>(e.g., Spin change or band-gap closure/electronic excitation) | $\Delta E_{tr} \sim -P_{tr}\Delta V_{tr} + \Delta E_{electroni}$ | Electronic transitions occur on ps. time scales, but can be kinetically limited due to strains associated with transition: viscous relaxation may be required for transition to go to take place. |




Courtesy: Jeanloz

Gleason *et al.*, 2015

# Highlights from recent experiments

*Crust*

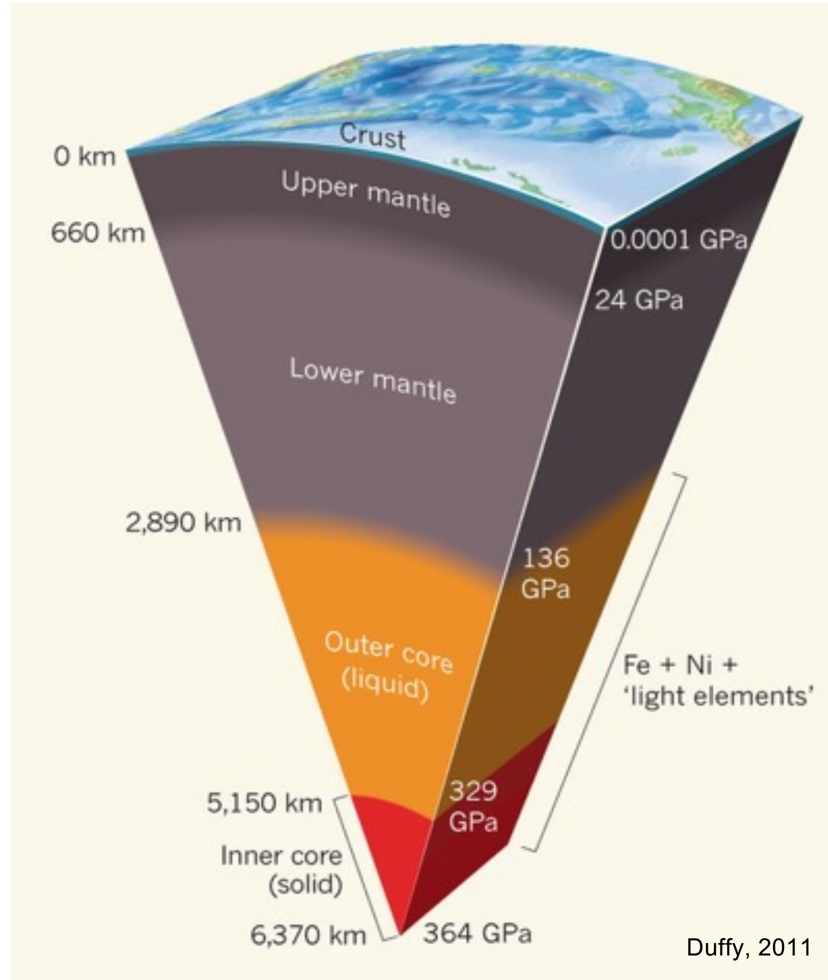
- Crystallization/amorphization kinetics in $SiO_2$

*Mantle*

- Dynamics of spin transitions in Fe-bearing silicates

*Core*

- Texture and deformation mechanisms of iron



Duffy, 2011

# Highlights from recent experiments

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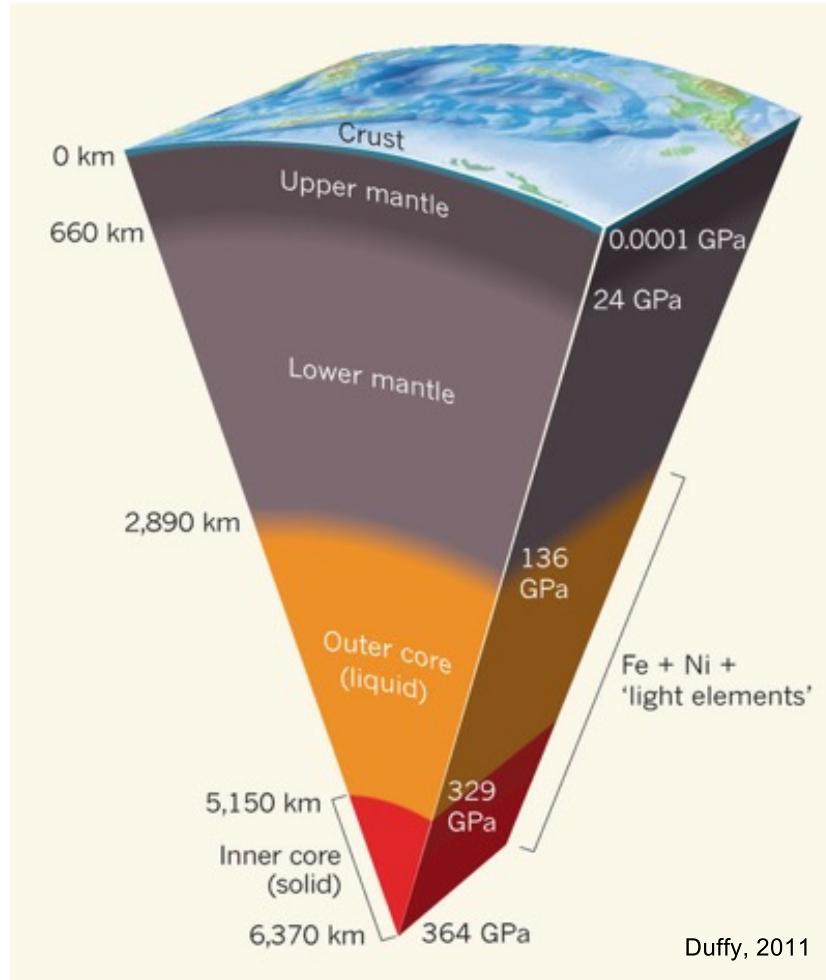
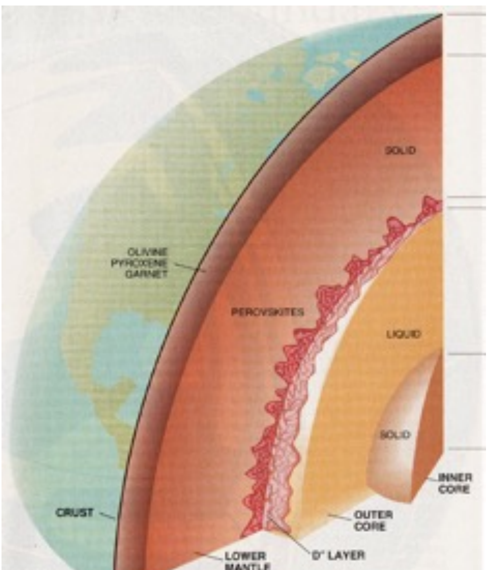
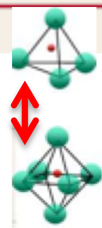


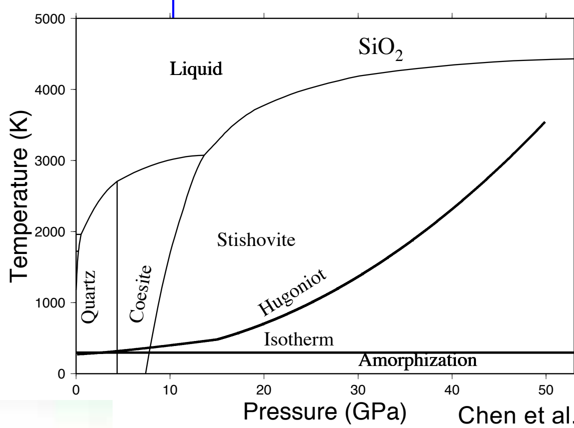

Duffy, 2011

# Dynamics of Transitions in $SiO_2$




Wadsworth Publishing Co., 1998






Chen et al., 1999

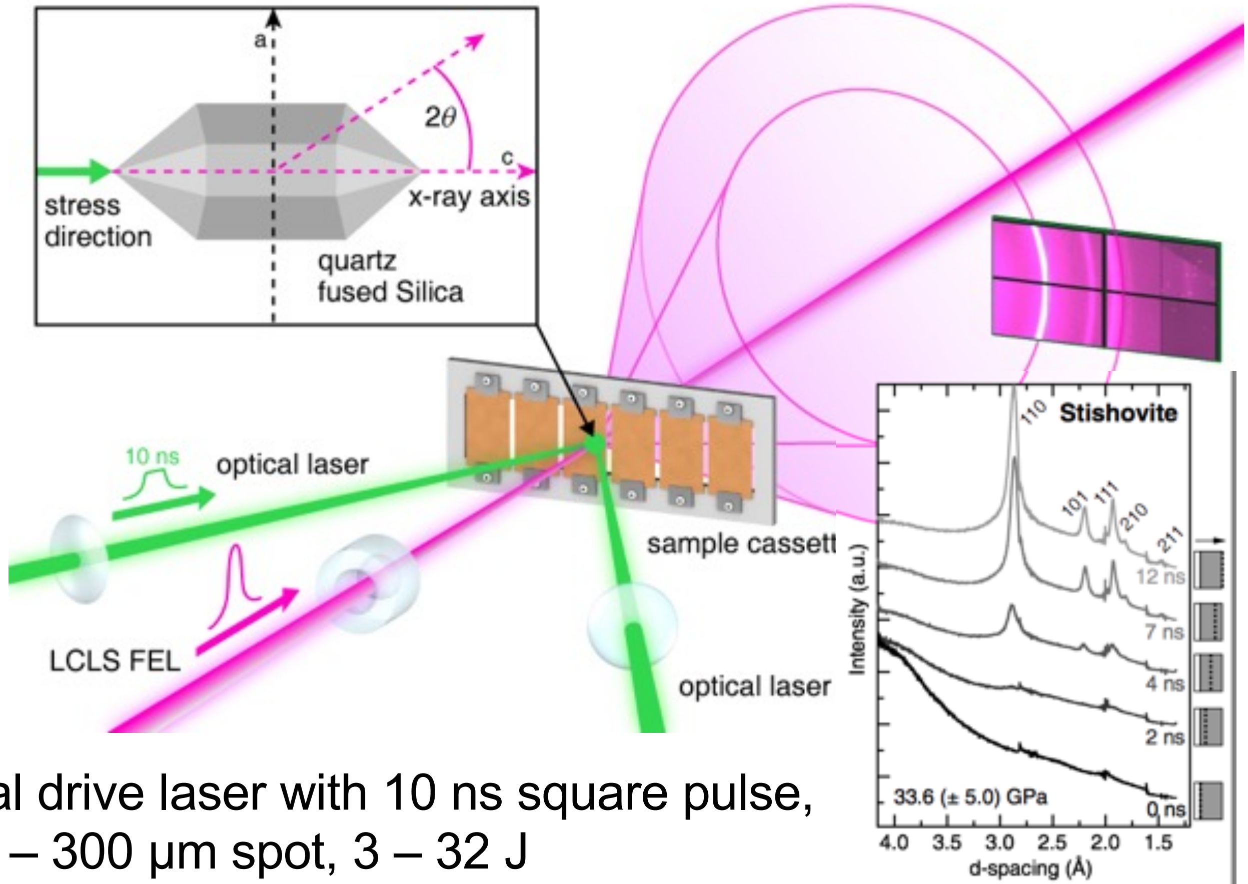
## Phase transition kinetics to stishovite

- Microstructure
- Nucleation
- Grain size
- Grain growth rate
- Transformation mechanism


## Mineralogy of impact craters & shock metamorphism

- Behavior of α-quartz
- Diaplectic glass formation vs. high pressure crystalline polymorphs

