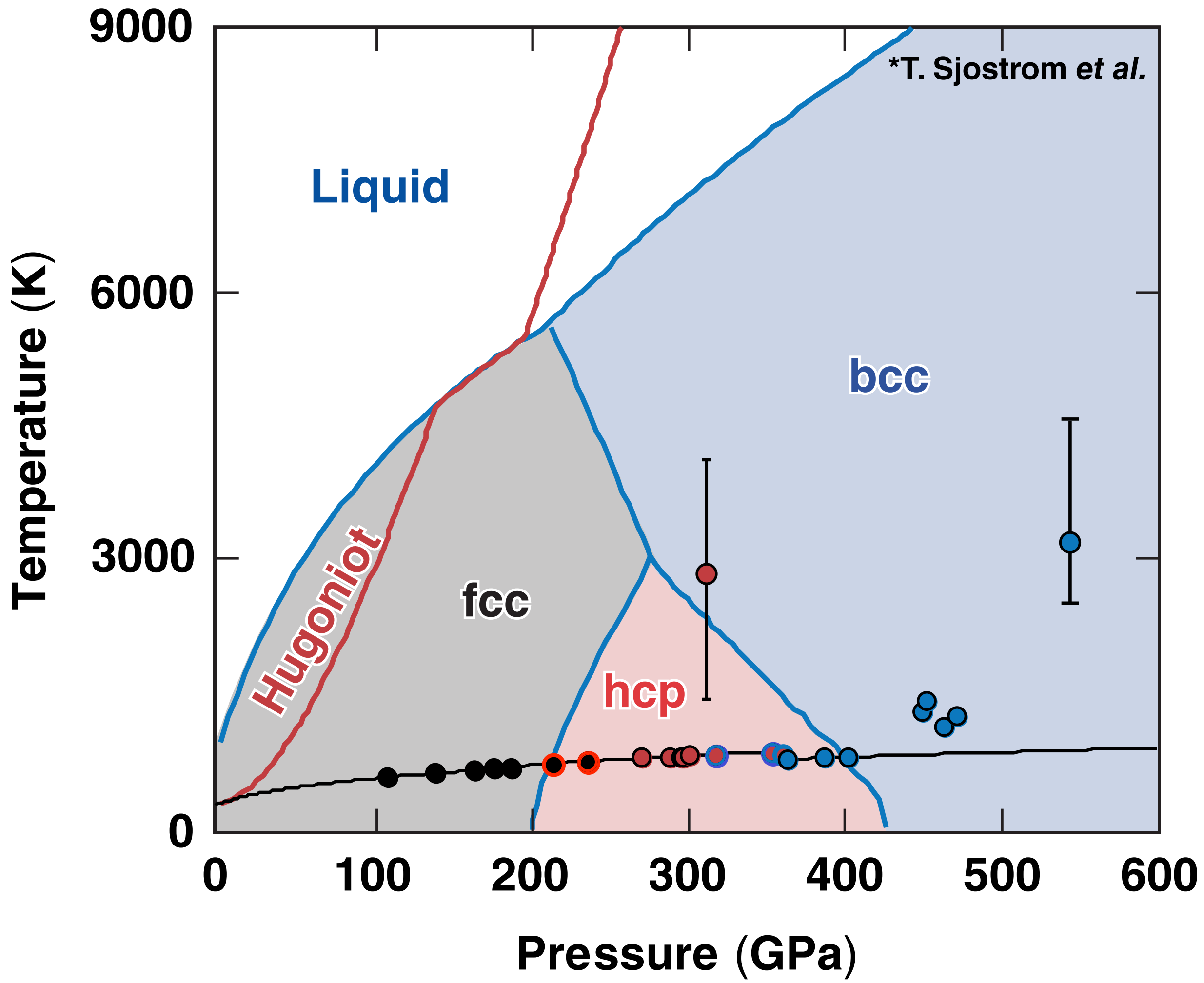
Observation of a New High-Pressure Solid Phase in Dynamically Compressed Aluminum



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Division of Plasma Physics
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We present the first *in-situ* high-pressure observation of bcc aluminum

- Aluminum and other prototypical *sp*-bonded materials are predicted to transform into complex, open, and incommensurate structures at multiterapascal pressures
- High-power lasers ramp compressed Al and nanosecond *in-situ* x-ray diffraction (XRD) measured the crystal structure at pressures of 111 GPa to 547 GPa
- The fcc–hcp and hcp–bcc phase transformations are observed at 216$\pm$9 GPa and 321$\pm$12 GPa, respectively
- Texture evolution shows that even on nanosecond time scales, atoms can rearrange in the spaces between close-packed planes

fcc: face-centered cubic
bcc: body-centered cubic
hcp: hexagonal close packed

Collaborators

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D. E. Fratandouno, R. Smith, R. Kraus, J. H. Eggert, F. Coppari, A. Jenei, D. C. Swift, M. C. Gregor, and P. M. Celliers

Lawrence Livermore National Laboratory

Outline

- OMEGA diffraction experiments
- NIF* experiment
  - dual backlighter
- Texture evolution

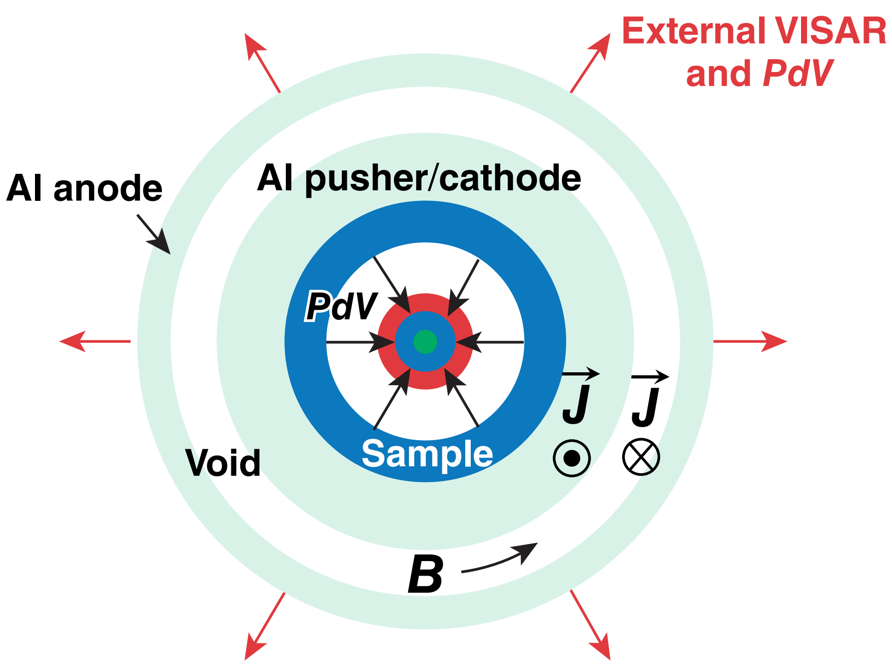
*NIF: National Ignition Facility

Outline

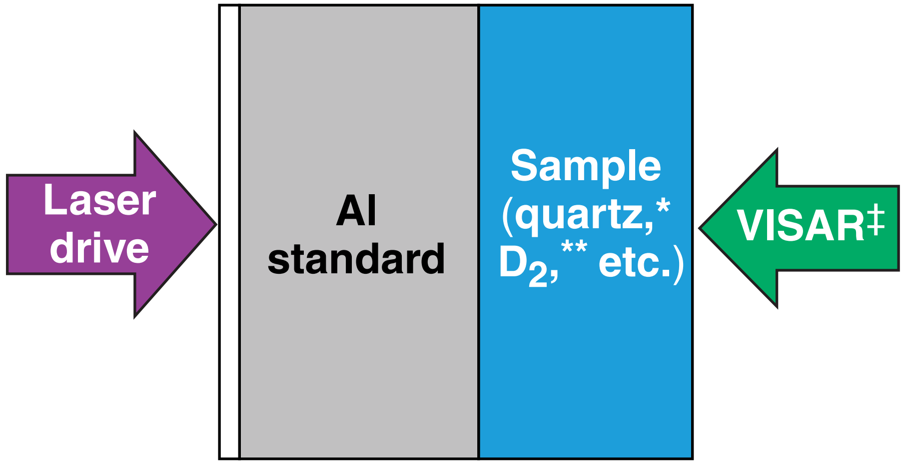
- **OMEGA diffraction experiments**
- NIF experiment
  - dual backlighter
- Texture evolution