# Pump-probe diagnostics

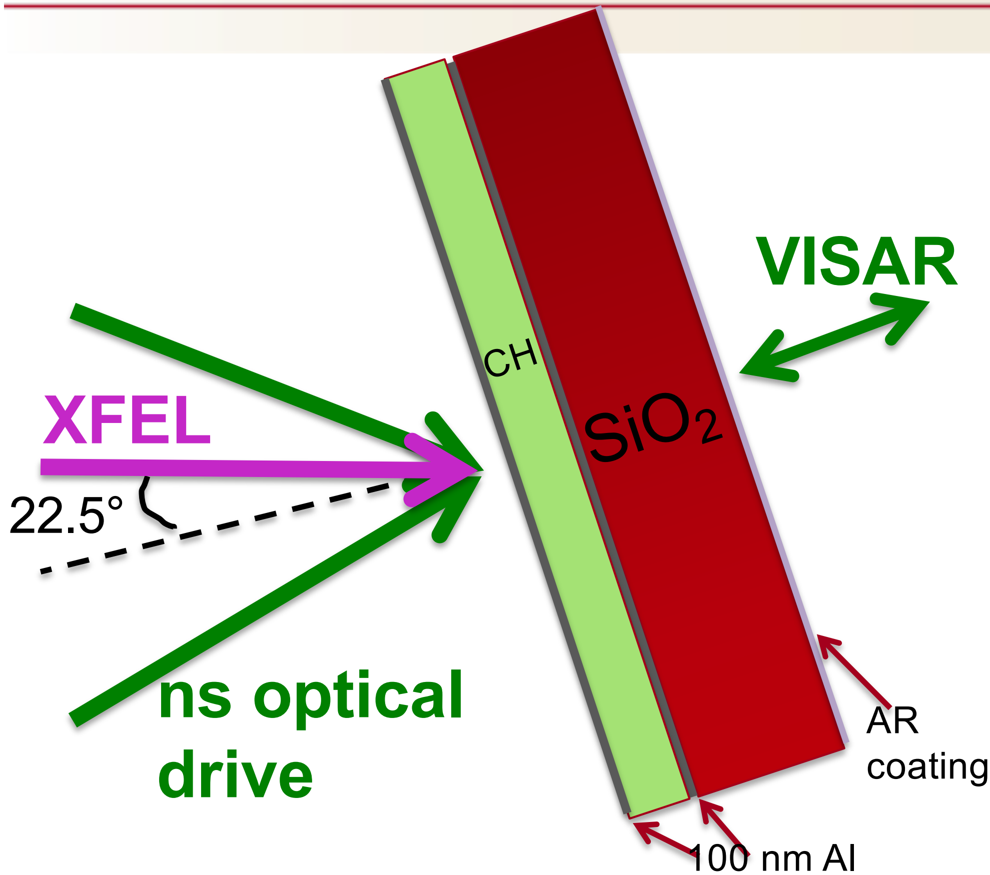



**Pump**: optical drive laser with 10 ns square pulse,
200 – 300 μm spot, 3 – 32 J

**Probe**: -LCLS XFEL with 60 fs pulse, 8 keV
-50 μm spot
-VISAR

Gleason *et al.*, 2015

# Targets

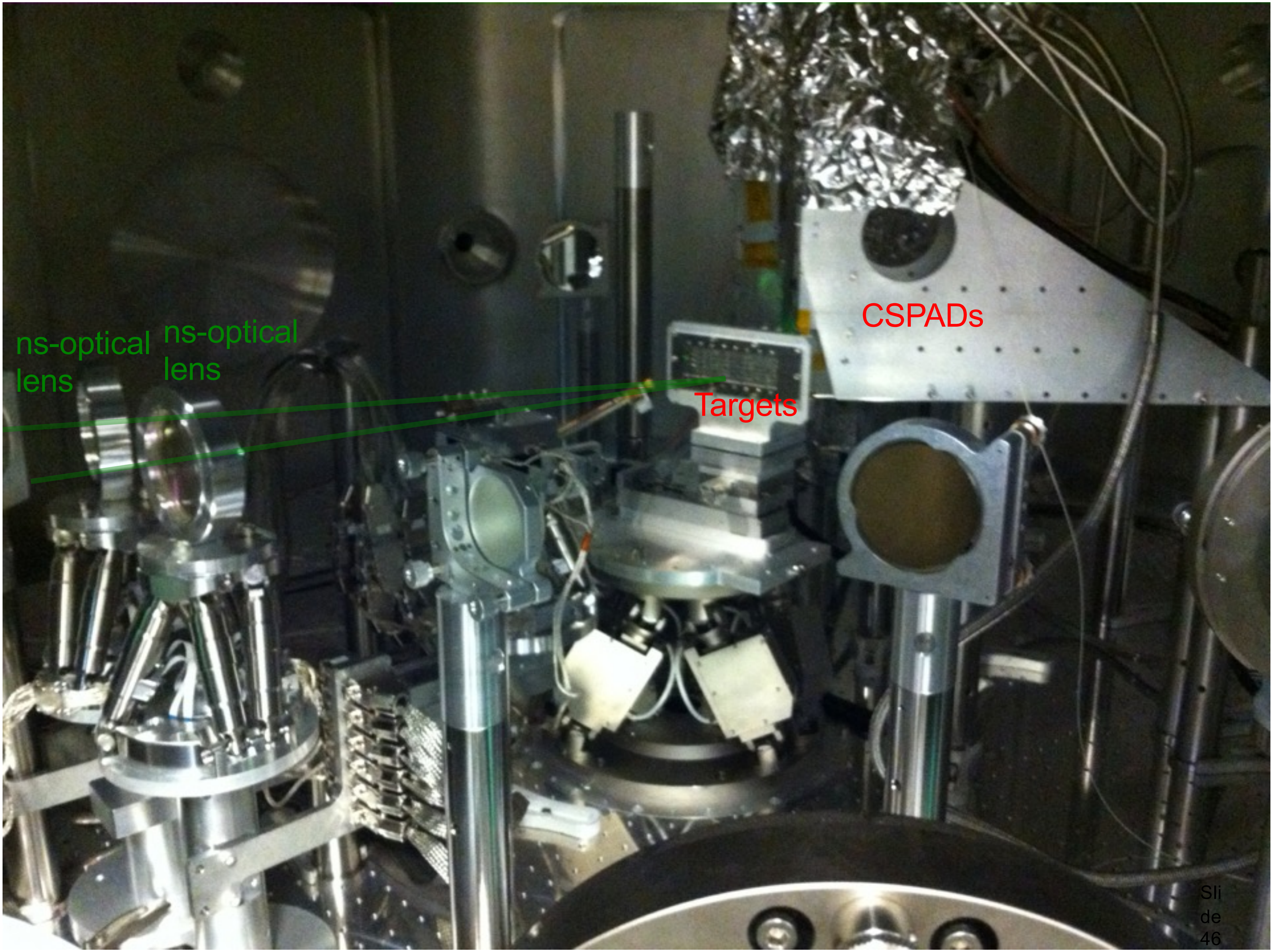


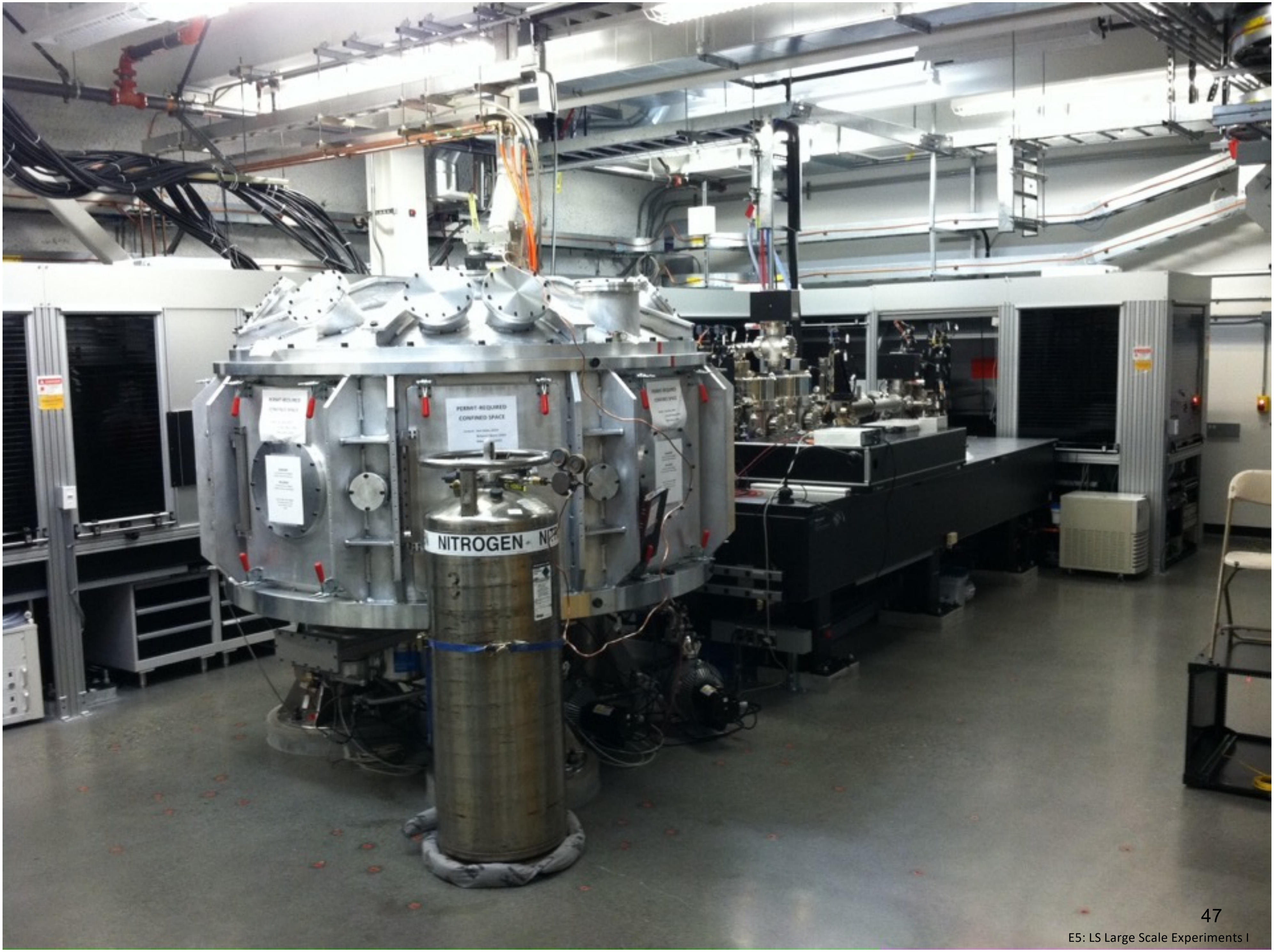


**X-ray window (ablator):**
- parylene (10 µm)

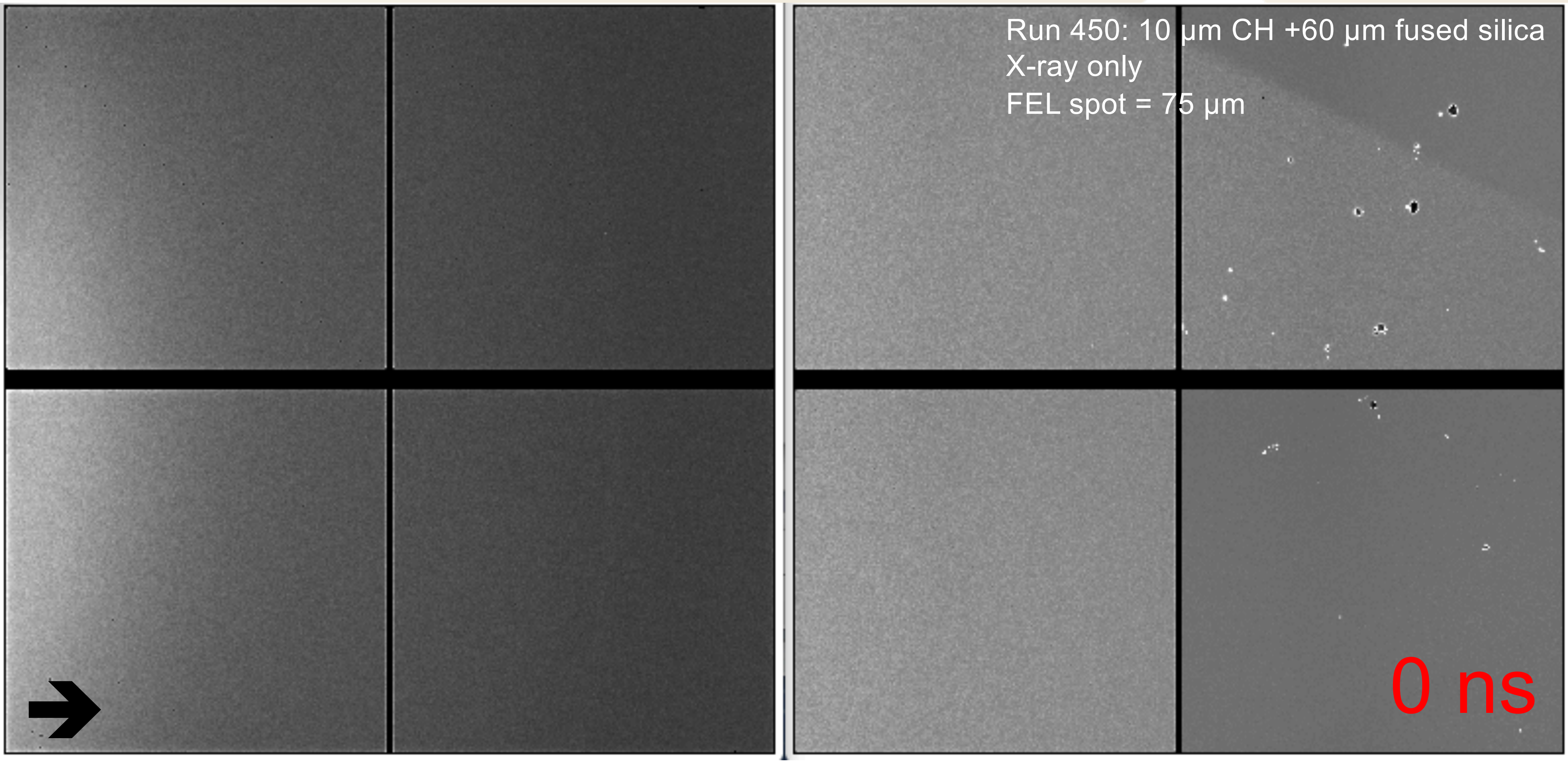
**$SiO_2$, 60 µm:**
-fused silica (amorphous)
-single-crystal *c*-cut quartz

*Ablator layer on a target is used to smooth out any hot spots in the drive laser and ensure more homogeneous ablation and uniform shock.*


ns-optical lens
ns-optical lens
Targets
CSPADs

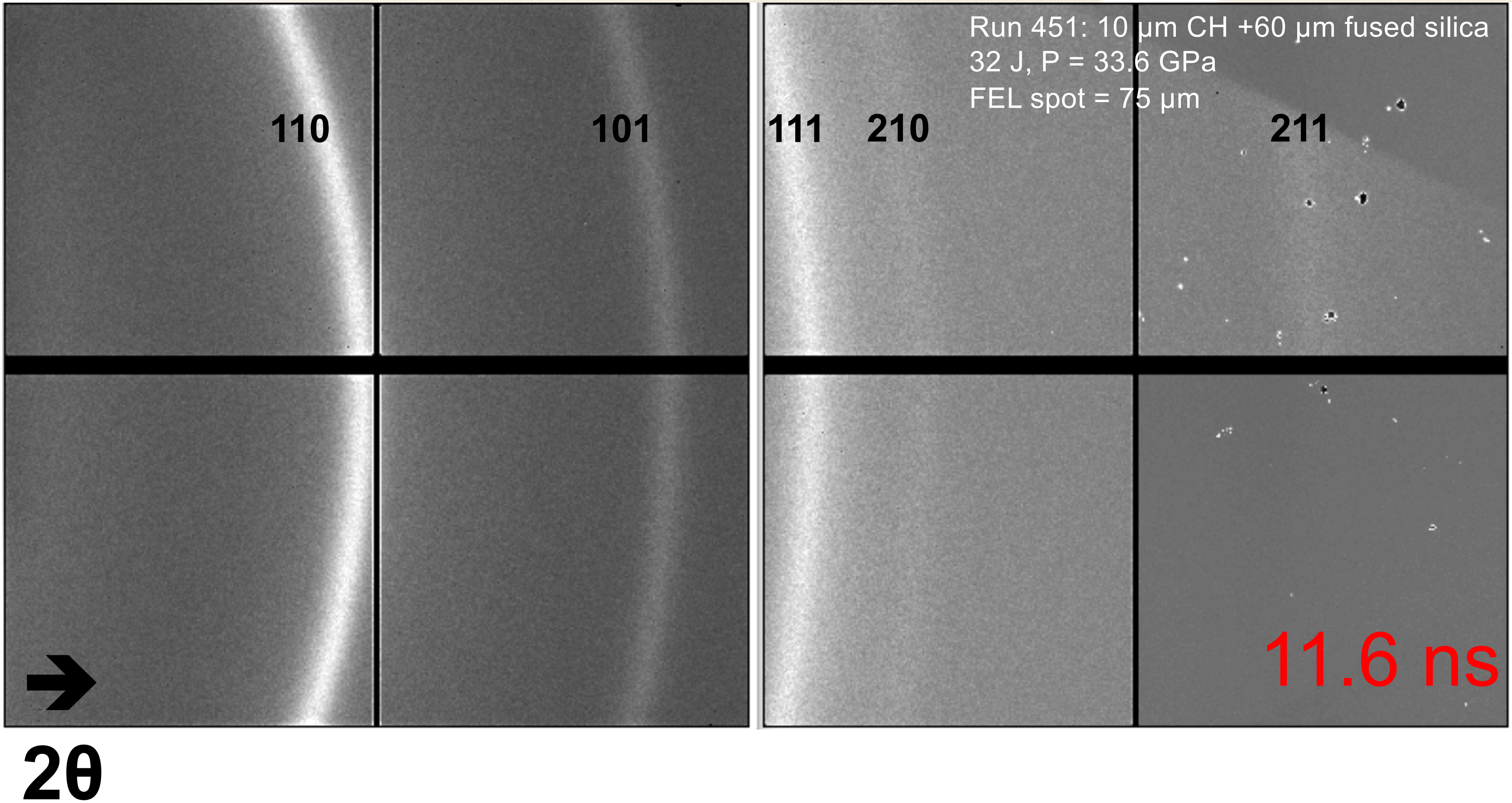

PERMIT-REQUIRED
CONFINED SPACE
NITROGEN

# Fused silica to stishovite

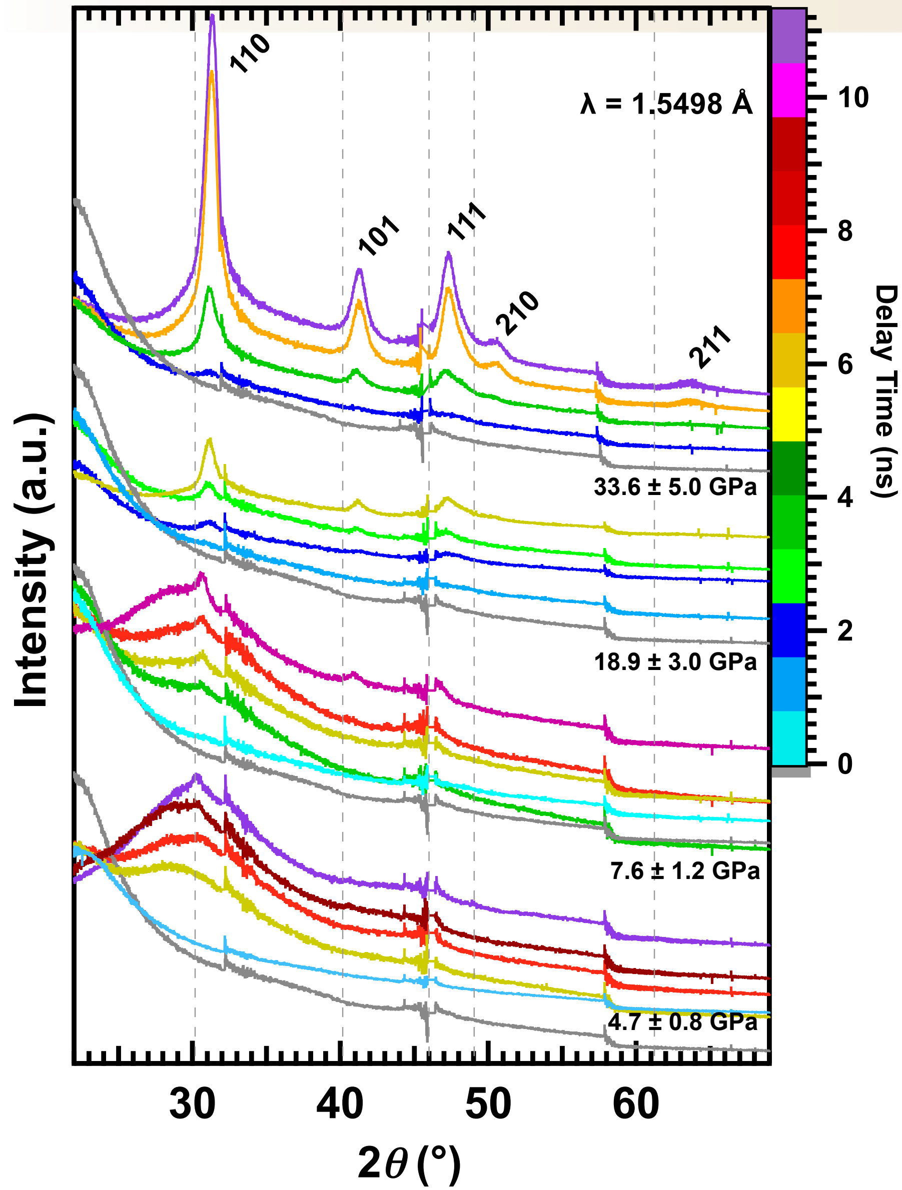



2θ

# Fused silica to stishovite



# Fused silica to stishovite: on compression




-randomly oriented grains
(Andrault *et al*., 2003)