The high-pressure EOS of many materials are referenced to the Al EOS*,**

Cylindrical implosion pusher†



Impedance-match standard

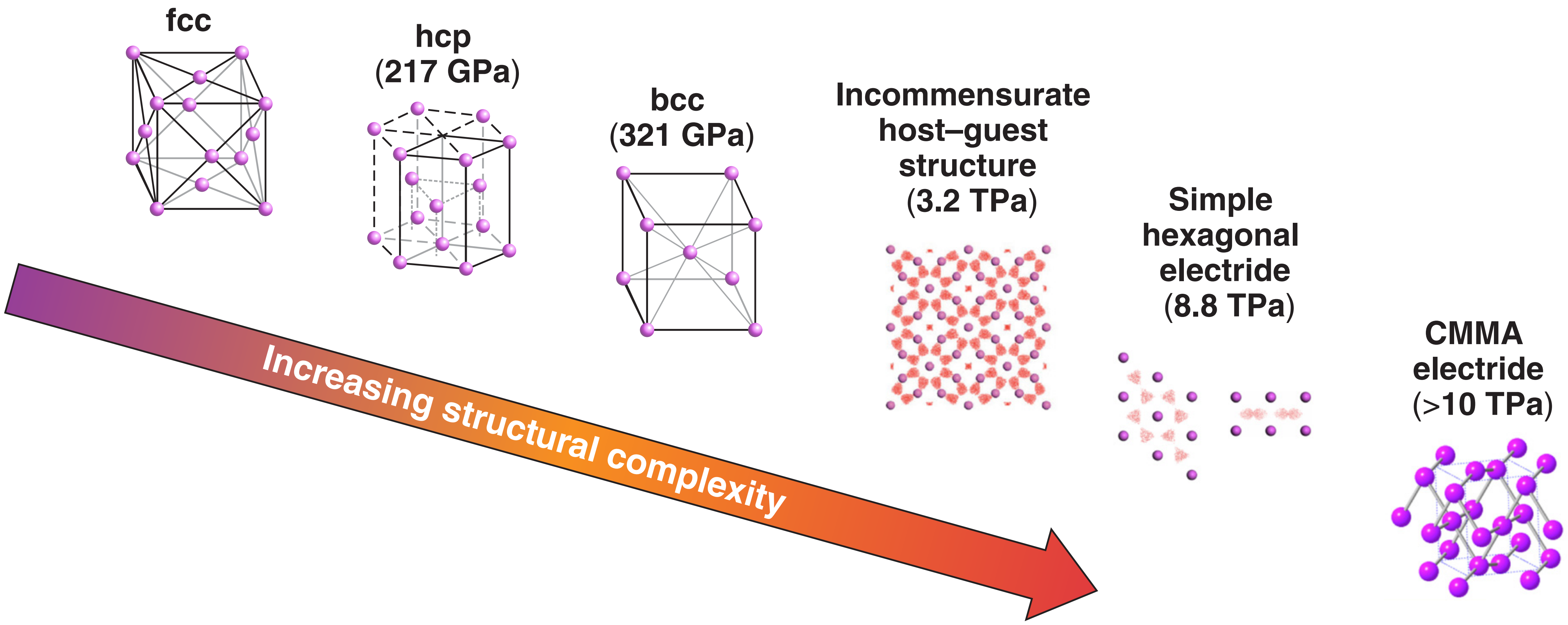


Accurate knowledge of the Al equation of state (EOS) is required to avoid the introduction of systematic errors in high-energy-density (HED) measurements.

*Hicks *et al.*, Phys. Plasmas 12, 082702 (2005).
**Hicks *et al.*, Phys. Rev B 79, 014112 (2009).
†R. W. Lemke *et al.*, J. Appl. Phys. 119, 015904 (2016).
‡VISAR: velocity interferometer system for any reflector

E26645

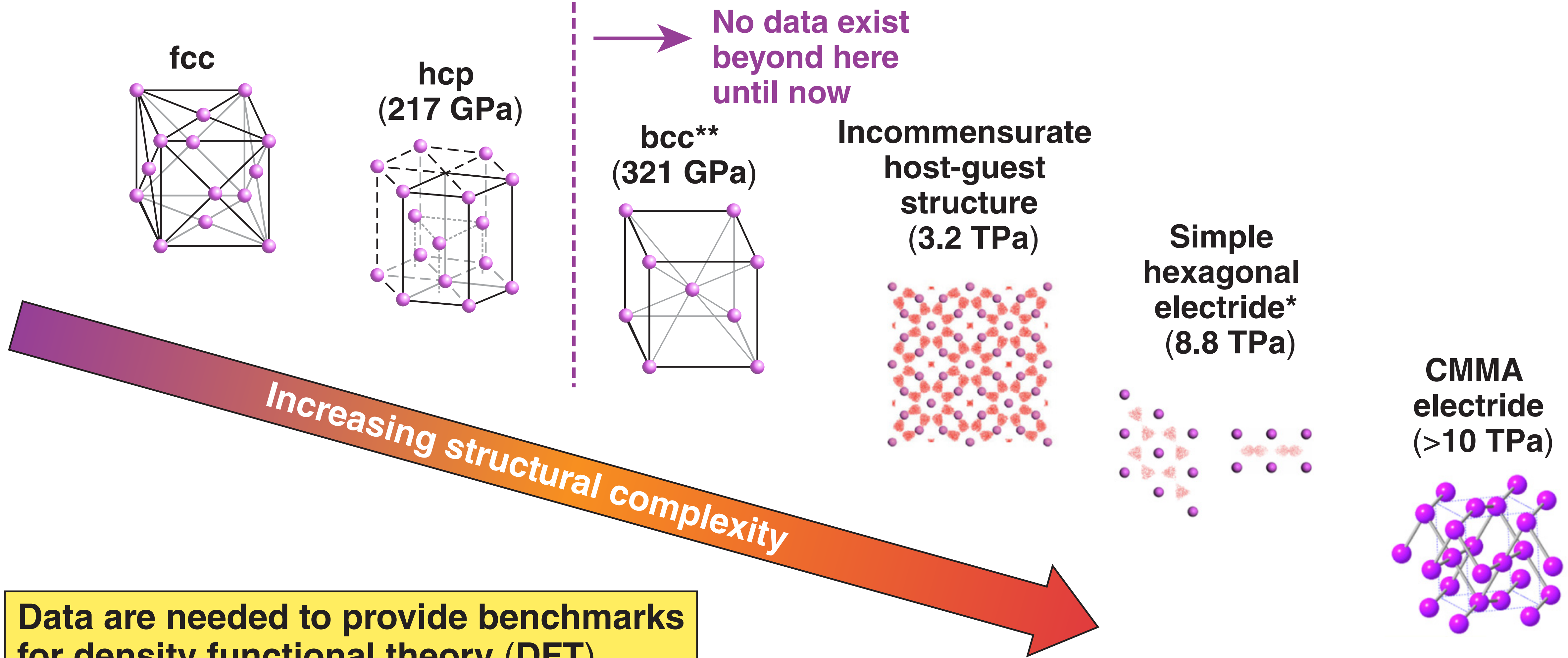
Aluminum and other prototypical *sp*-bonded materials are predicted to transform into complex, open, and incommensurate structures at multiterapascal pressures



C. J. Pickard and R. J. Needs, Nat. Mater. 9, 624 (2010).

E26646

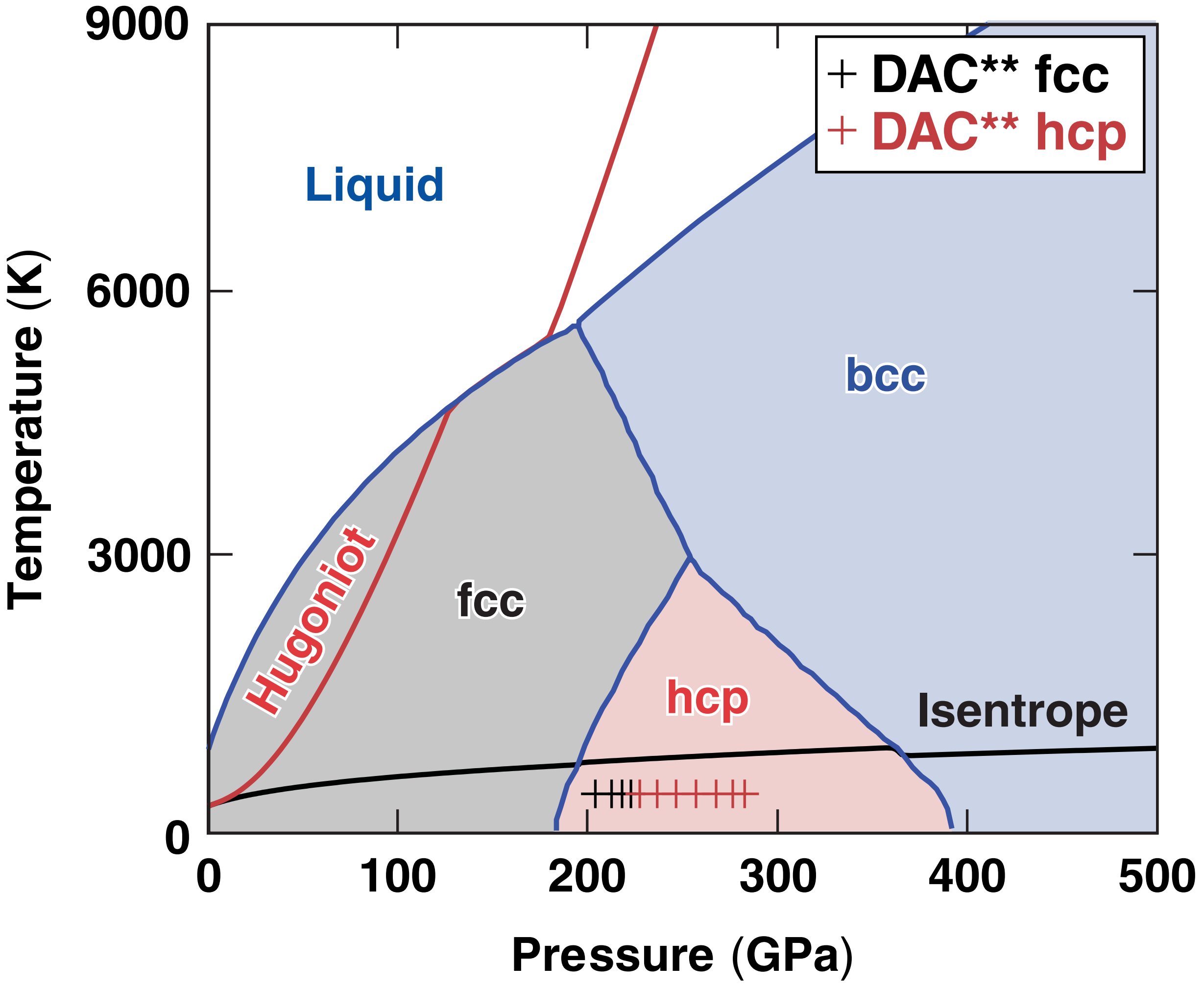
Aluminum and other prototypical *sp*-bonded materials are predicted to transform into complex, open, and incommensurate structures at multiterapascal pressures



Data are needed to provide benchmarks for density functional theory (DFT).

C. J. Pickard and R. J. Needs, Nat. Mater. 9, 624 (2010).
*X. Gong *et al.*, PO5.00007, this conference.
**D. N. Polsin *et al.*, "The First Observation of the bcc Phase in Aluminum Compressed to 559 GPa," to be published in Physical Review Letters.

Aluminum is predicted* to undergo fcc–hcp and hcp–bcc solid–solid phase transitions as it is compressed at low temperatures



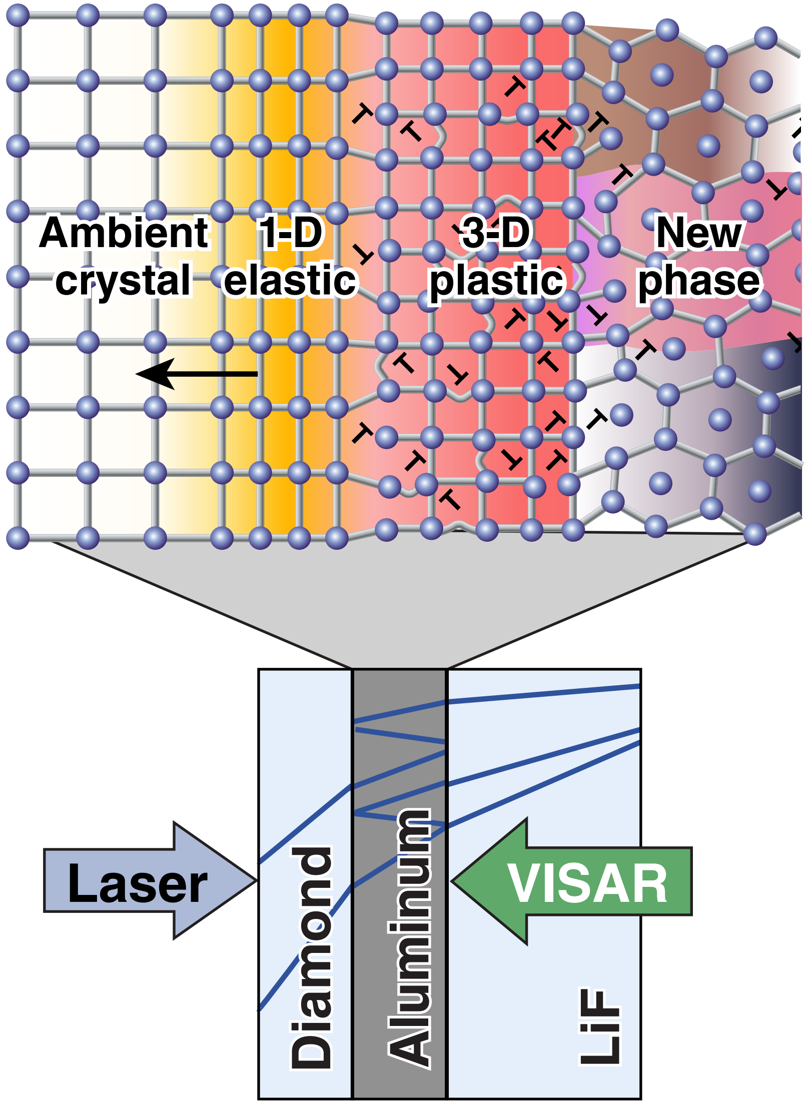
- Solid x-ray diffraction experiments are limited to 125 GPa along the principal Hugoniot because of shock melting
- Diamond-anvil cell (DAC) experiments measured the fcc–hcp transition at 217 GPa and 297 K

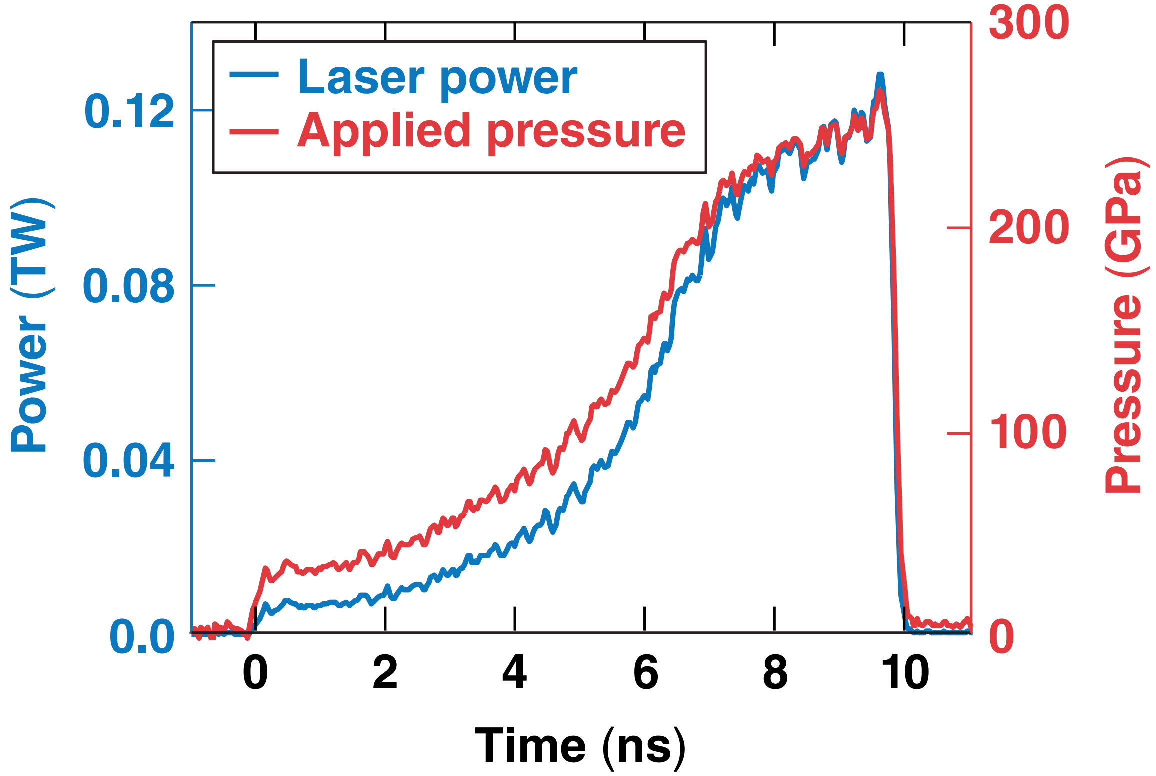
*T. Sjostrom, S. Crockett, and S. Rudin, Phys. Rev. B 94, 144101 (2016).
**Y. Akahama *et al.*, Phys. Rev. Lett. 96, 045505 (2006);

E26342a

Ramp (shockless) compression is used to access high-pressure, low-temperature states

Ramp compression



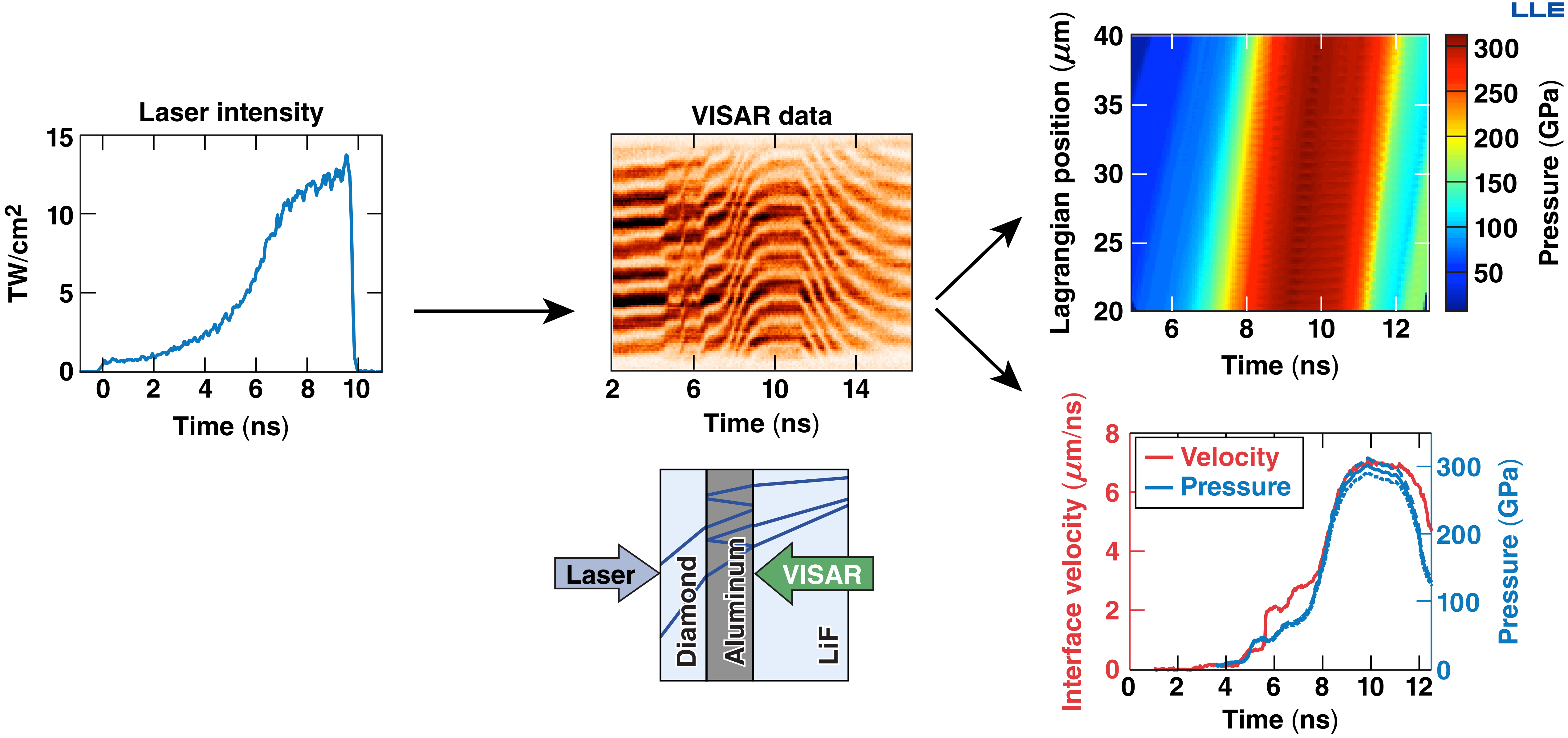


$^*P$ (GPa) = 42 $[I$ (TW/cm^2)$]^{0.71}$

E26648

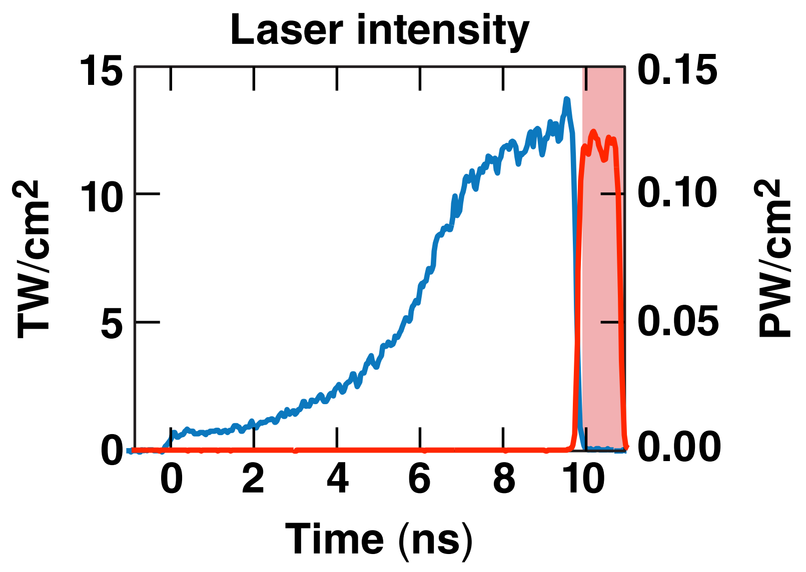
*D. E. Fratanduono *et al.*, J. Appl. Phys. 110, 073110 (2011).