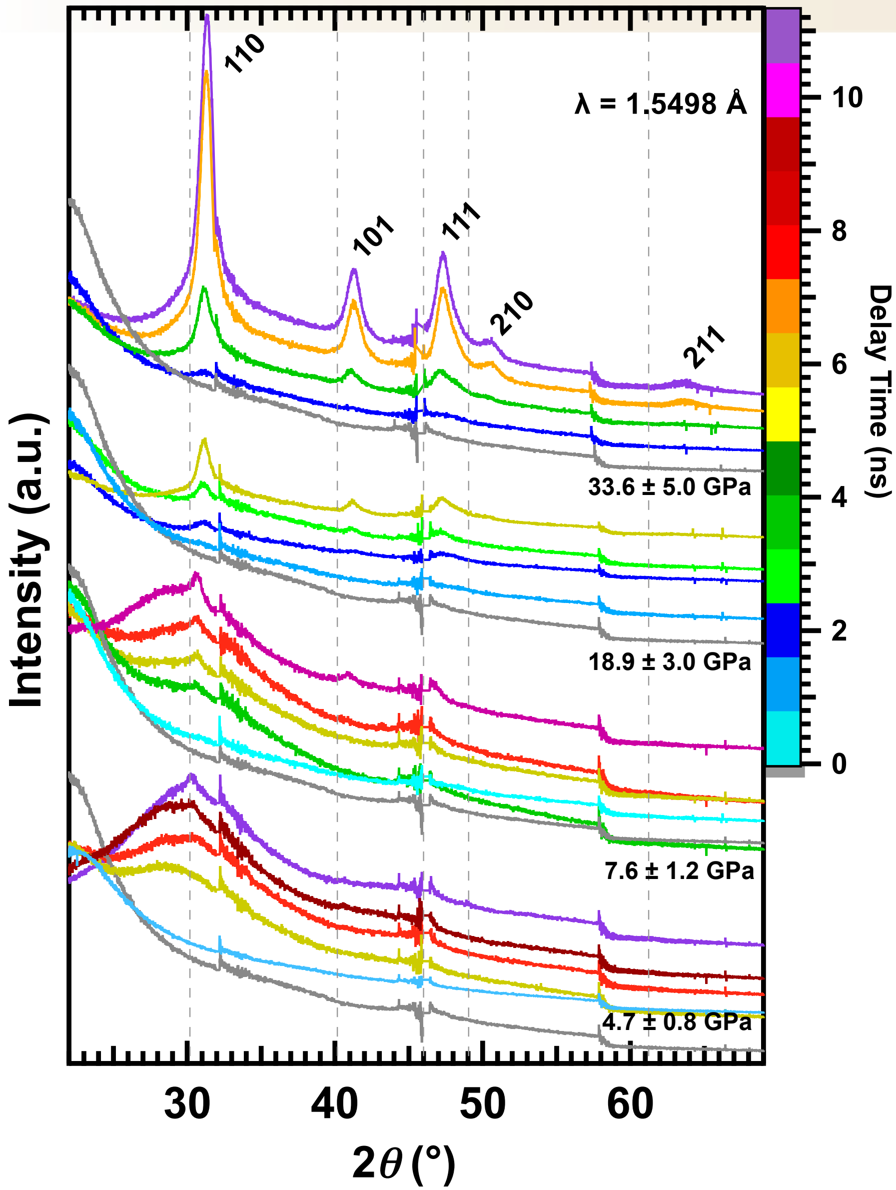
-fine-grain size

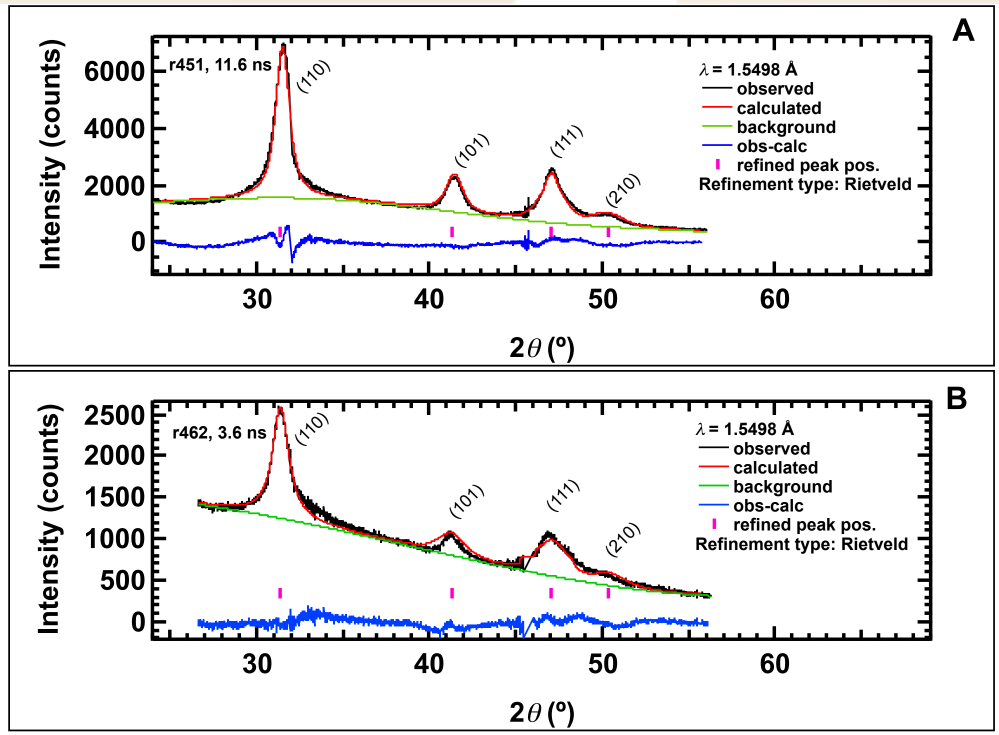
-compressed amorphous + crystalline

-crystallinity develops at later times

Gleason *et al*., 2015

# Fused silica to stishovite: on compression



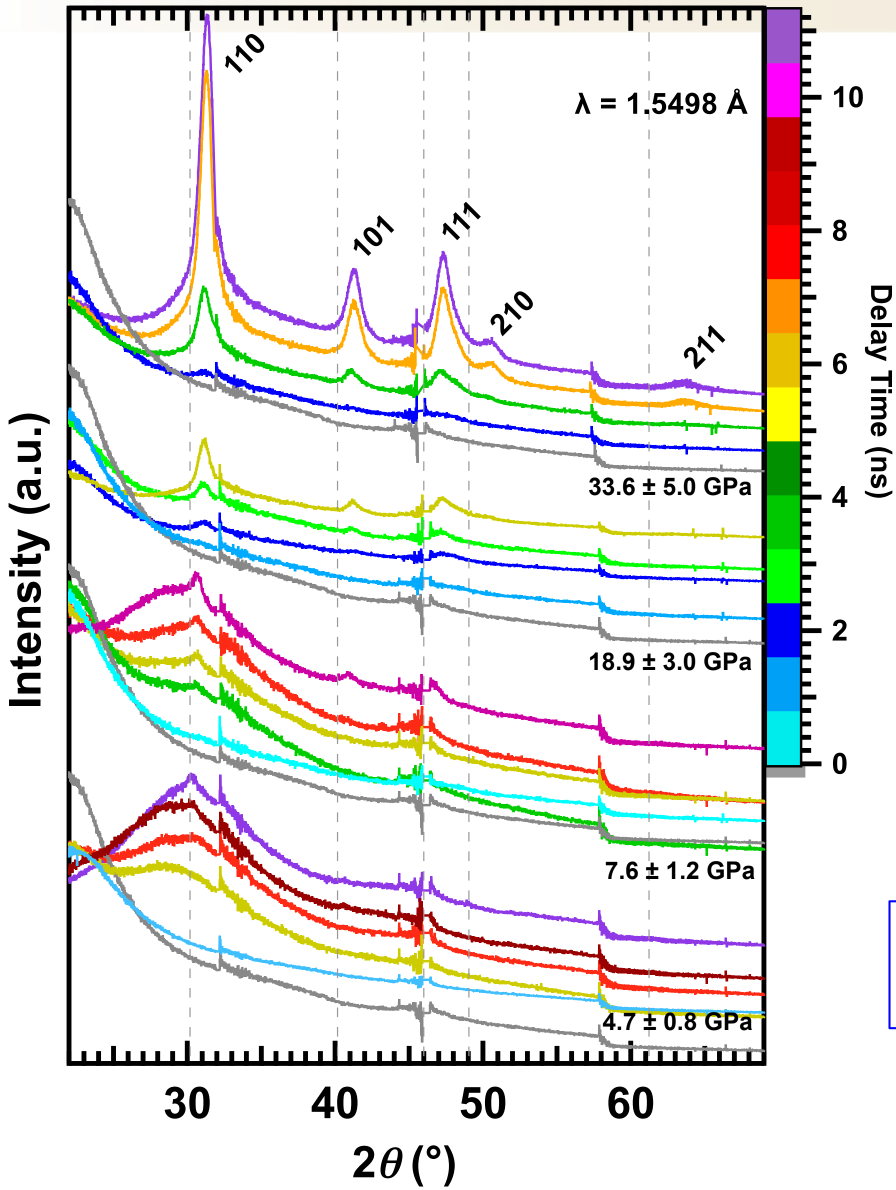



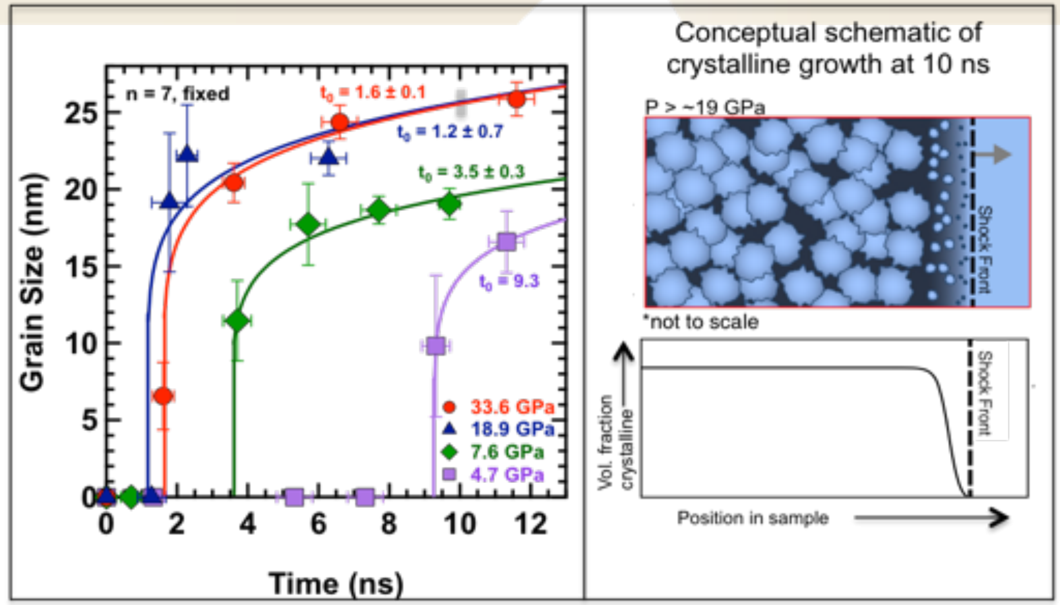

Rietveld refinement

-General Structure Analysis System (GSAS) Larson & VonDreele, 1994

Gleason *et al.*, 2015

# Fused silica to stishovite: on compression




$$D = k(t-t_0)^{1/n}$$

Huang *et al.*, 2003;
Zheng *et al.*, 2009

$D$ = particle size
$k$ = temperature-dependent material constant appropriate to exponent $n$
$t_0$ = nucleation time

n > 4 coalescence events rather than diffusion-related growth

Gleason *et al.*, 2015

# Question 6

True or false: Time-resolved X-ray diffraction peak widths are sensitive to both grains size change and strain.

a. True

b. False

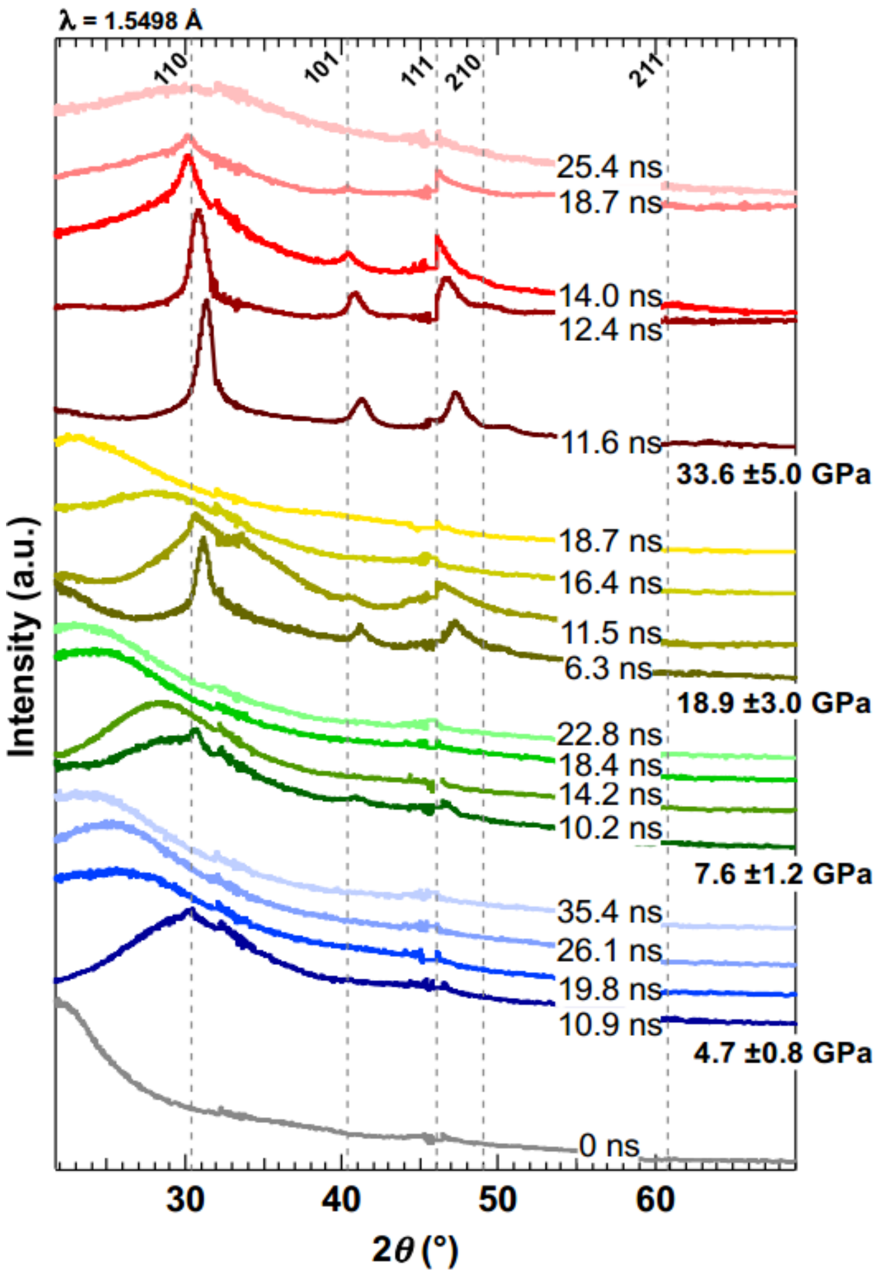
# Question 6

True or false: Time-resolved X-ray diffraction peak widths are sensitive to both grains size change and strain.