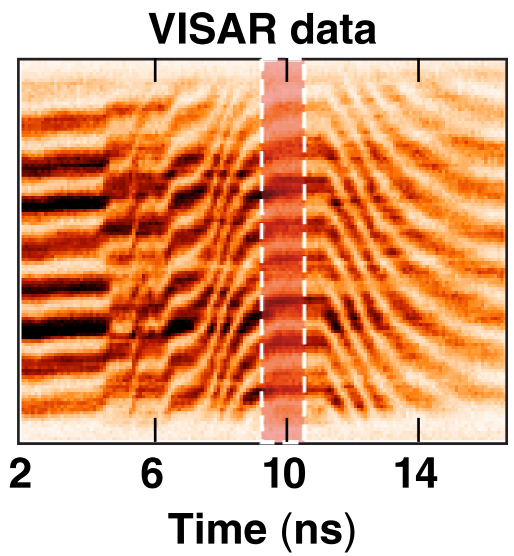
Pressure distributions in the Al samples are calculated using the measured Al–LiF interface velocities

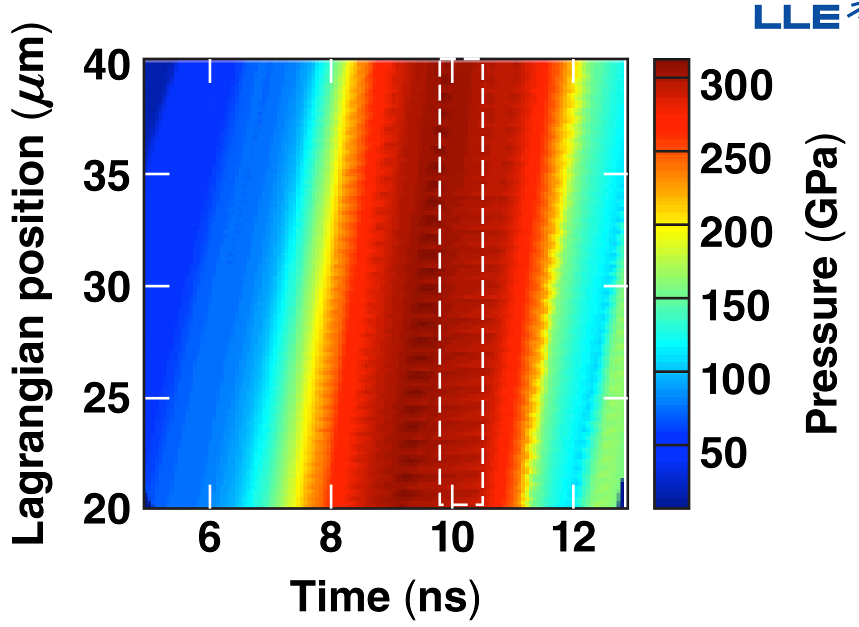


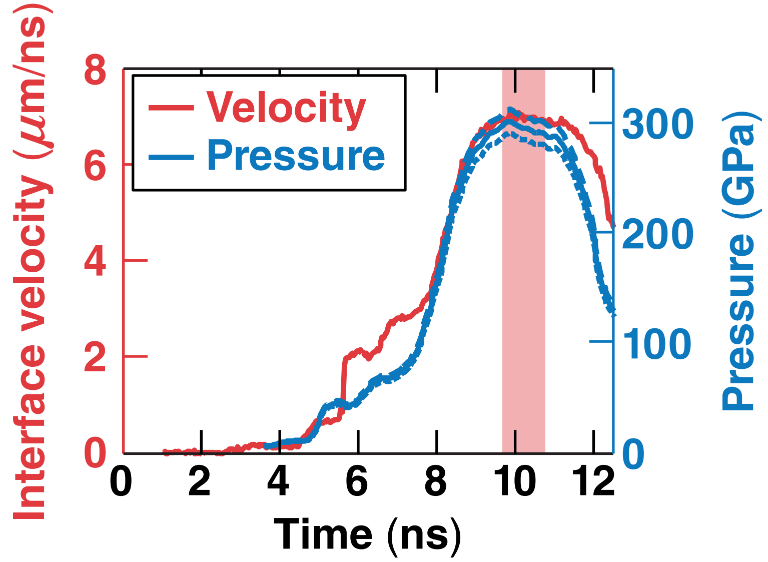
E26649

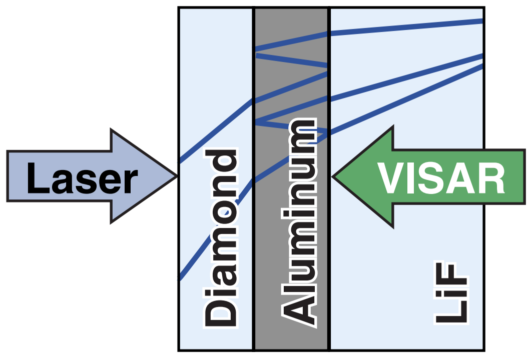
The x-ray backlighter was timed to probe the uniform pressure plateau in the Al pressure profile





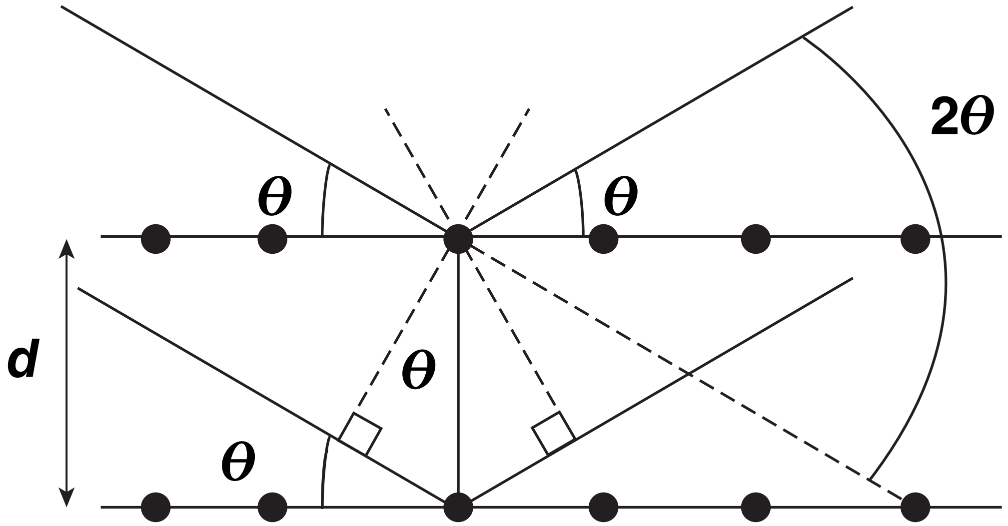




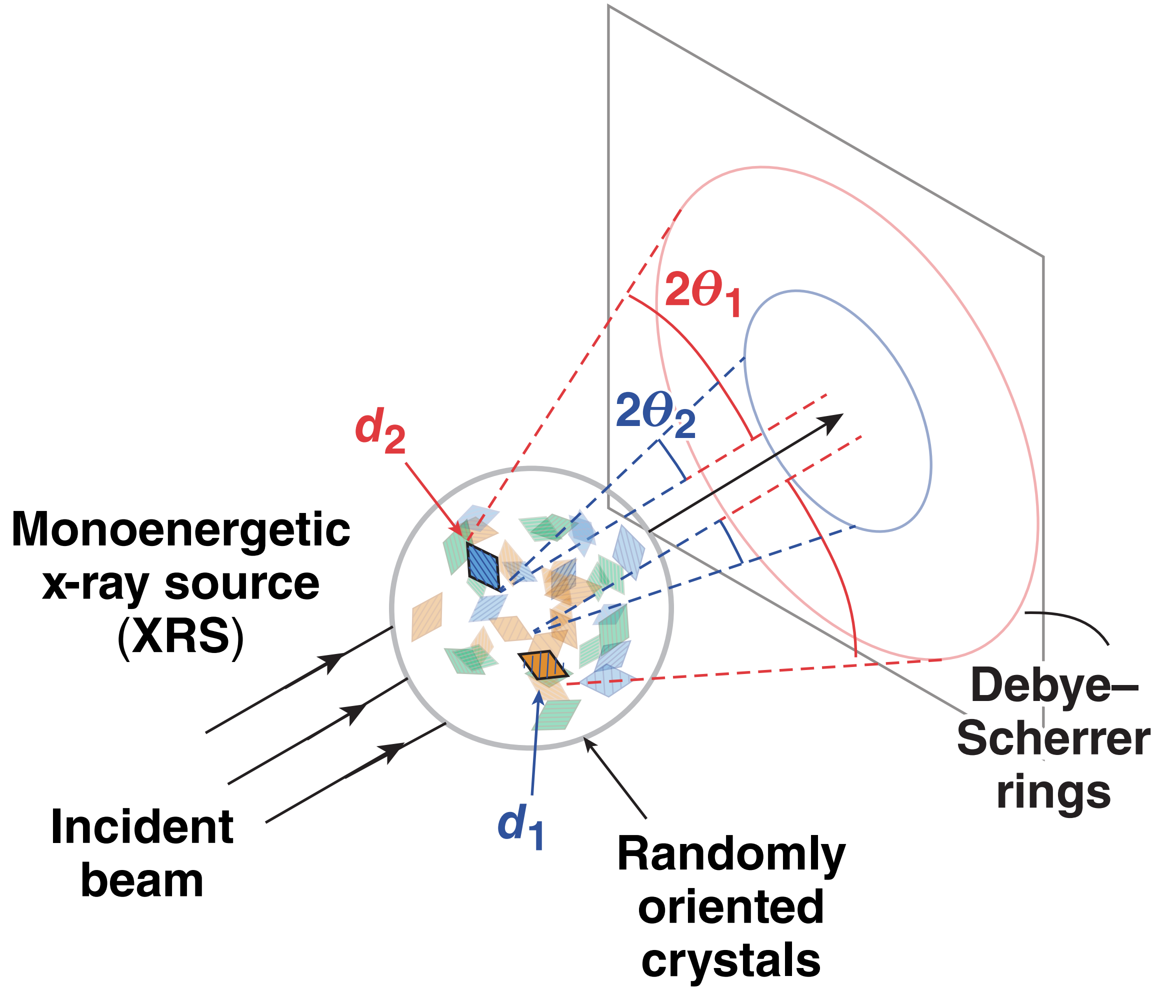


The sample is at a uniform, solid, high-pressure state at the time of the x-ray probe.