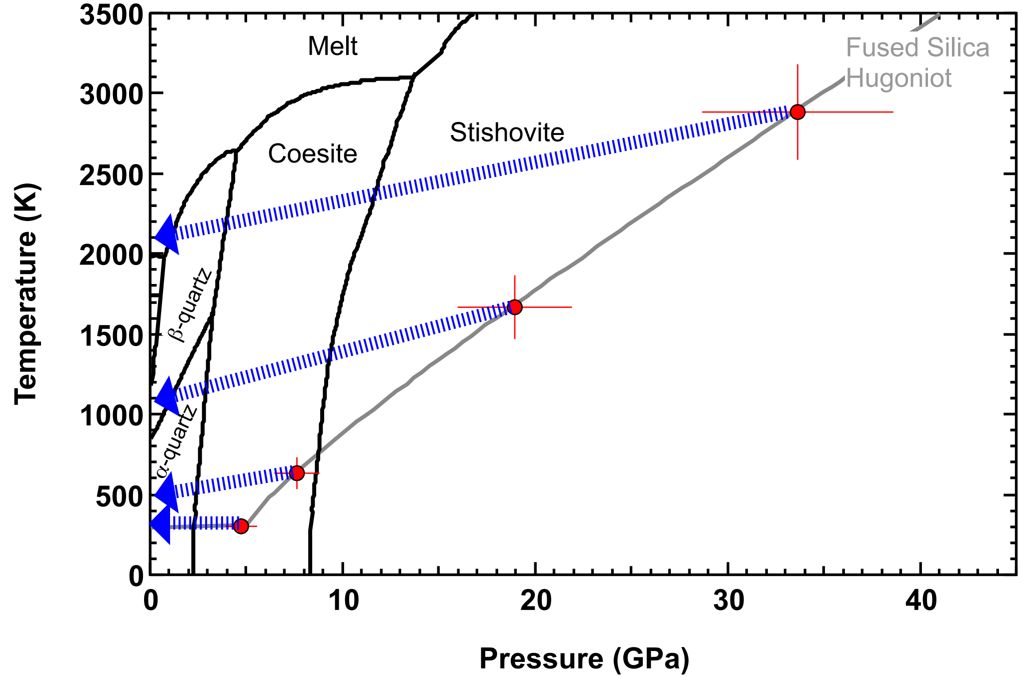
a. True

b. False

# Fused silica to stishovite: on release



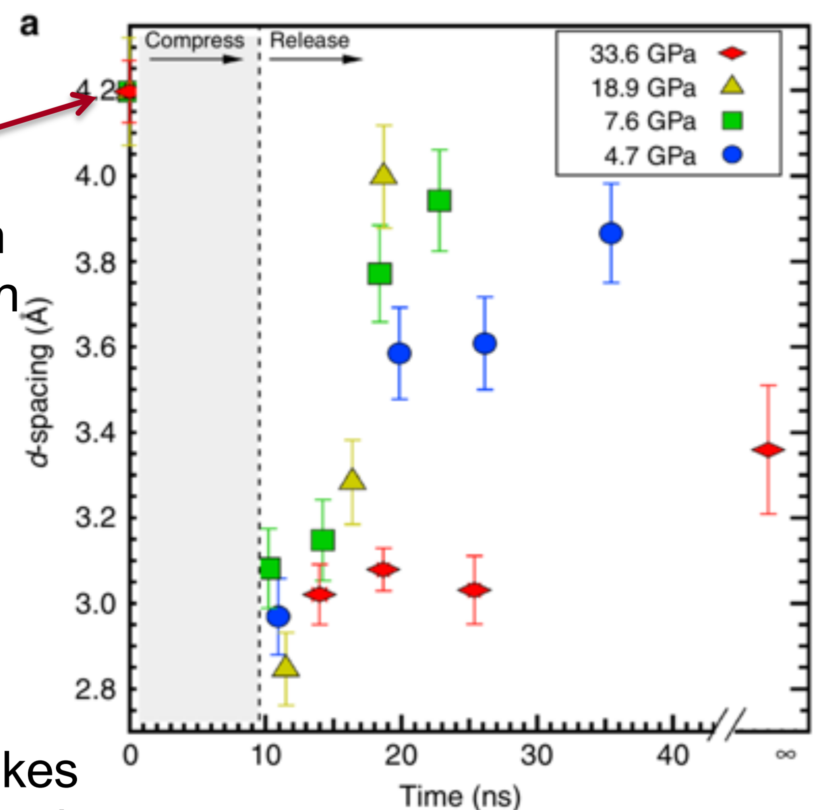

**Amorphization on release !!!**




Gleason *et al.*, 2017

# Fused silica to stishovite: on release

Ambient condition
4-fold coordination

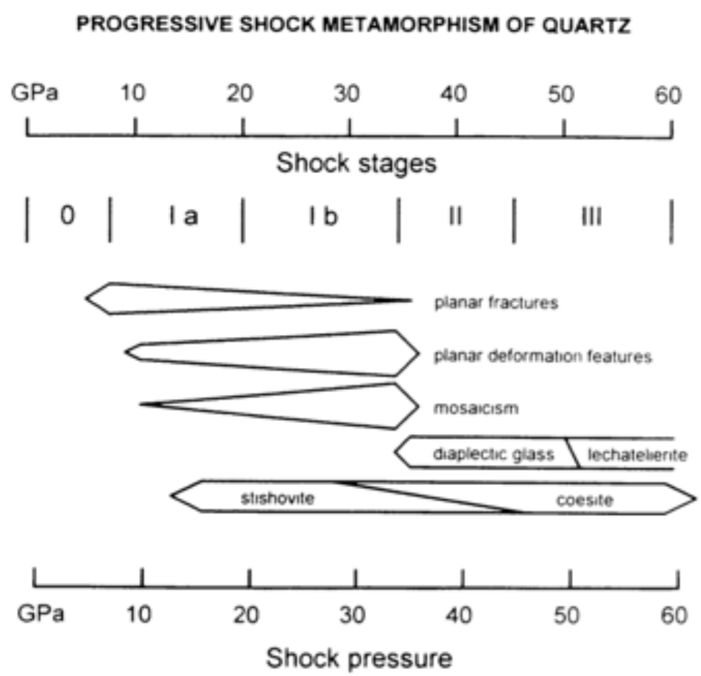



Recovered sample,
Higher order
coordination?

2 trends?
-phase reversion takes longer from lower peak pressure
-lock in a higher coordination for the highest peak pressure

Gleason *et al.*, 2017

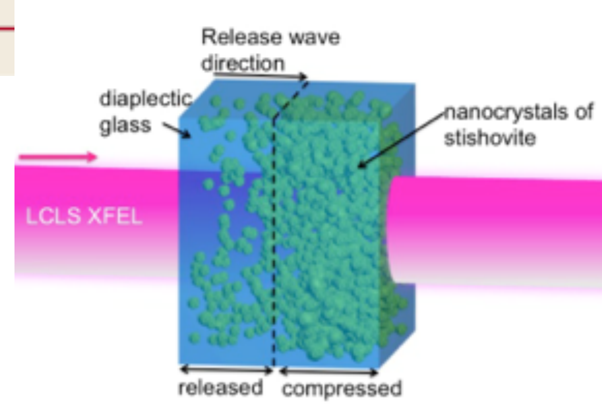
# Fused silica to stishovite: on release

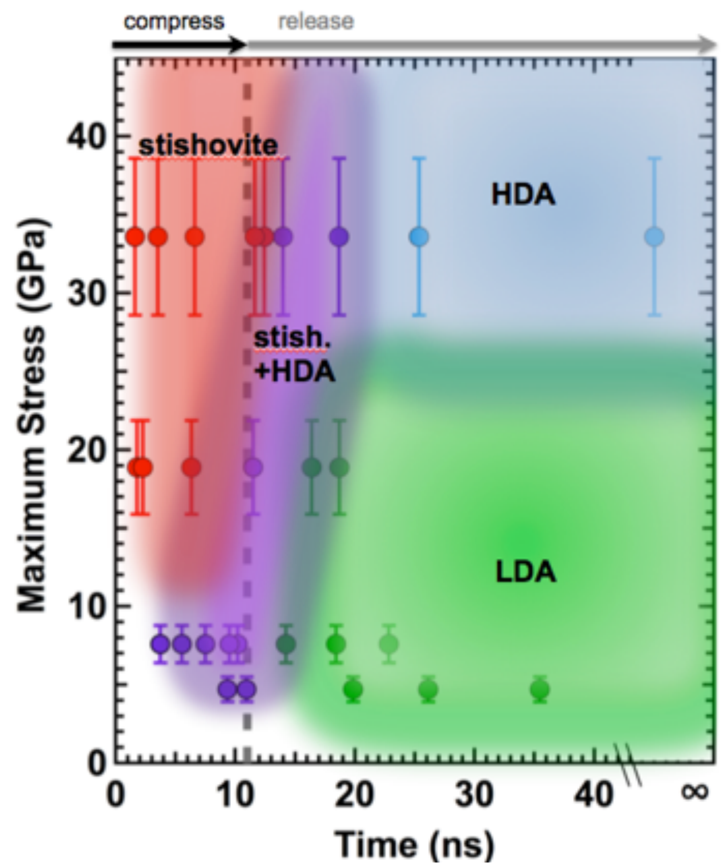



IG. 28. Pressure calibration of shock effects in quartz based on experimental ata (for references see text); shock stages after Stöffler (1971a, 1984).

Stoffler and Langenhorst, 1994

-New constraints on impact crater mineralogy and shock stages



# Highlights from recent experiments

*Crust*

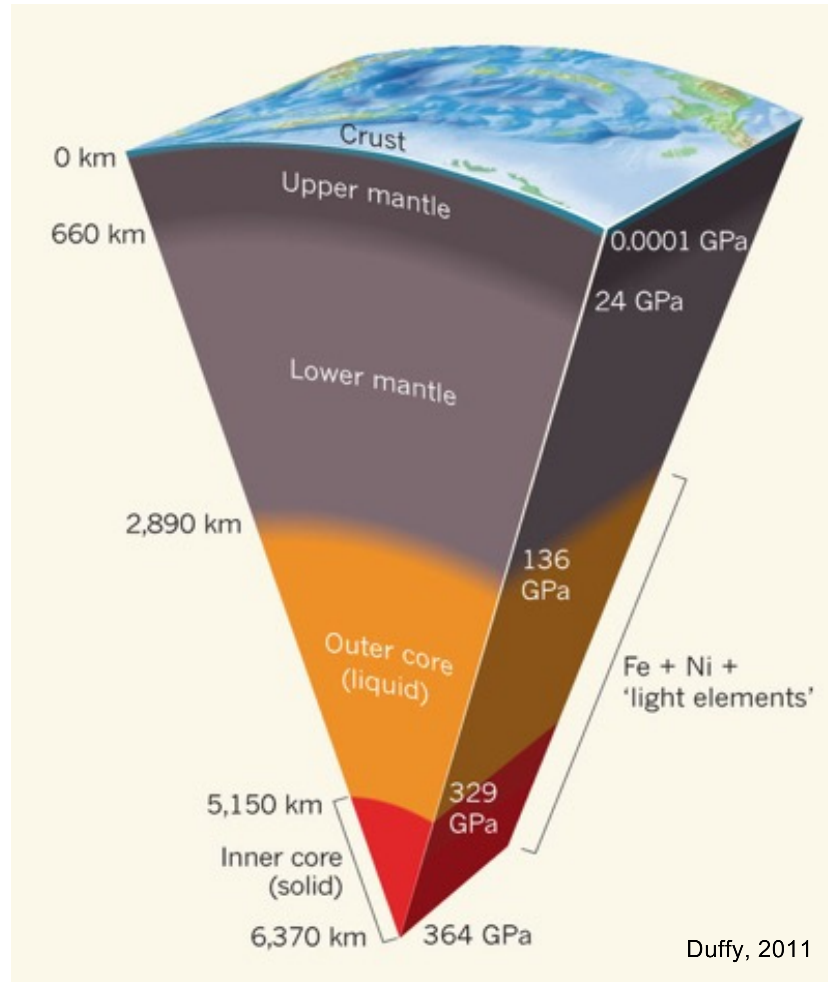
- Crystallization/amorphization kinetics in $SiO_2$

*Mantle*

- Dynamics of spin transitions in Fe-bearing silicates

*Core*

- Texture and deformation mechanisms of iron

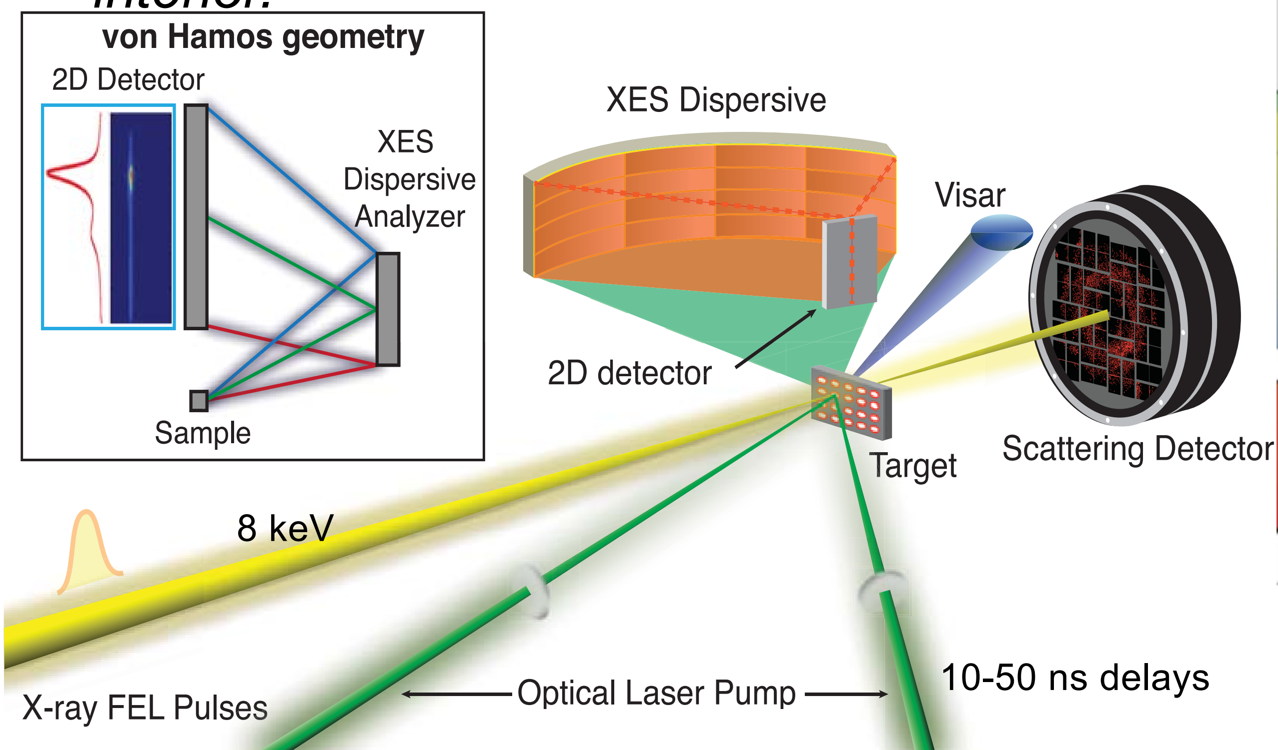



Duffy, 2011

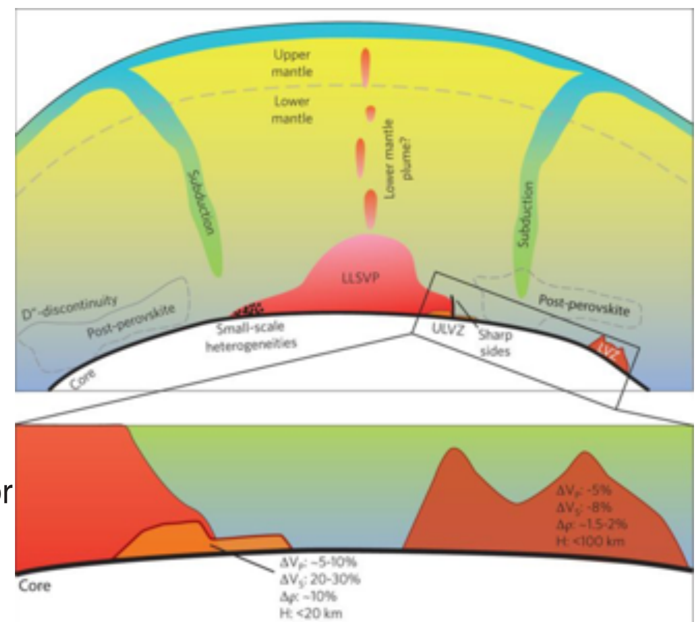
# Spin transitions in Fe-bearing silicates

PI: R. Alonso-Mori, SLAC

*Goal: Discovery experiment to determine feasibility of collecting X-ray emission spectra during laser shock compression and measure spin transitions in Fe-bearing silicates with implications for the Earth's interior.*