Monoenergetic x rays incident on an ideal powder sample will diffract in rings of uniform intensity at angles 2θ with respect to the x-ray beam



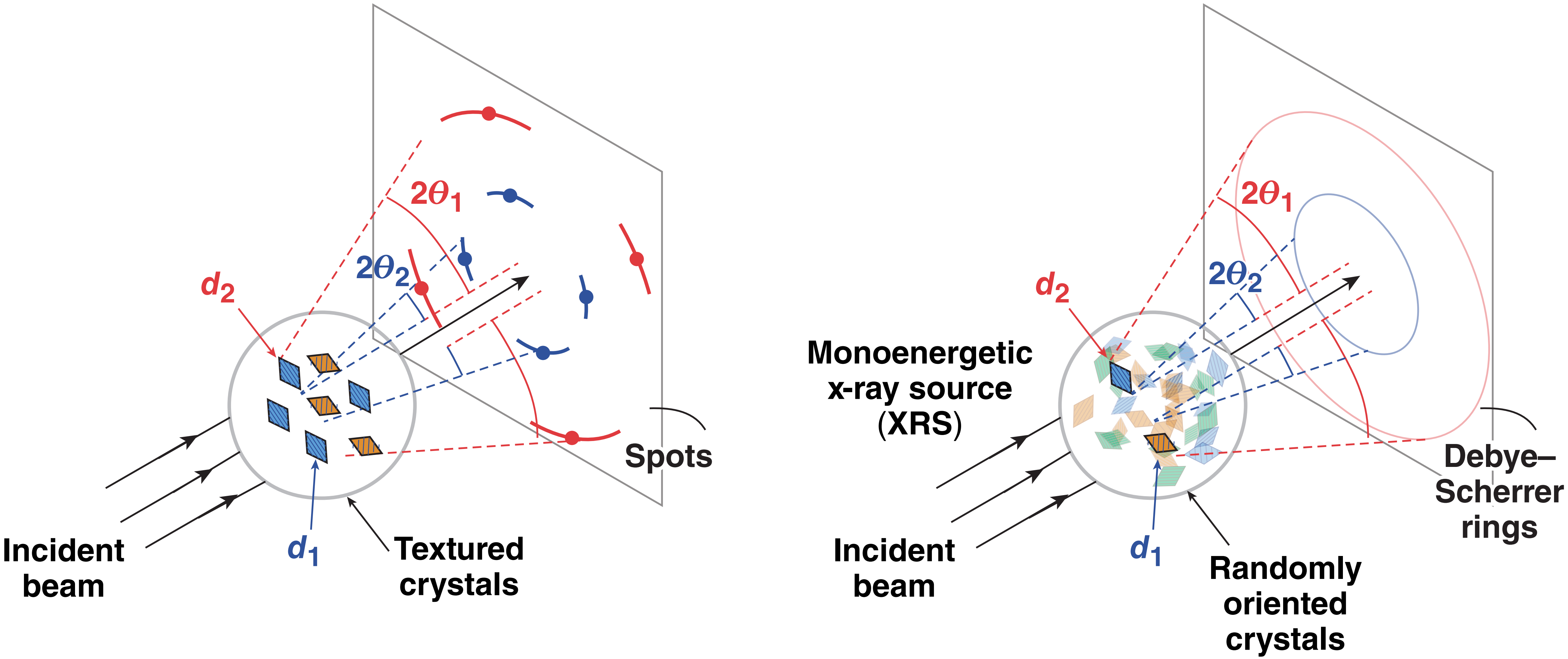
$$n\lambda = 2d \sin\theta$$



Compression of interatomic spacing (*d* spacing) is determined by measuring diffraction angles (2θ) and x-ray wavelength (λ).

E25408d

Monoenergetic x rays incident on an ideal powder sample will diffract in rings of uniform intensity at angles 2θ with respect to the x-ray beam

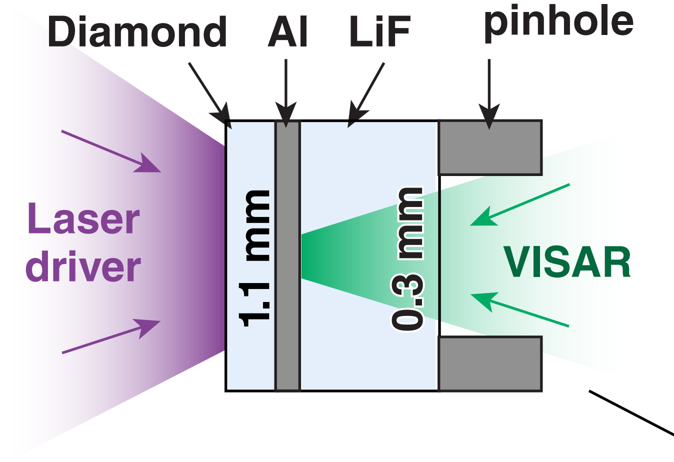


Textured foils diffract into spots rather than continuous rings.

E25408e

The powder x-ray diffraction image plate (PXRDIP)* diagnostic is used to record diffraction patterns on OMEGA EP

Target



X-ray source

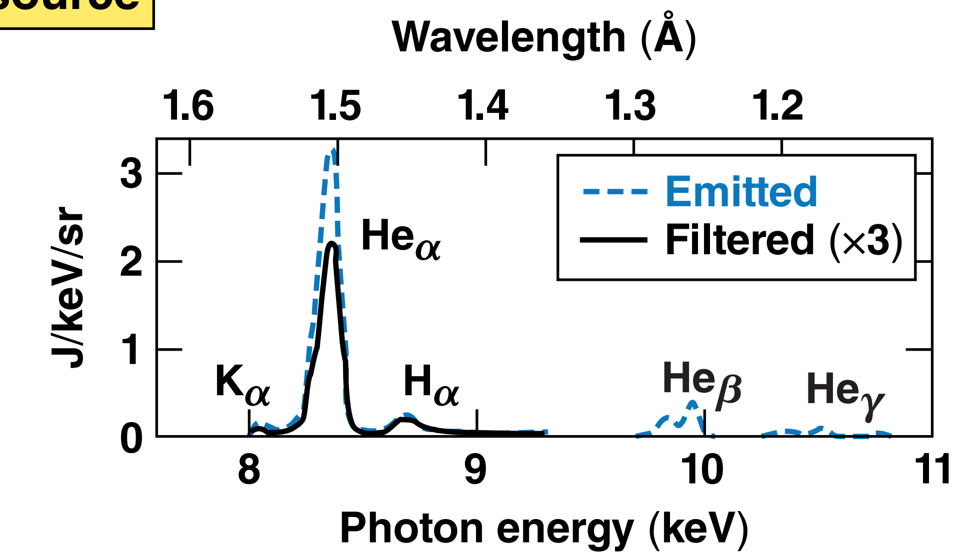
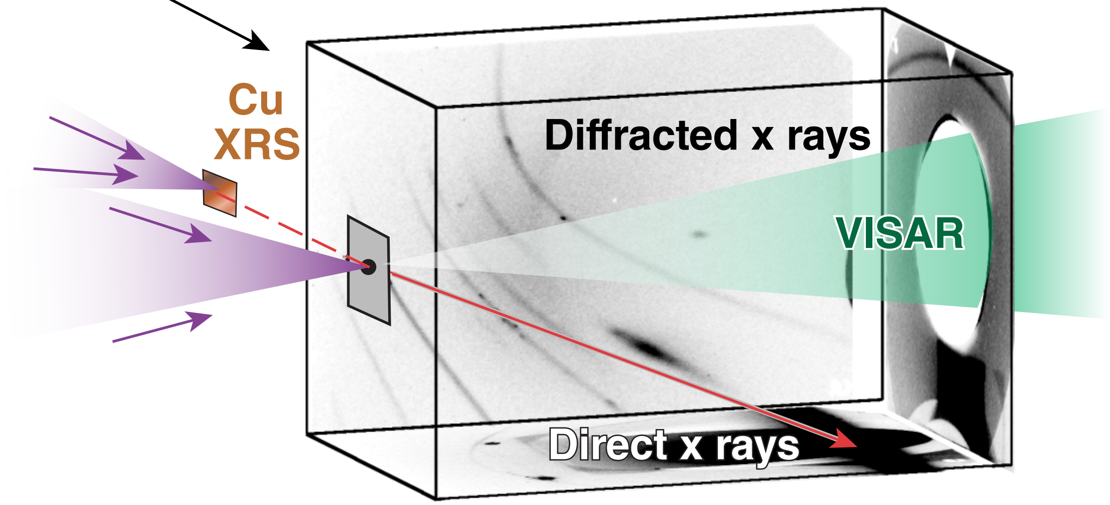


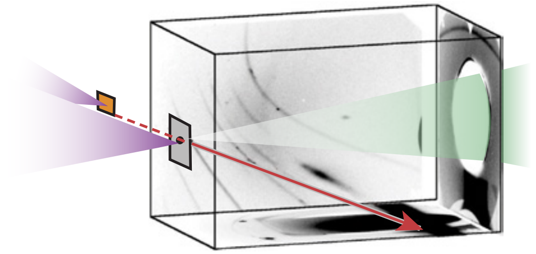
Image-plate data

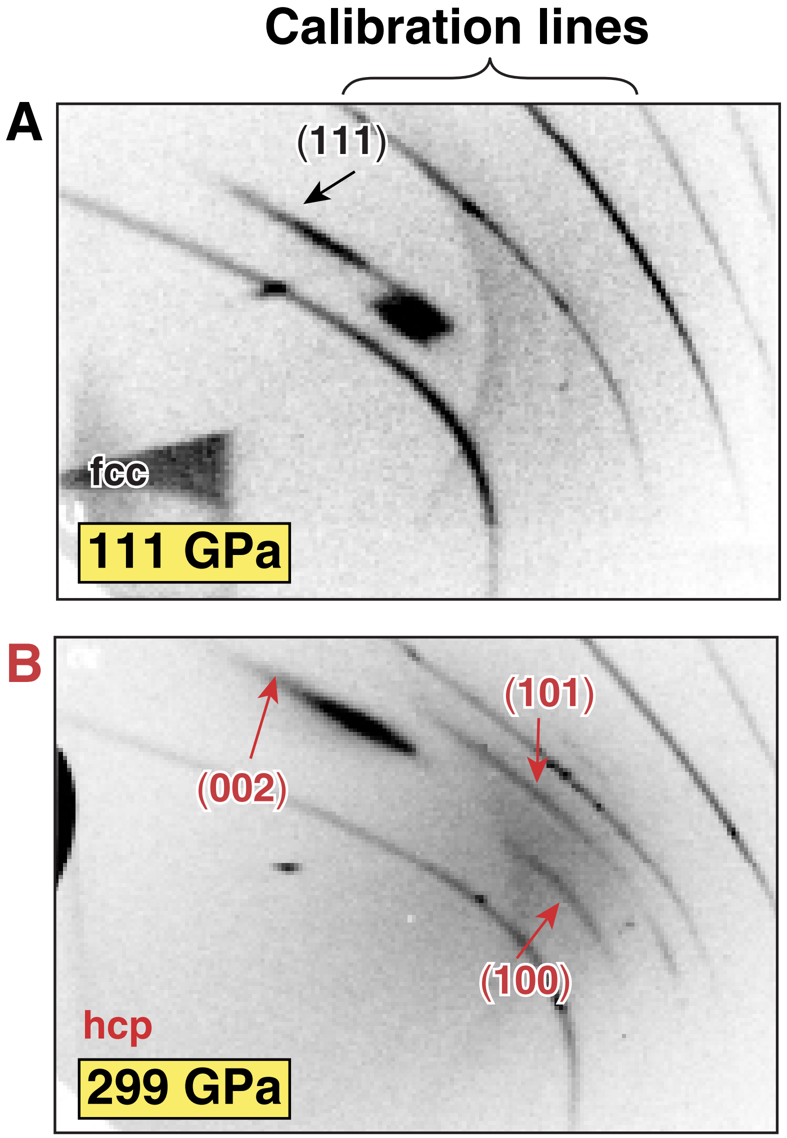


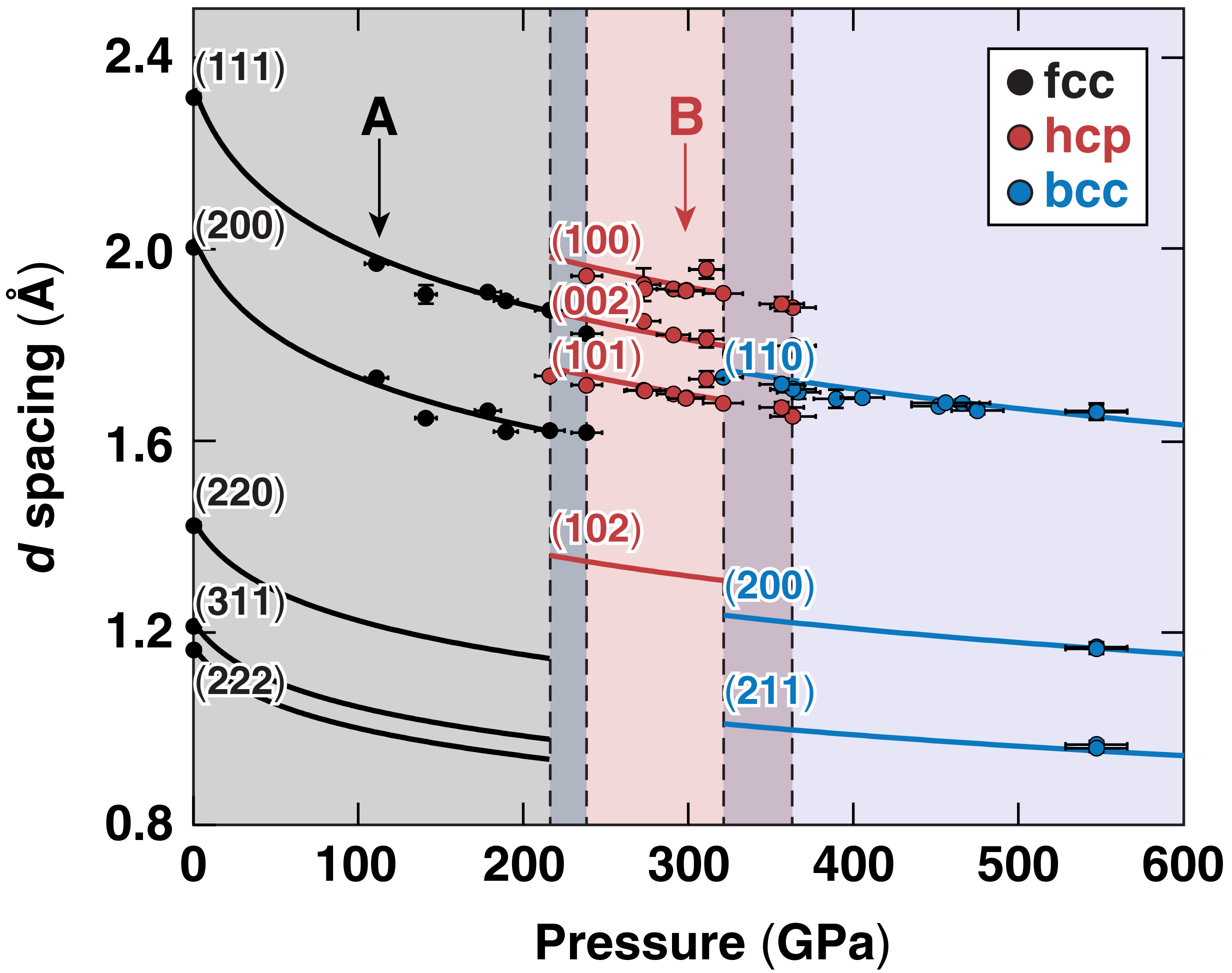
E26652

*J. R. Rygg *et al.*, Rev. Sci. Instrum. 83, 113904 (2012).

When pressure was increased from 111 GPa to 299 GPa, two diffraction lines were newly observed, consistent with hcp aluminum and distinct from fcc