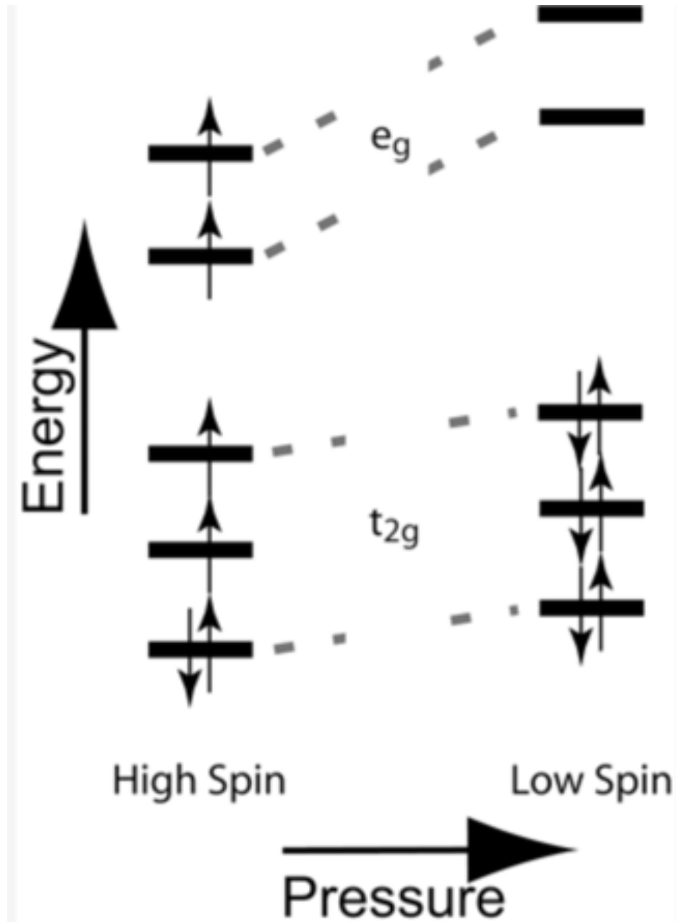



Adapted from Alonso-Mori et al., 2012




Rost, 2013

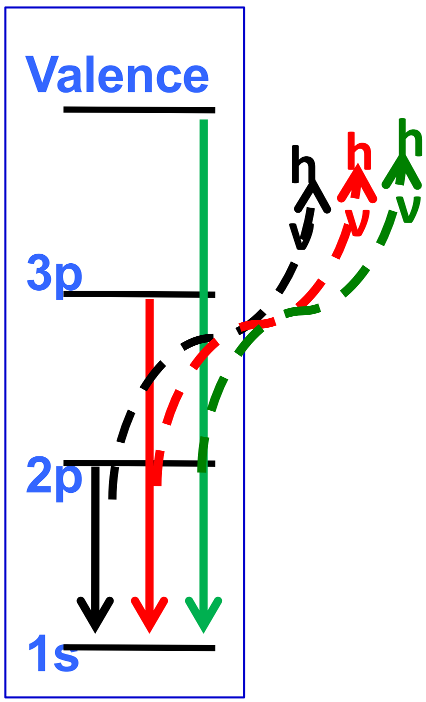
# X-ray emission spectroscopy: spin transition in iron




Speziale et al., 2005

# X-ray emission spectroscopy: spin transition in iron

SLAC

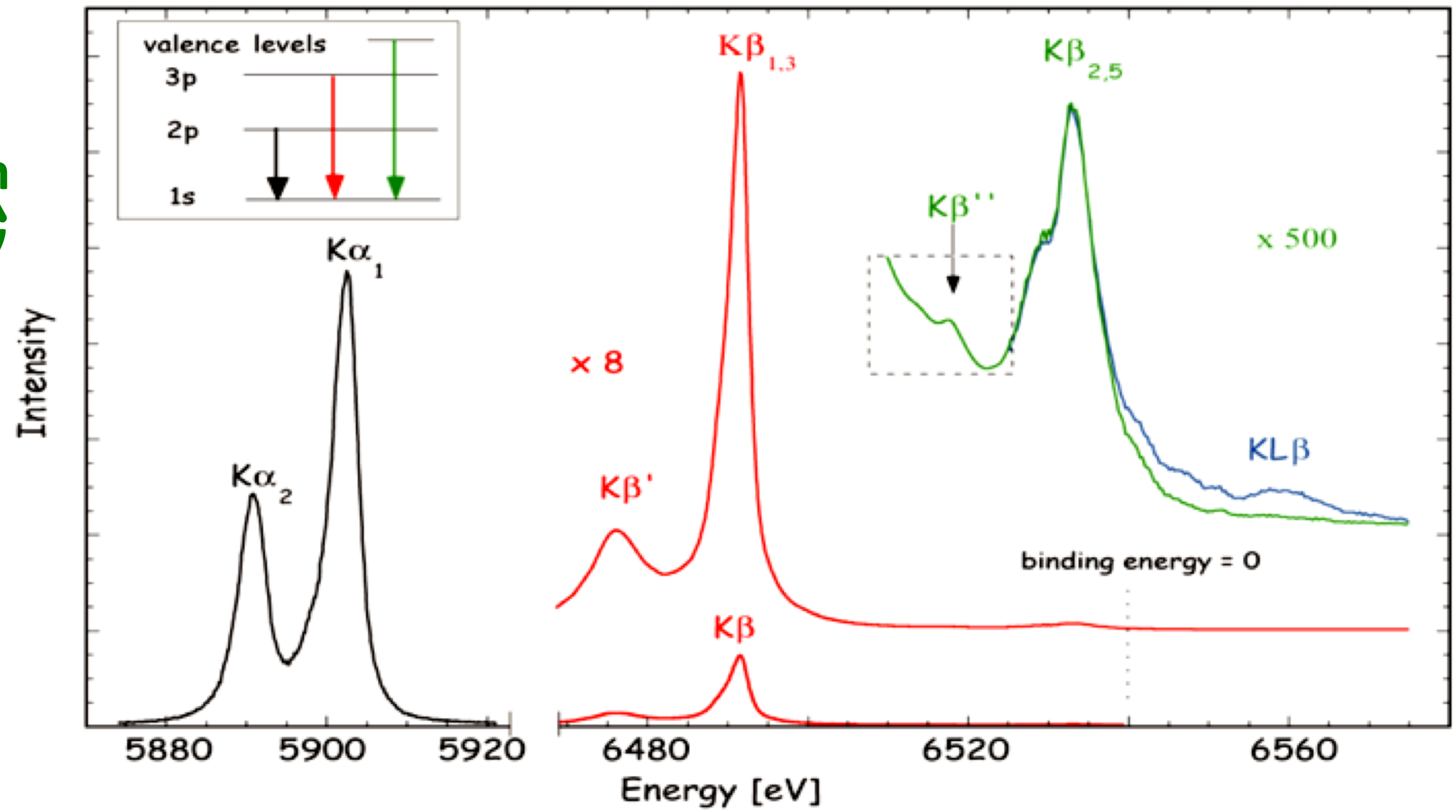



3p to 1s (Kβ)

Oxidation state

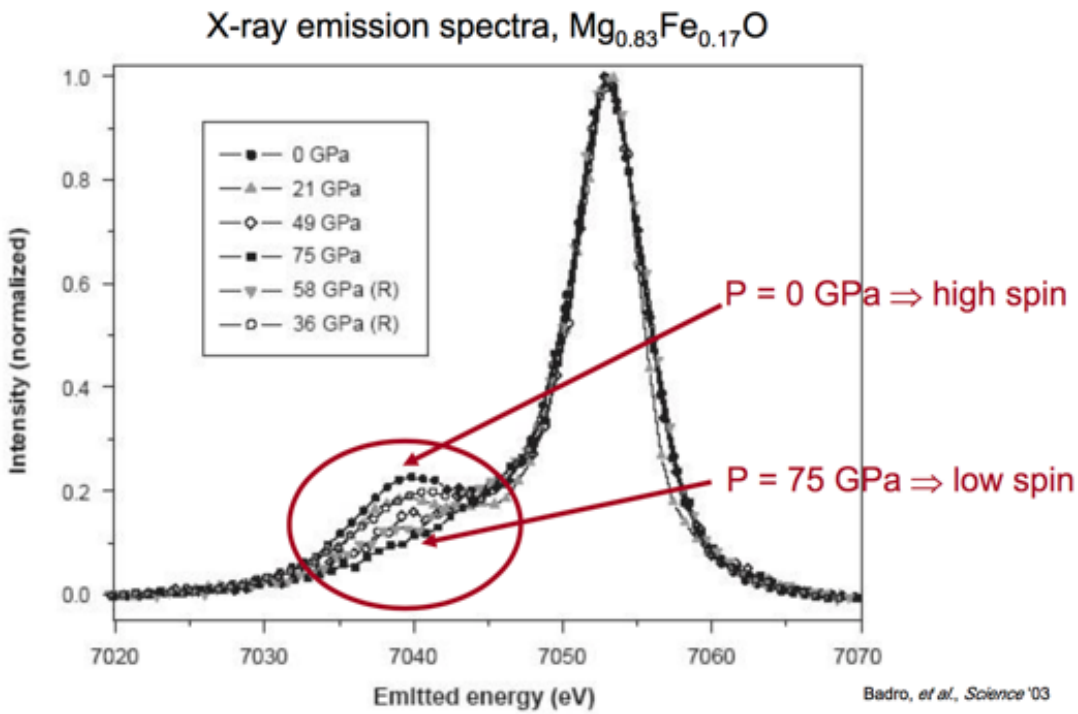
Oxidation and spin state

Chemical sensitivity

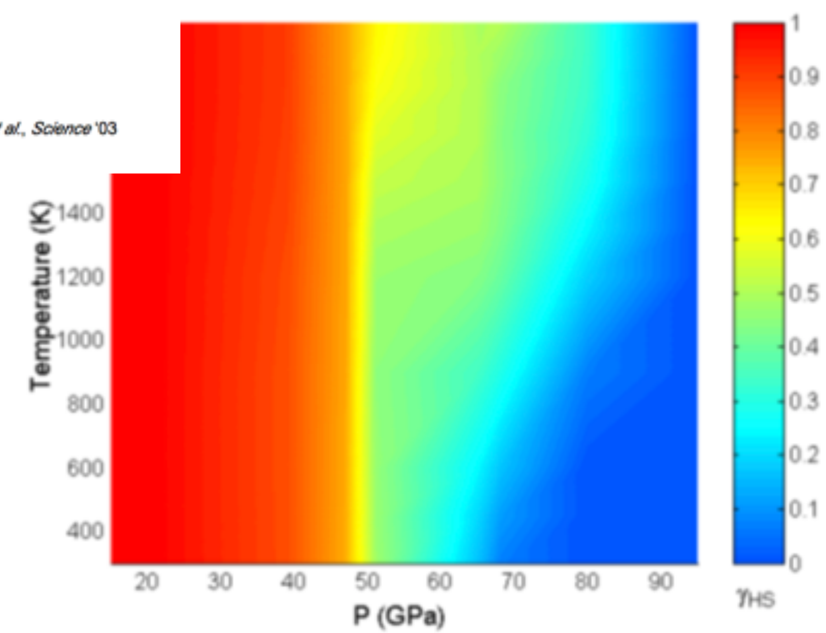



Courtesy R. Alonso-Mori

# X-ray emission spectroscopy

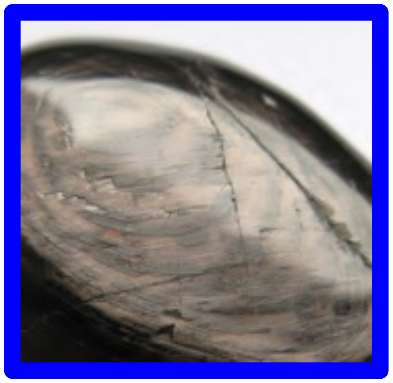


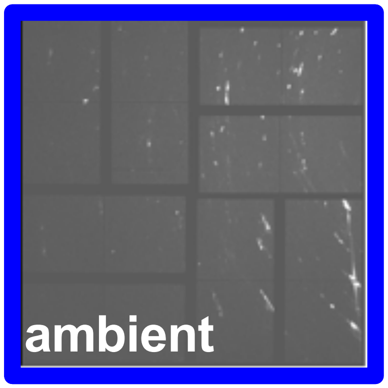

Badro, *et al.*, *Science* '03




Lin, *et al.*, *Science* TBP

# Spin transitions in Fe-bearing silicates

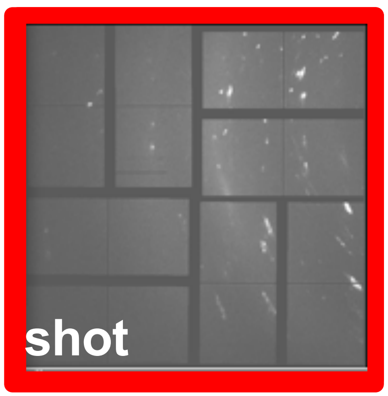


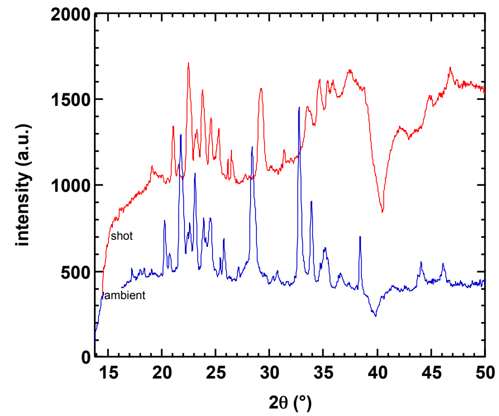



Run 314

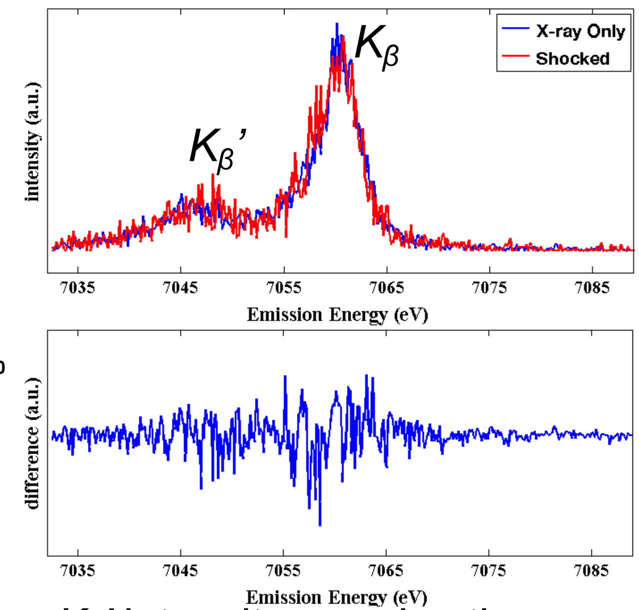
~40 GPa, 900 K

→17% compression of starting material at 10 ns delay




## Single shot spectrum




$K_\beta$' intensity remains the same →$Fe^{3+}$ stays **high spin**

# Highlights from recent experiments

*Crust*

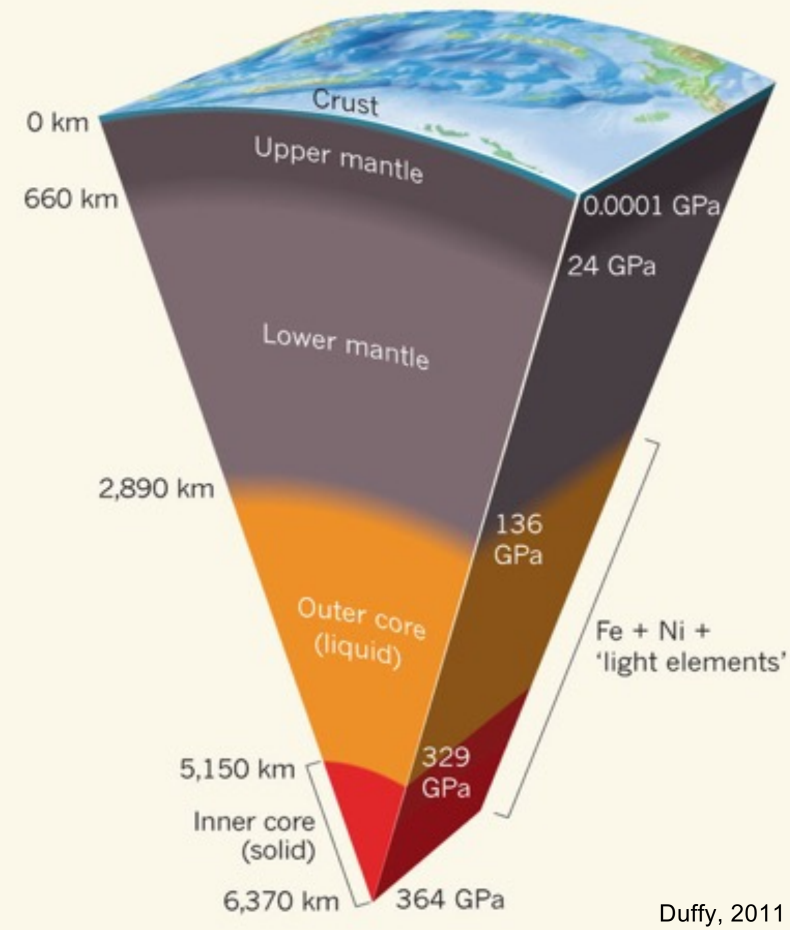
- Crystallization/amorphization kinetics in $SiO_2$

*Mantle*

- Dynamics of spin transitions in Fe-bearing silicates

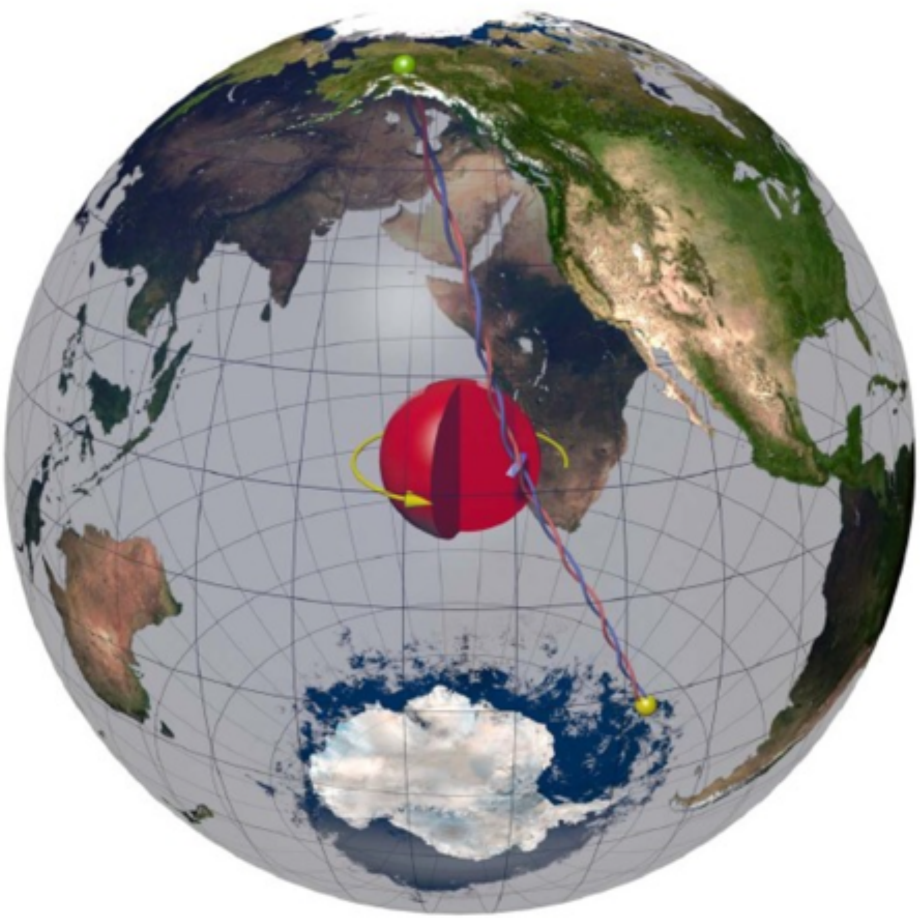
*Core*

- Texture and deformation mechanisms of iron




Duffy, 2011

# Earth's inner core

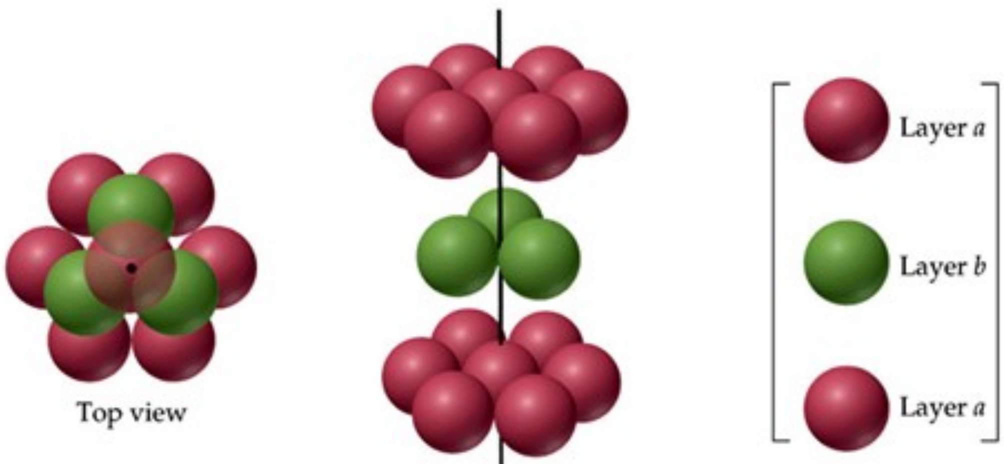


Tkalcic, 2015

- 1220 km radius
- Crystallization of Fe-alloy due to Earth's cooling
- Pressure range: 330 – 365 GPa
- Temperature: ~ 6000 K

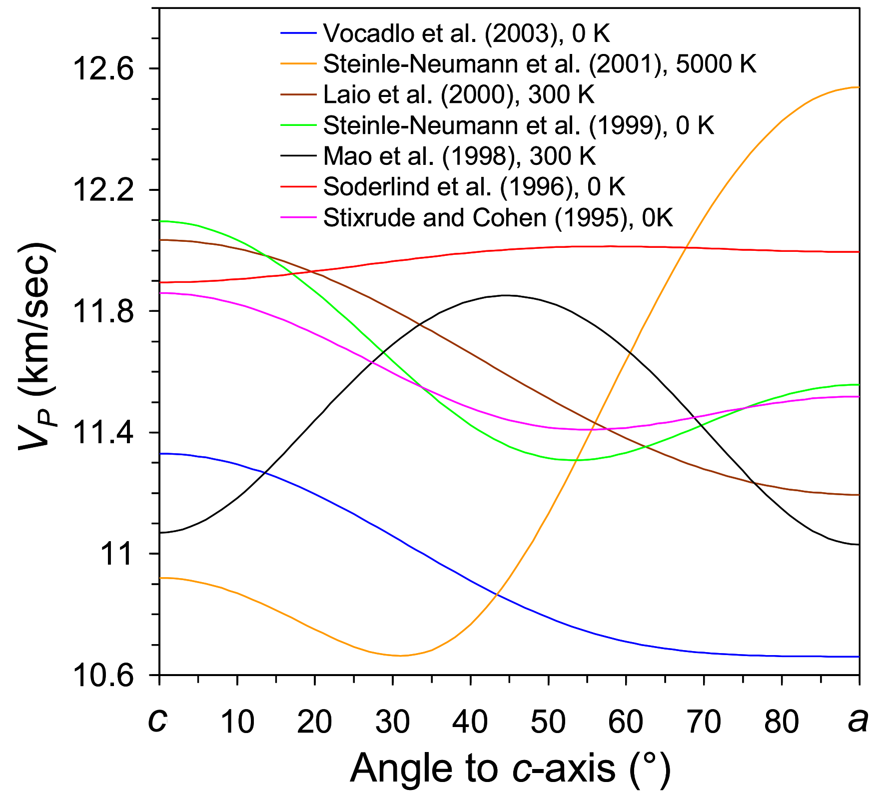
# Earth's inner core

SLAC




www4.nau.edu/meteorite/Meteorite/Book-GlossaryH.html

What mechanisms induce anisotropy in the inner core?

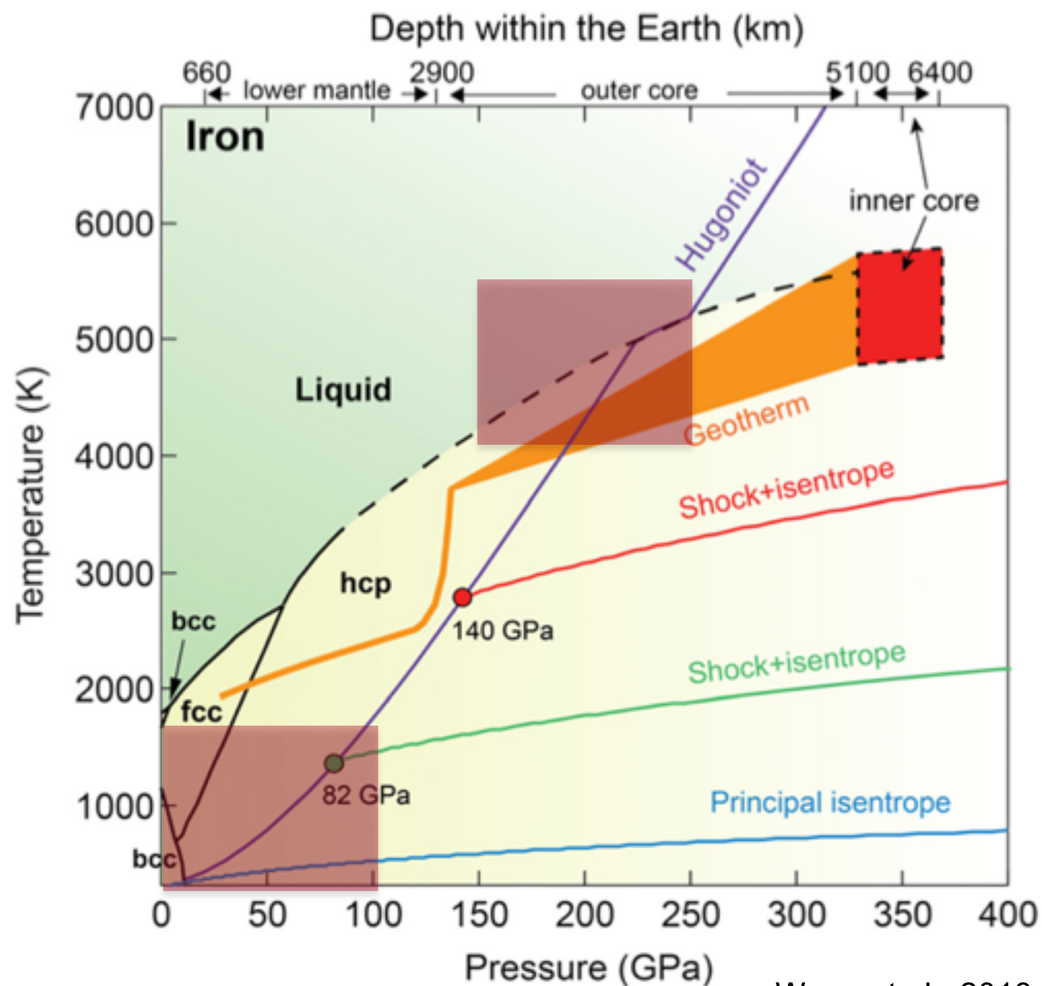



W. Mao *et al.*, 2008

# Earth's inner core

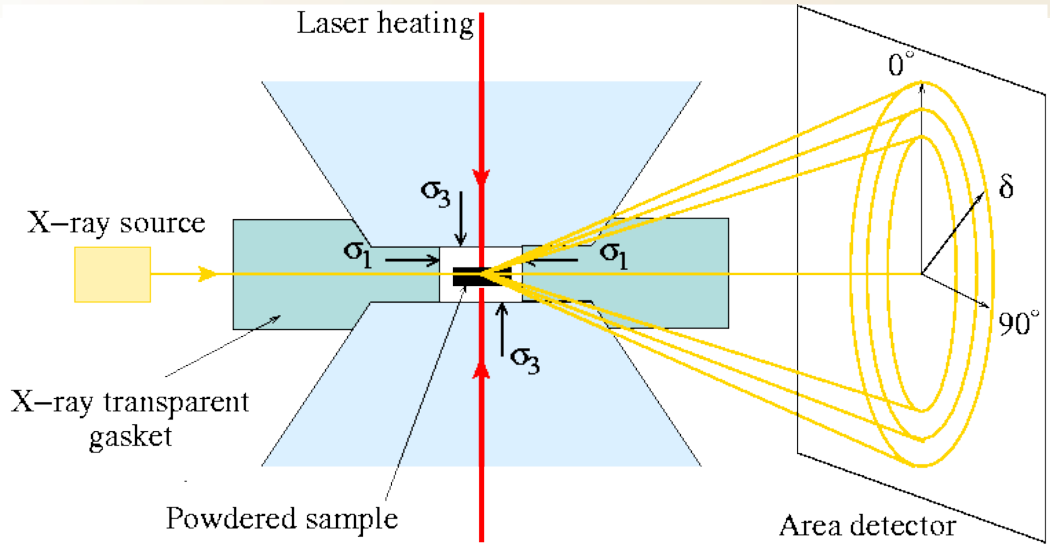
*Goal*

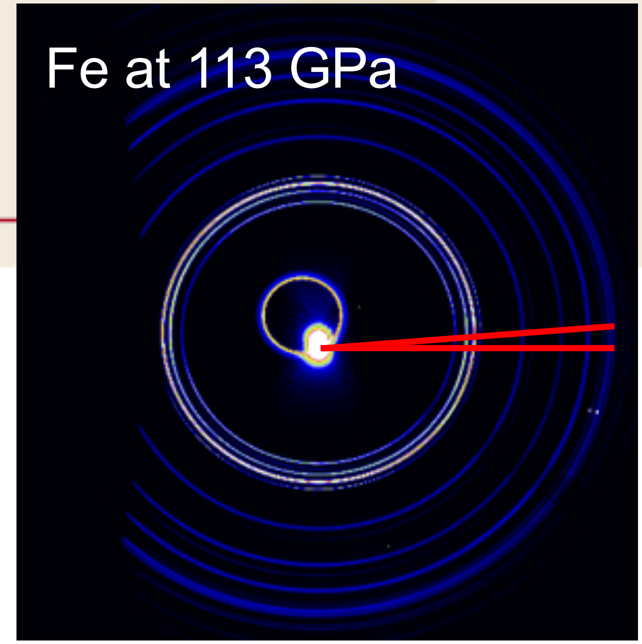
- Measure texture evolution and strength as a function of shock compression conditions.