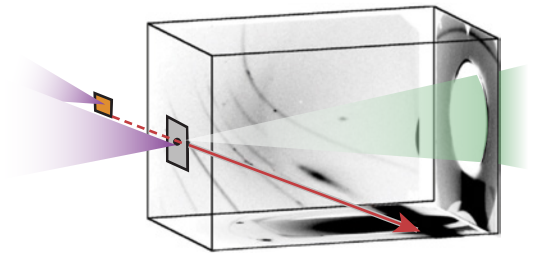


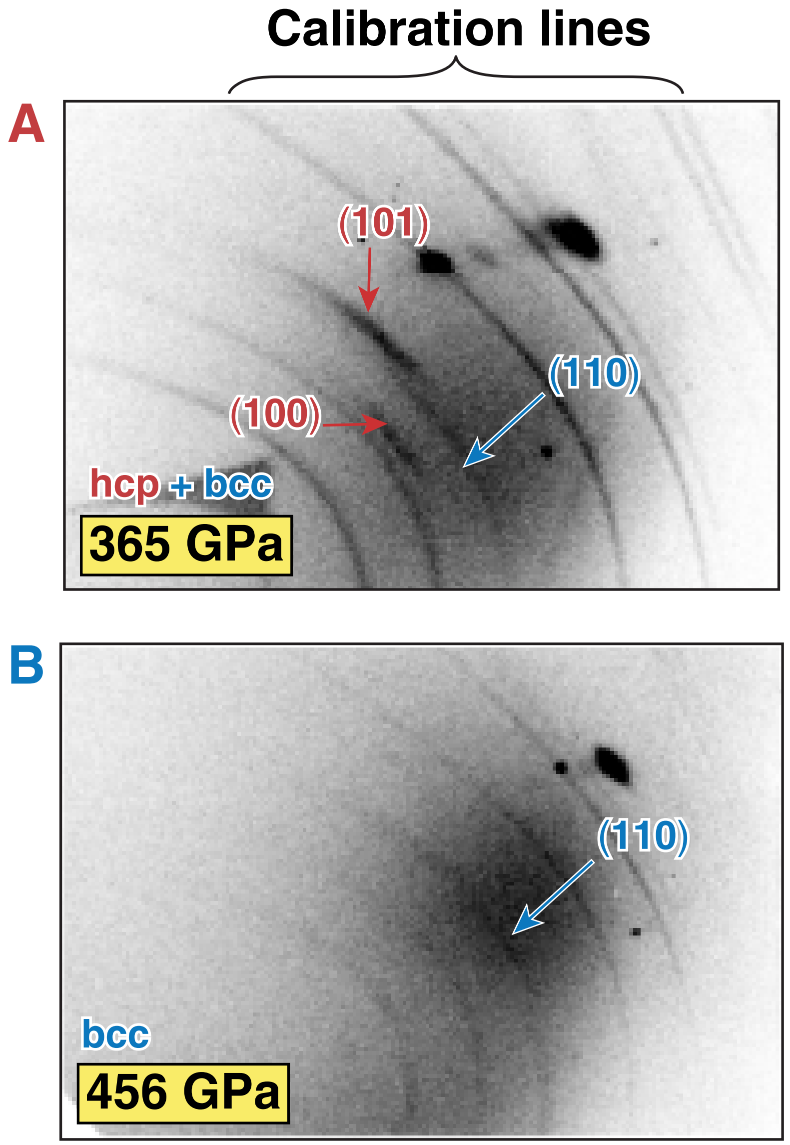


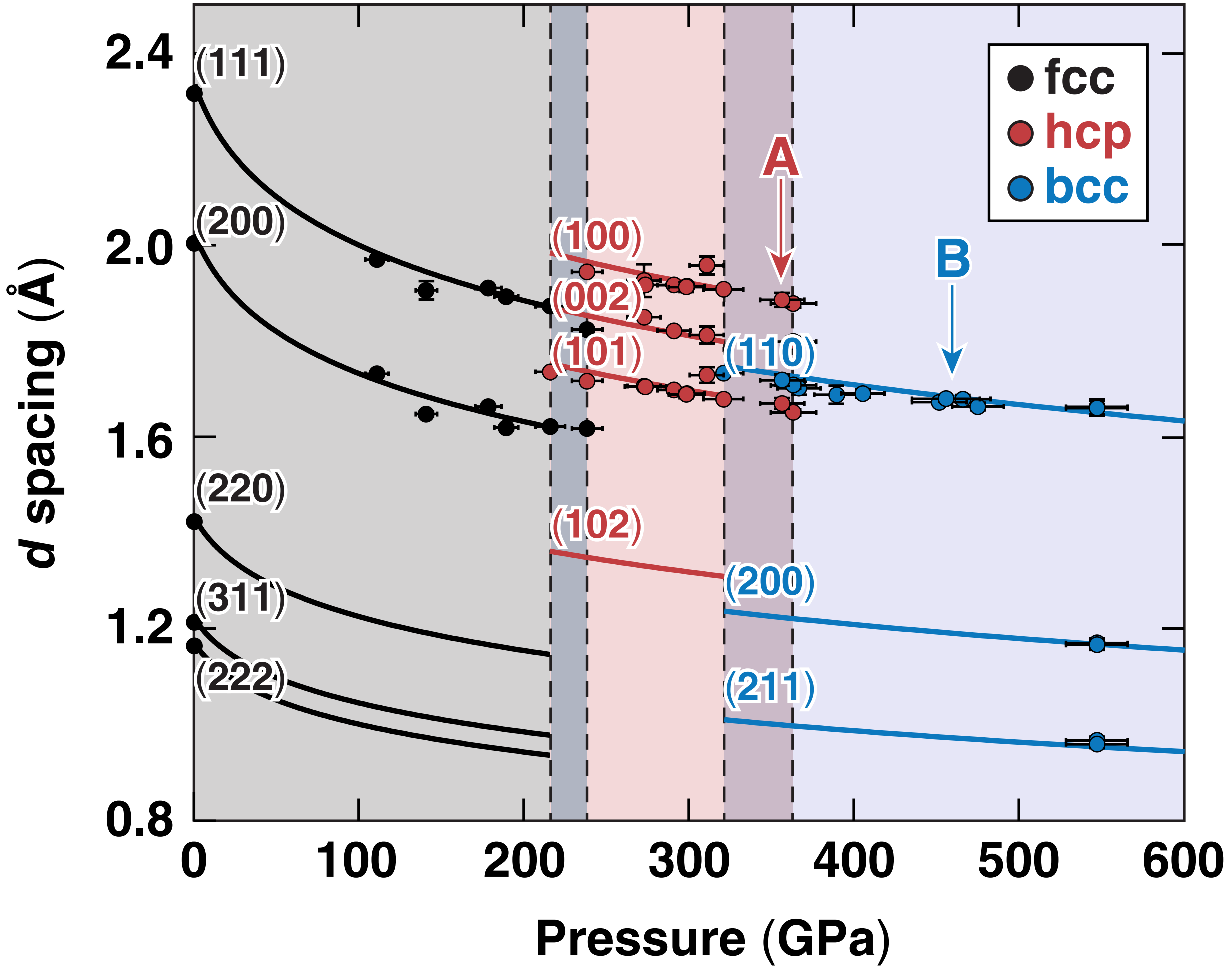


E26653

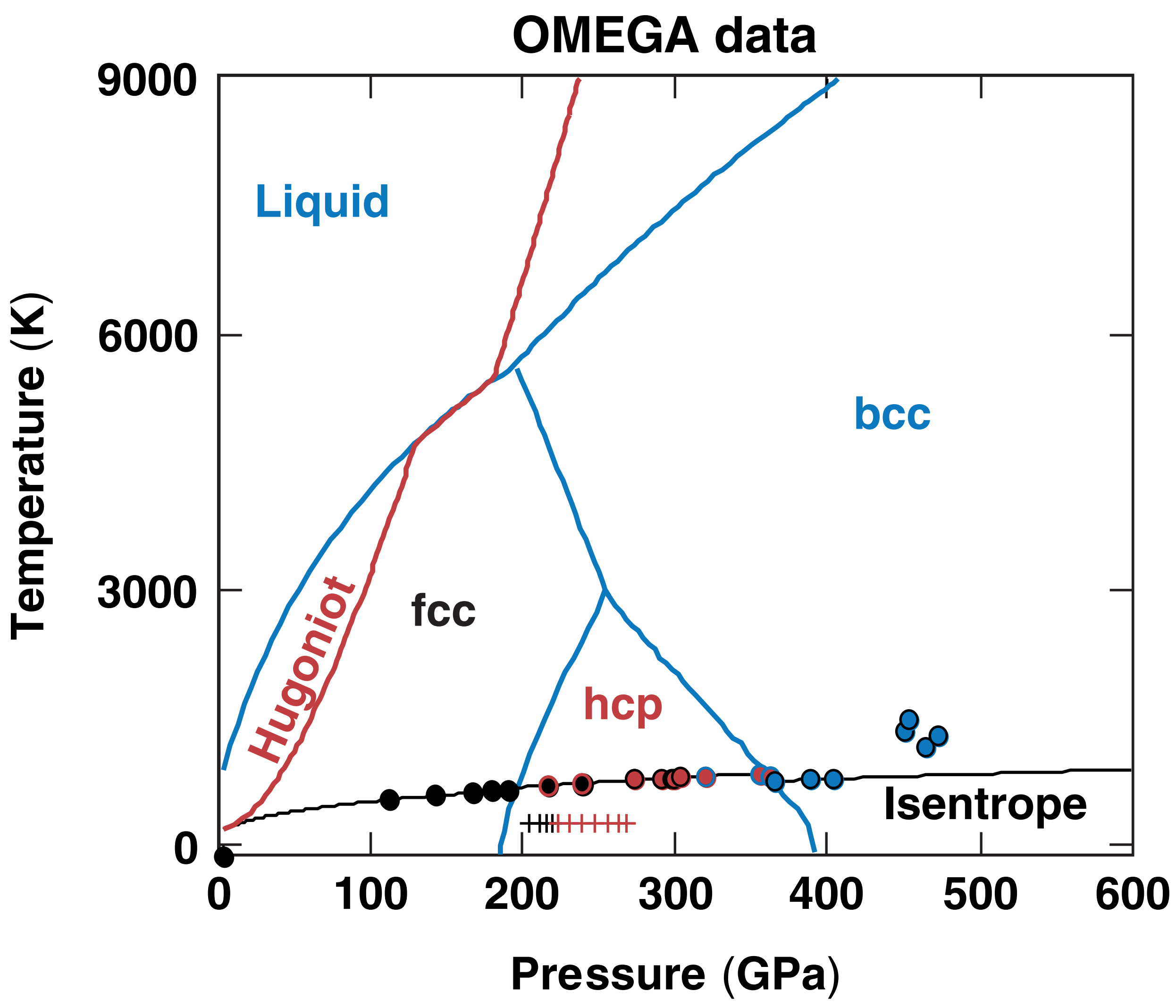
Above 321 GPa, a region of coexistence is observed, then a single intense line appears, consistent with (110) bcc aluminum