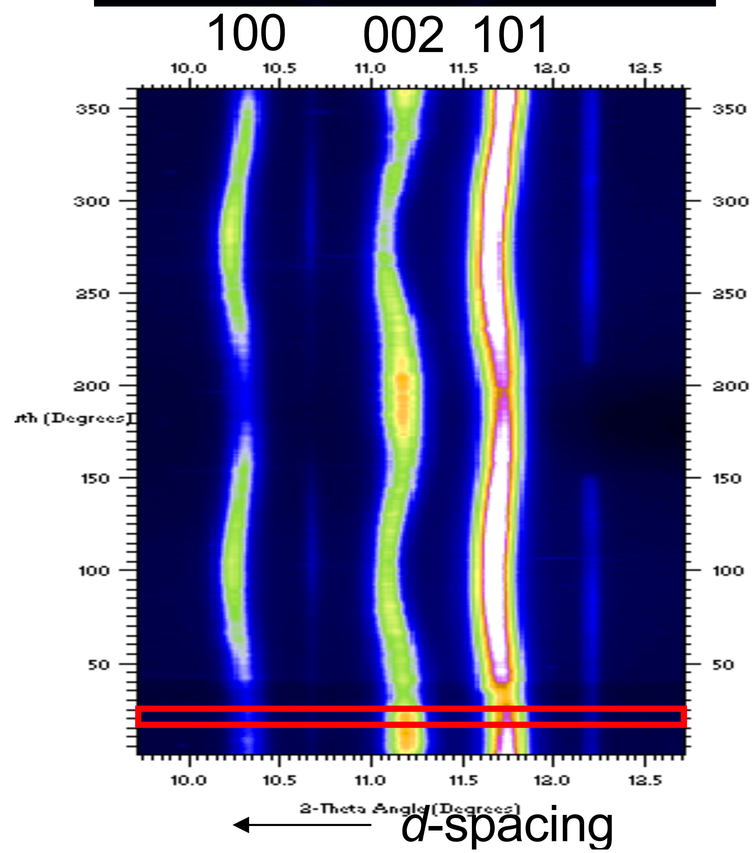



Wang et al., 2013

# Radial x-ray diffraction



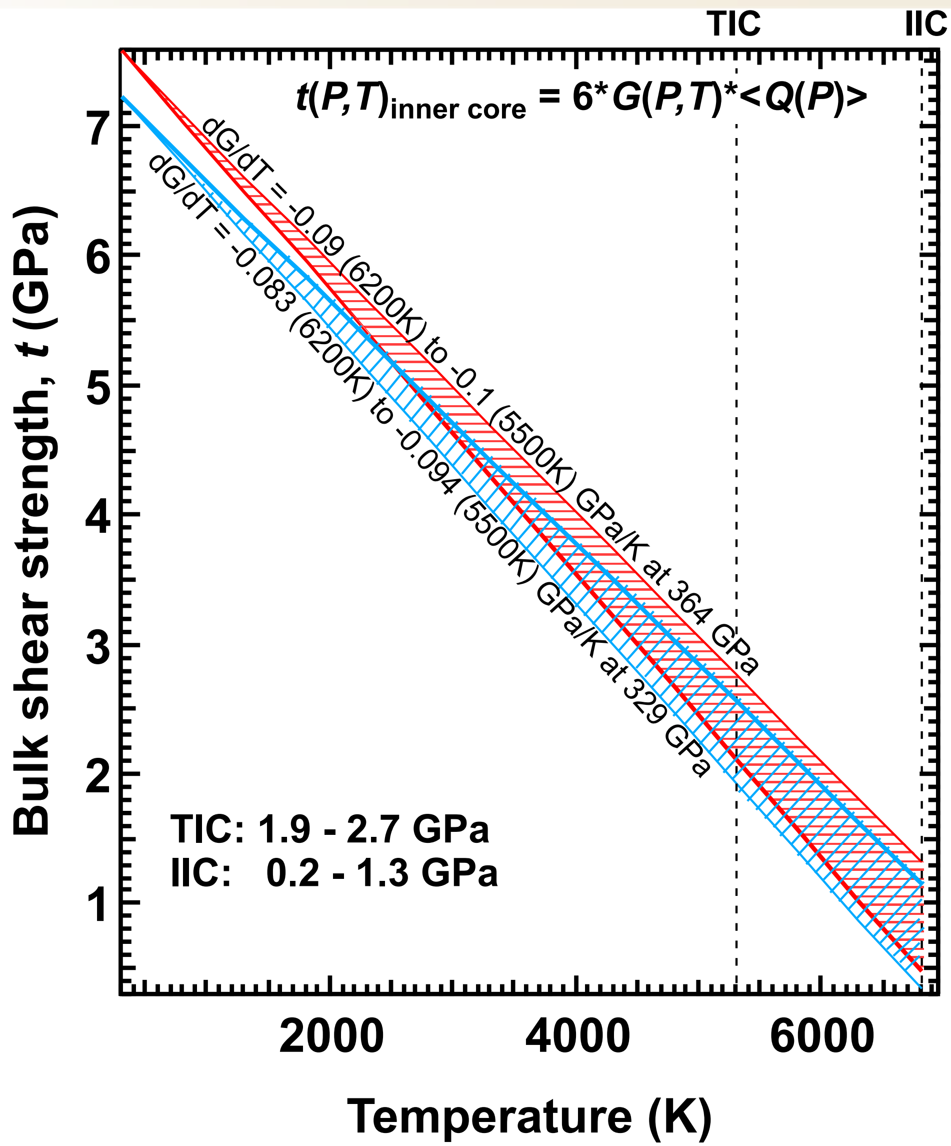



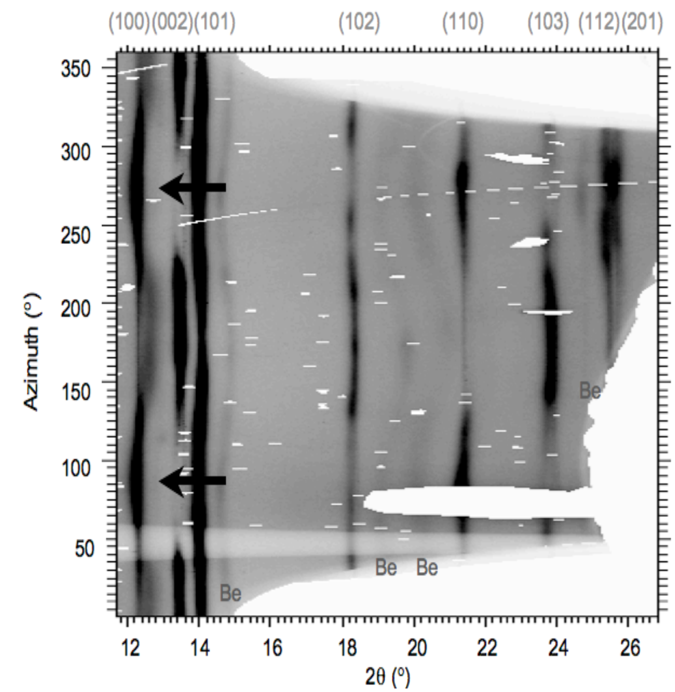

Magnitude of waviness
-- deviatoric strain & shear strength

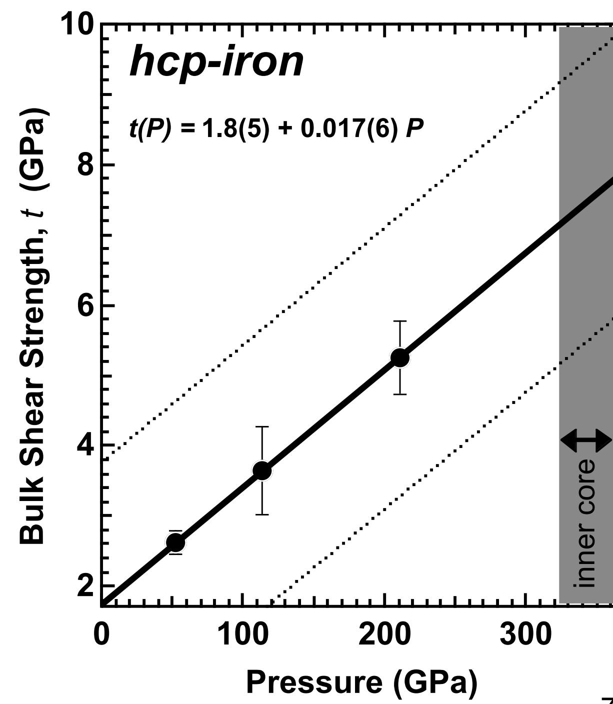
Magnitude dependence on *hkl*
-- elasticity tensor

Intensity vs. azimuthal angle
-- lattice preferred orientation

# Radial x-ray diffraction






Gleason and Mao, 2013

# Targets

SLAC

Varied:

-starting chemistry and phase

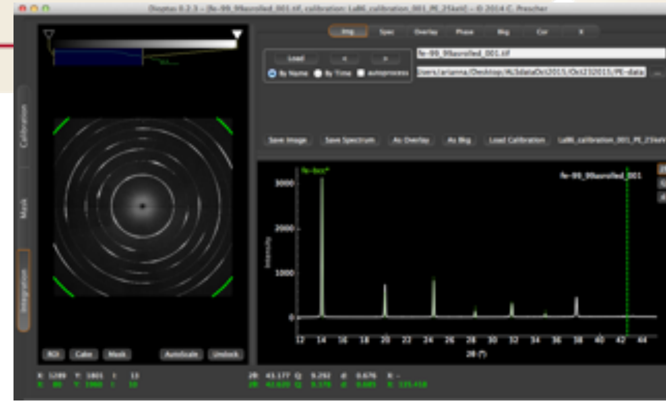
99.5%, 99.99%, steels, natural meteorites

-starting microstructure

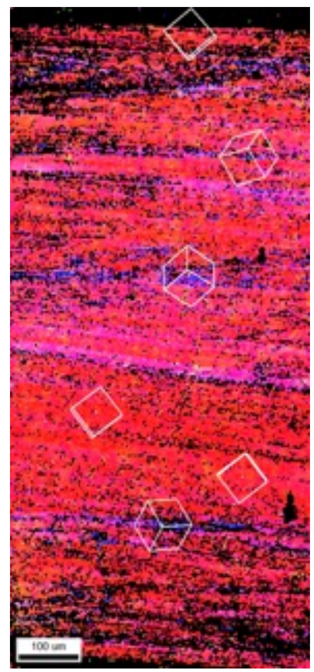
single-crystals, polycrystalline+texture, polycrystalline random orientation, grain size

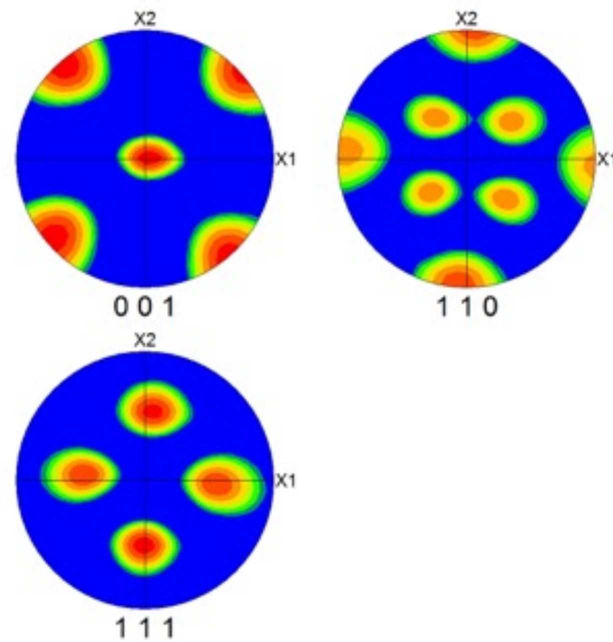
-processing history

annealed, hardened, as-rolled, sputtered



Goodfellow
99.99% Fe
As-rolled





# Looking forward: New Era in Materials Genomics

SLAC

**Connecting structure, properties and performance.**
***How do materials transform/deform/fail under extreme conditions?***

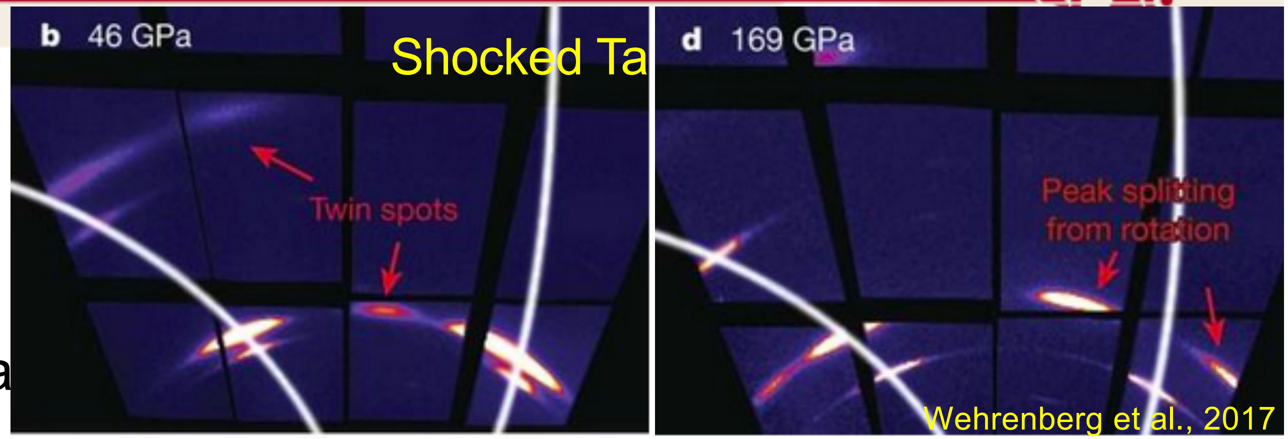
- Visualization of transformation/deformation mechanism
  - Twinning
  - Texture
  - Mosaicity

- Synergy of datasets → New materials properties correlations
  - XRD + spectroscopy + imaging

- Kinetics models
  - Nucleation mode tied to molecular dynamics (MD) simulations/density functional theory (DFT) & synthetic data

# Real-time visualization of transformation & deformation mechanisms

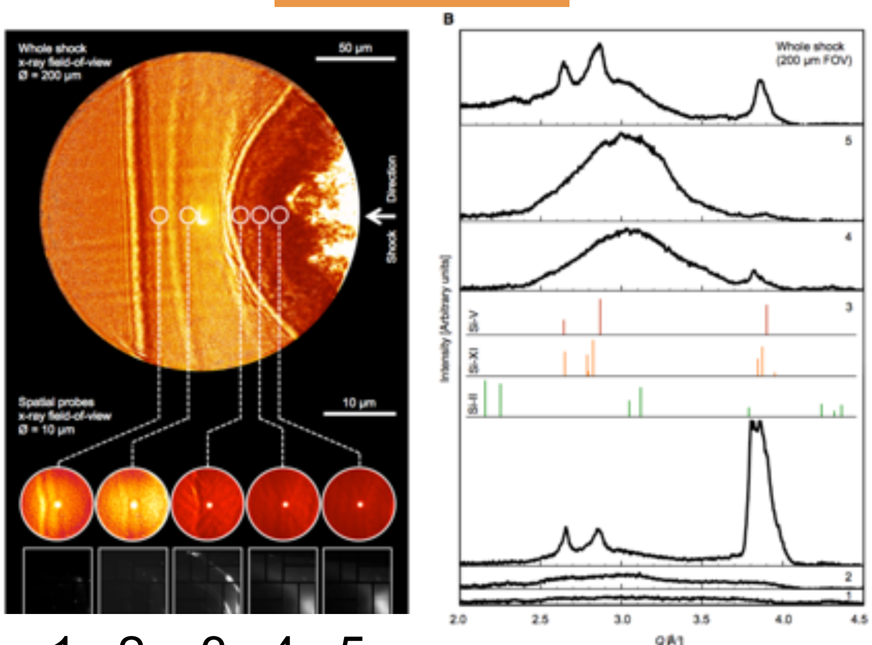
- **Twinning**
  - Timescale: picoseconds
  - Transition from twinning to dislocation-slip plasticity above 150 GPa
- **Texture**
  - Dynamic strength
  - Polycrystal plasticity models
- **Mosaicity prediction**
  - Fracture and rotation of crystallites in a brittle materials
  - Elastic-plastic transitions



# Synergy of datasets: looking for new materials properties correlations

- **XRD + x-ray spectroscopy**
  - meV-resolution inelastic X-ray scattering: transport properties + lattice structure
  - X-ray emission spectroscopy: electronic- vs. lattice-structure changes
- **XRD + coherent diffractive X-ray imaging**

Shocked Si




1 2 3 4 5

*Brown et al., 2019*

# Kinetics models leading to more predictive models

- Kinetics models (e.g., Johnson-Mehl-Avrami-Kolmogorov)

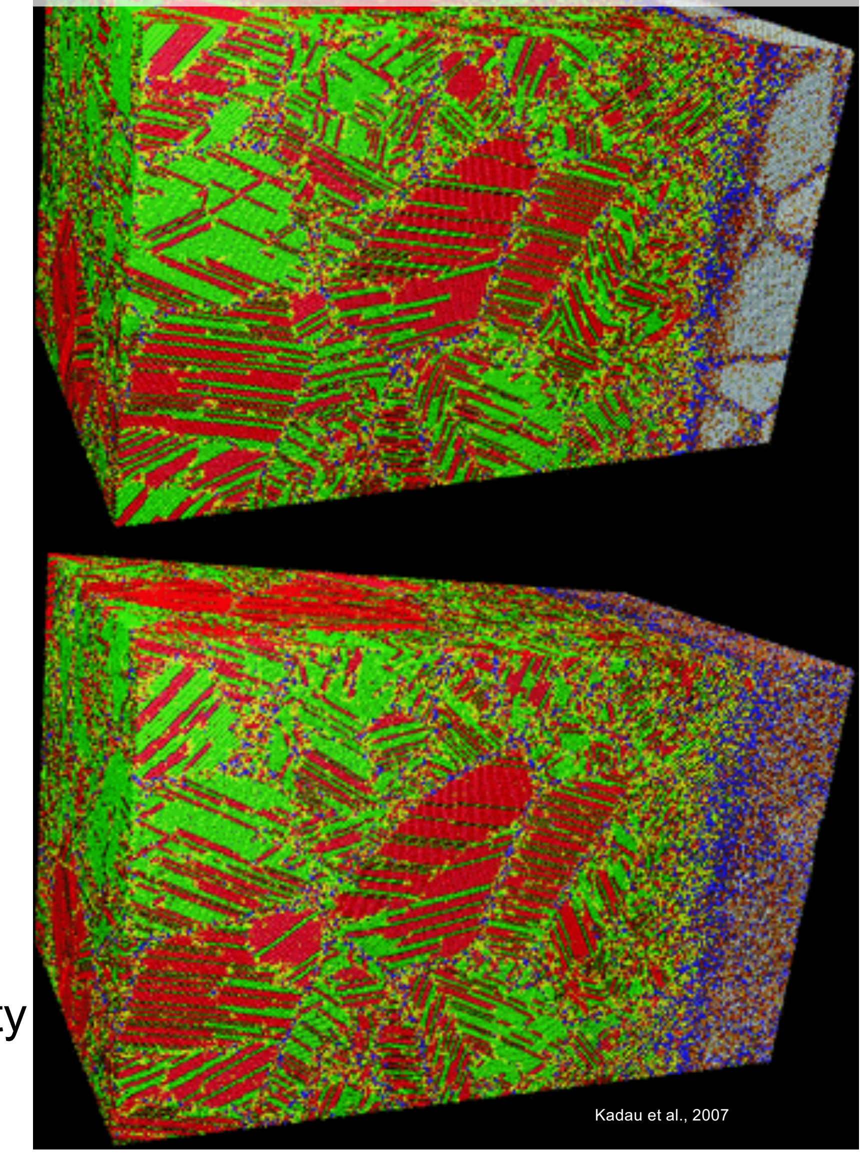
volume fraction with an exponential functional form,

$$\alpha(t) = 1 - \exp(-(k(t-\tau))^n, \quad (1)$$

where $\alpha(t)$ is the fraction of the material transformed as a function of time, $t$, $k$ is a crystallization rate constant, $\tau$ is incubation time, and $n$ is the JMAK kinetic exponent.

- Nucleation mode tied to MD/DFT & Synthetic data
  - Solidification – visualize the formation
  - Melting/resolidification
  - Far-from-equilibrium phenomena
  - Materials properties correlations
  - Tuning properties at the mesoscale
    - Role of impurities, defects, dislocation density
      →Works toward predictive capability

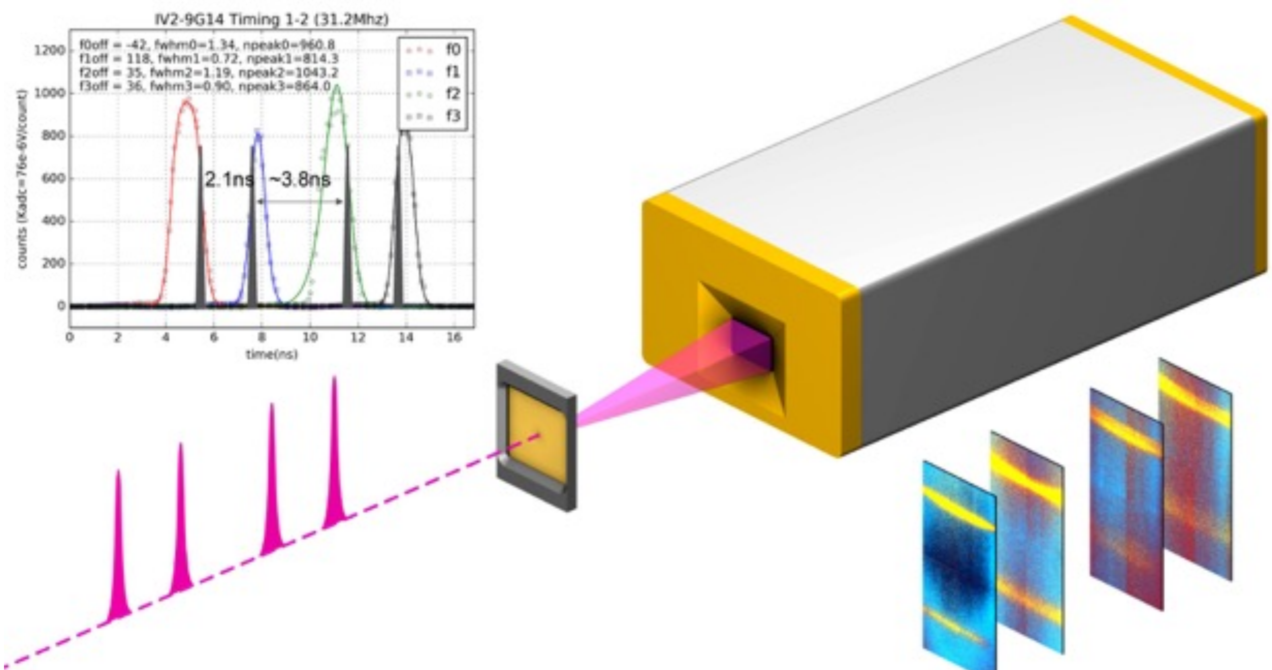
MD simulation of Fe phase transition

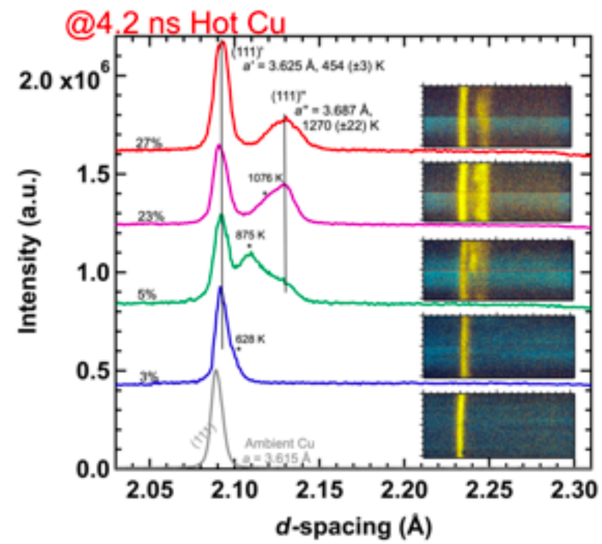


# Revolution in X-ray sources is enabling a revolution in WDM & HED Science

SLAC

New gated detector deployed at LCLS in 2019 measures nanosecond Cu heating



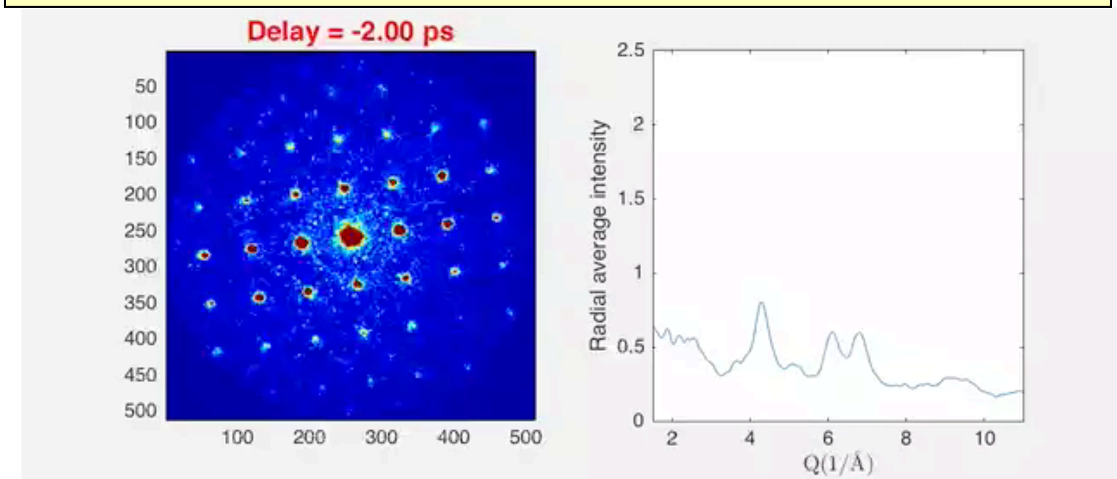




Hart et al., 2019

# Ultrafast Electron Diffraction has visualized the heterogenous to homogeneous melting transition

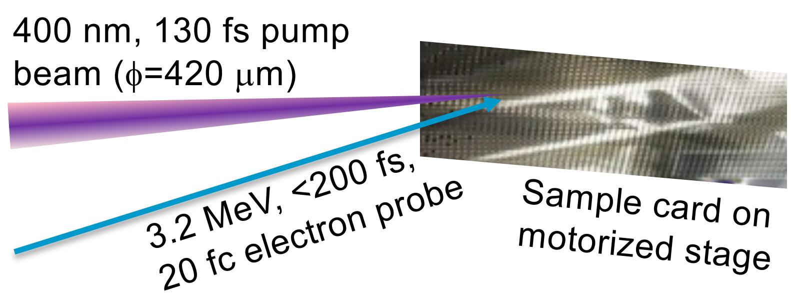
SLAC

**Observation of melting and formation of WDM**

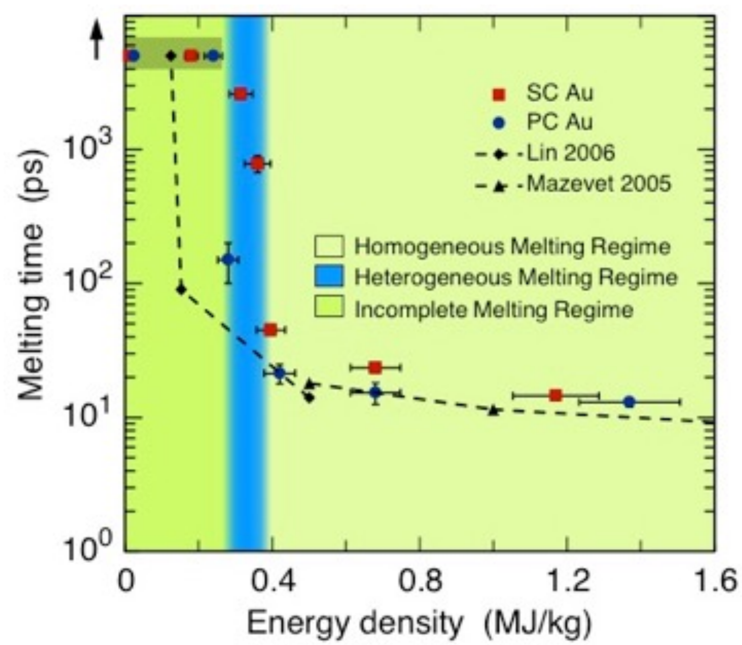



Data for 900 J/m$^2$ on Au

Mo et al., 2018




**Sensitive to nucleation sites (blue)**

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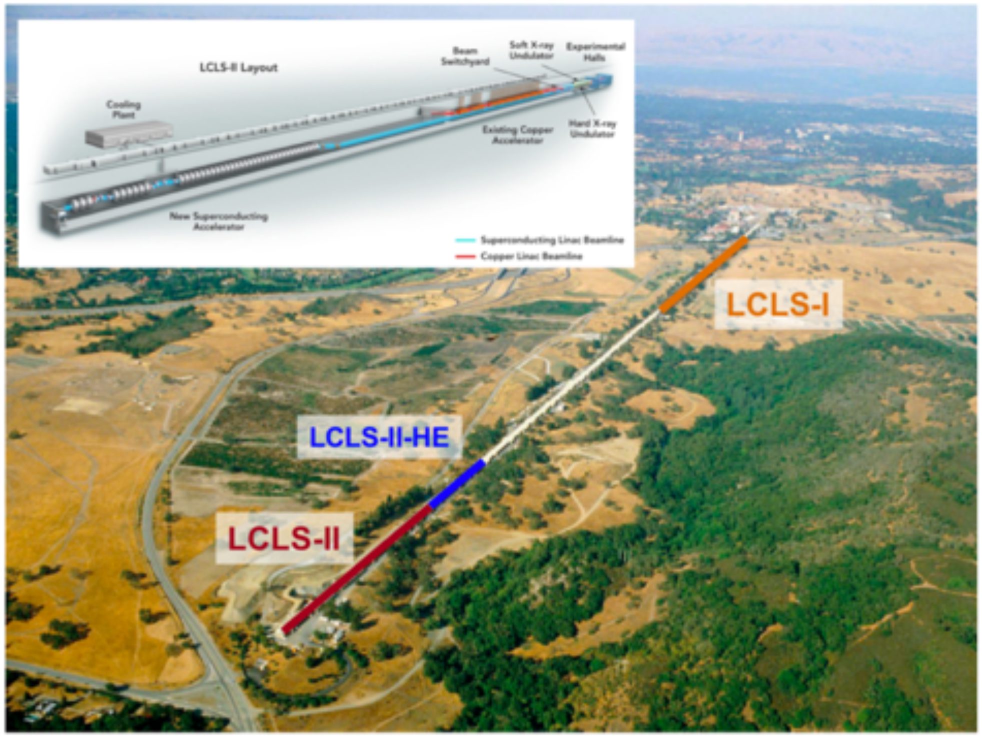
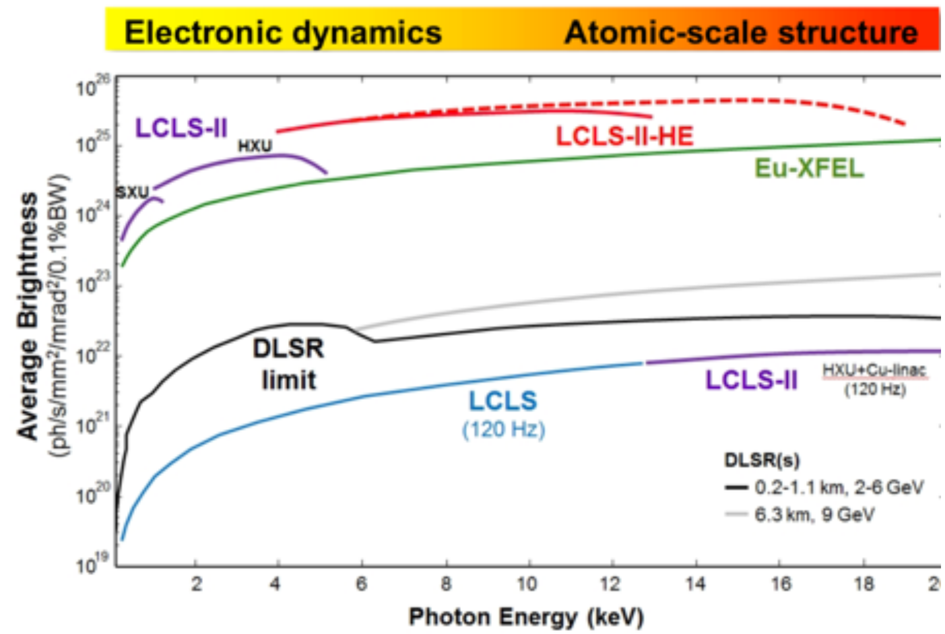
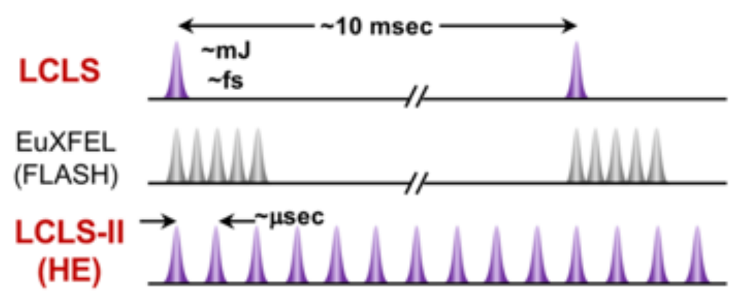
# LCLS-II and LCLS-II-HE will take us from 120 pulses per second to 1 million pulses per second






**LCLS-II now 75% complete; users in 2021**

**LCLS-II-HE received CD-1 in Sept 2018**

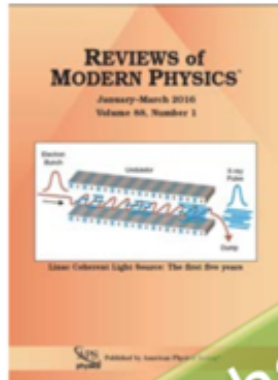
**Targeting mid-decade users**

# The X-ray laser revolution is set to drive a new era of Grand Challenge discovery science

U.S. DEPARTMENT OF ENERGY | Office of Science

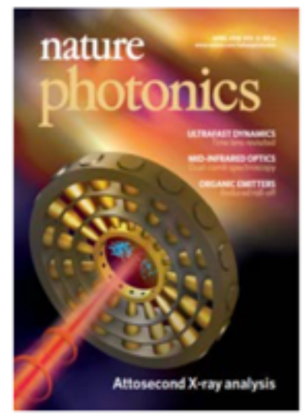
SLAC NATIONAL ACCELERATOR LABORATORY

**From early scientific impact,**

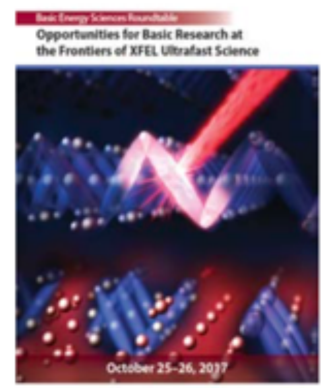



**… to unprecedented measurements,**


**… to accessing critical new regimes,**




**… to full exploitation and exploration of new frontiers**




**… IF we can figure out how to handle all the data!**

# Thank you for your attention!!

Collaborators:
- Cindy Bolme, Richard Sandberg, Don Brown – LANL
- Wendy Mao – Stanford University; SLAC
- Hae Ja Lee, Bob Nagler, Eric Galtier, Brice Arnold, Eduardo Granados, Zhou Xing, Despina Milathianaki, Sebastien Boutet, Roberto Alonso-Mori, Dimosthenis Sokaras, Thomas Kroll – SLAC
- Andrew Higginbotham – University of York
- Justin Wark – University of Oxford
- Andreas Schropp, Frank Seiboth, Christian Schroer – DESY
- James Hawreliak – Washington State University
- Dan Dolan, Chris Seagle, Tom Ao – Sandia National Lab
- Suzanne Ali, Peter Celliers, Amy Lazicki, Richard Kraus, Dayne Fratanduono, Jon Eggert, Rip Collins – LLNL
- many more

Funding: DOE; NSF