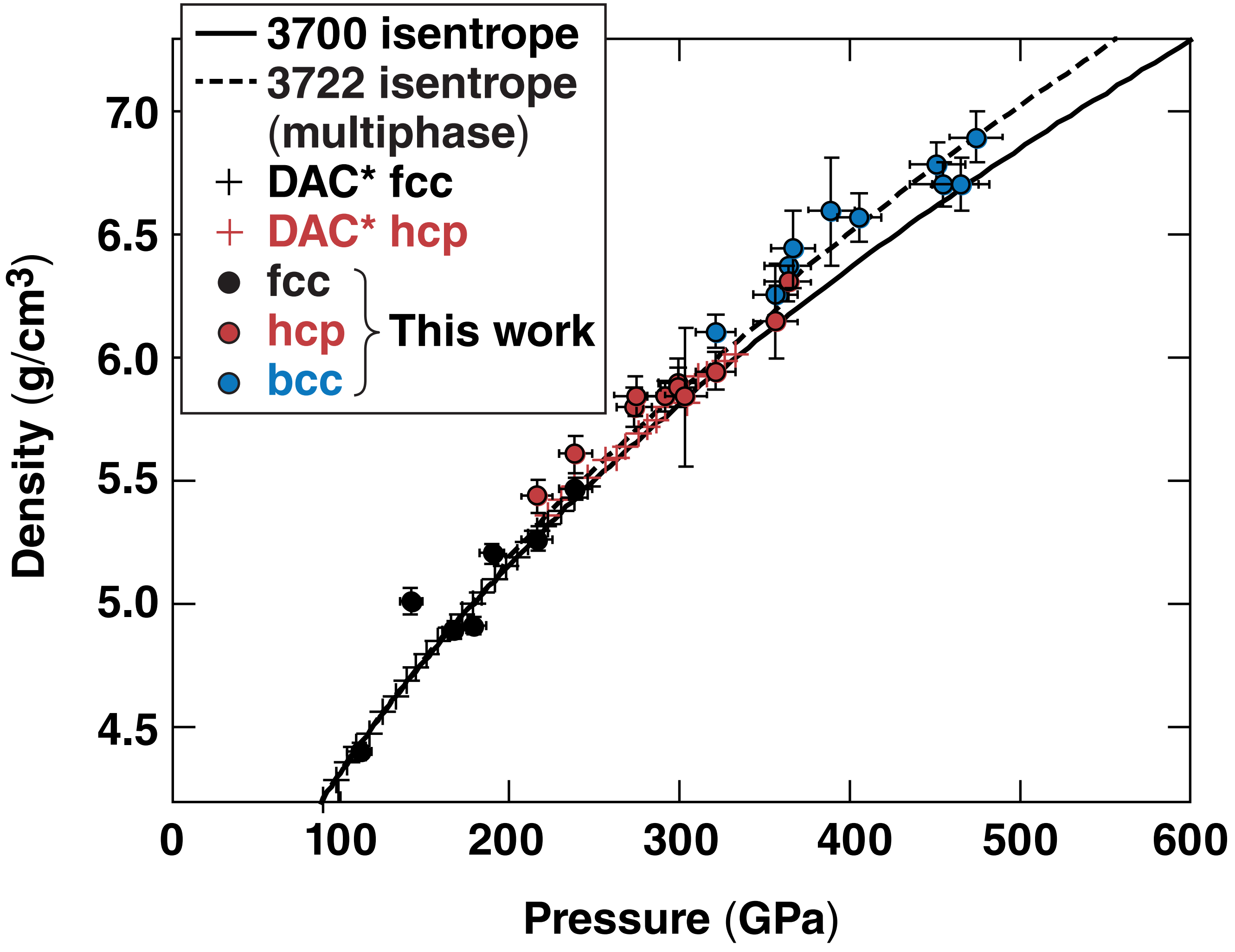






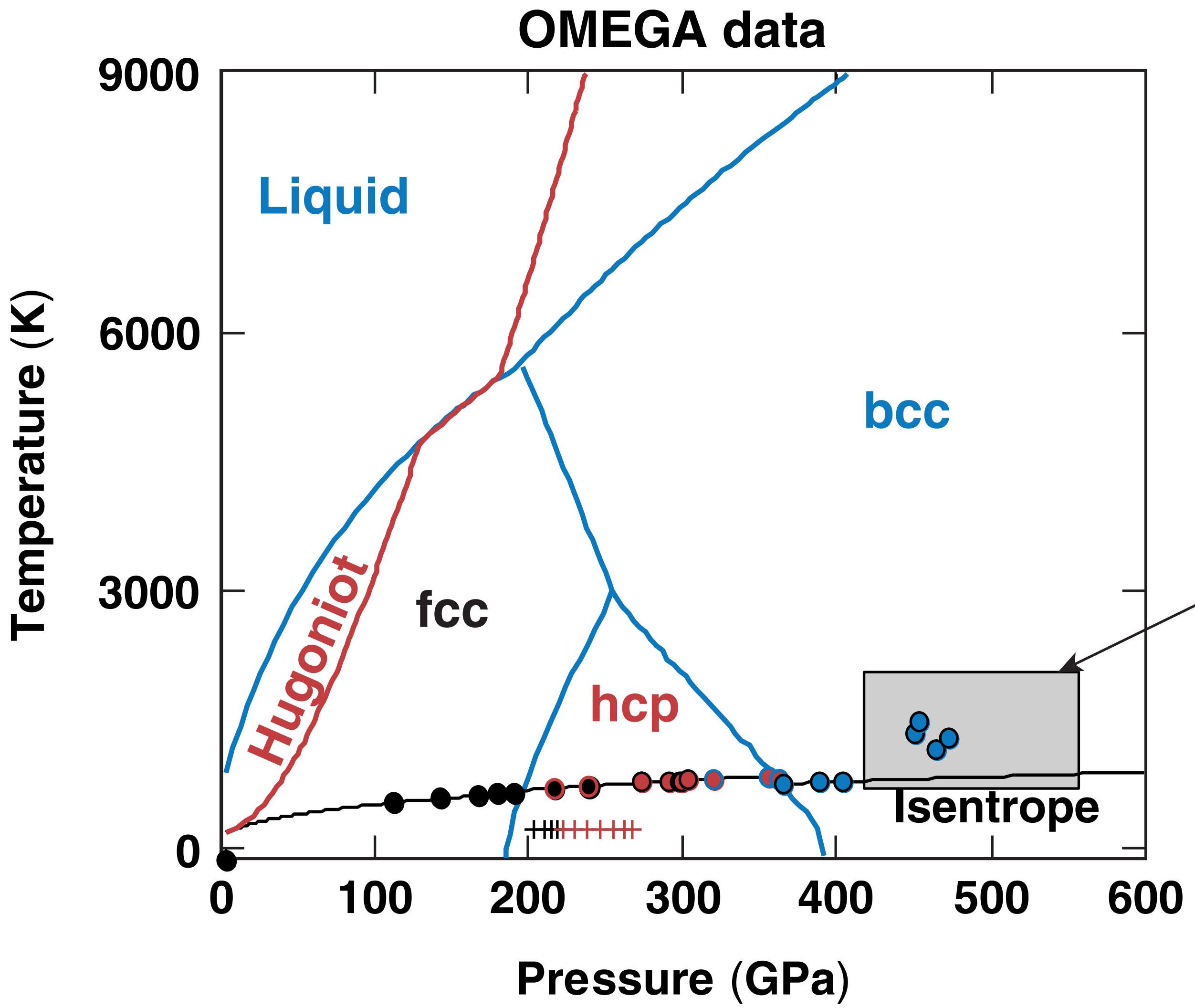
The fcc–hcp and hcp–bcc phase transformations are observed at 216±9 GPa and 321±12 GPa, respectively





*Y. Akahama *et al.*, Phys. Rev. Lett. 96, 045505 (2006).

The fcc–hcp and hcp–bcc phase transformations are observed at 216±9 GPa and 321±12 GPa, respectively



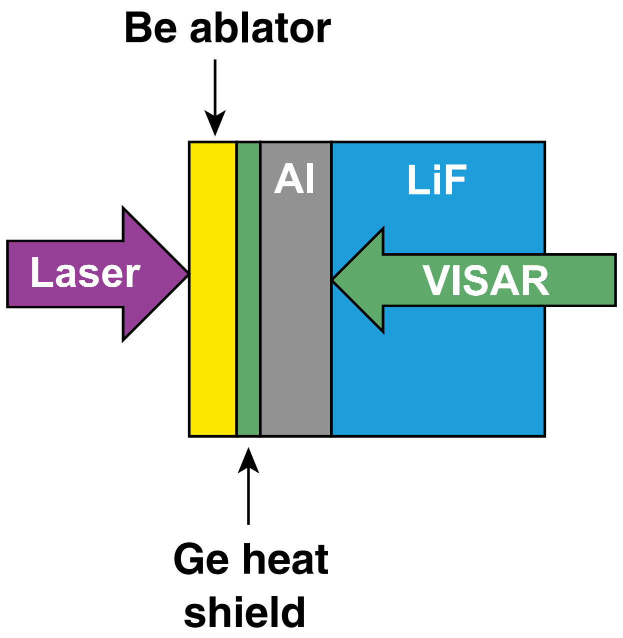
At higher pressures, the ramp is steeper and small shocks start to form. The aluminum still remains solid.

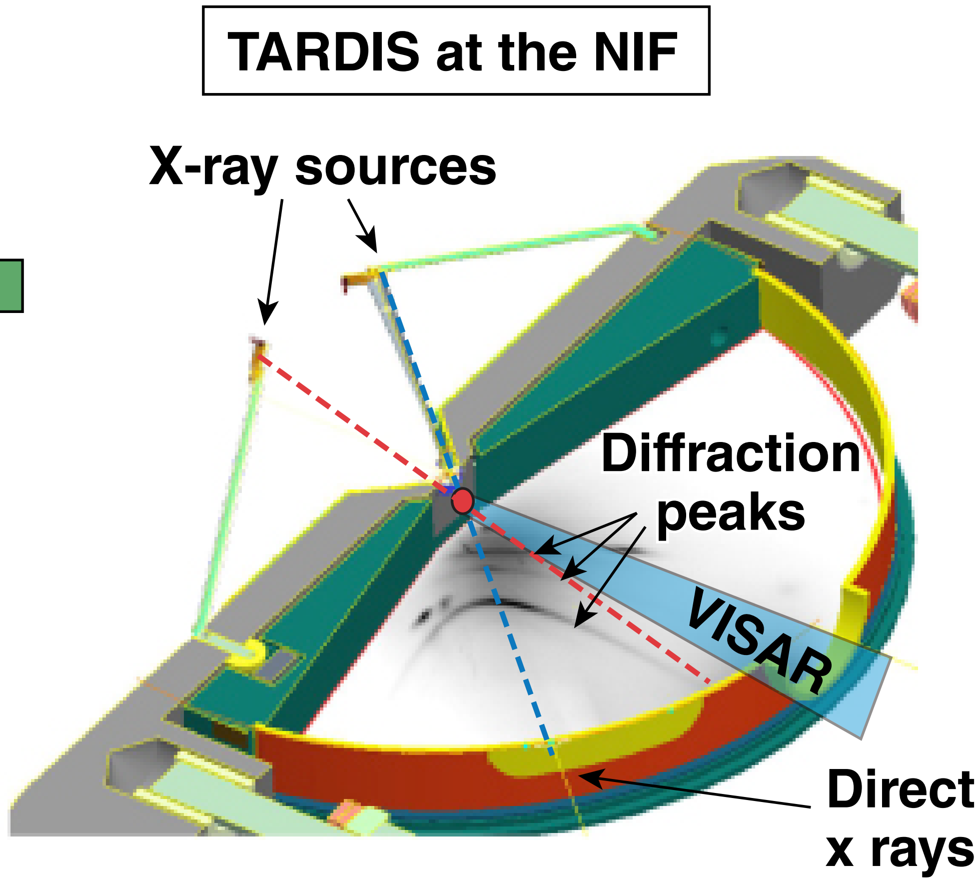
E26667a

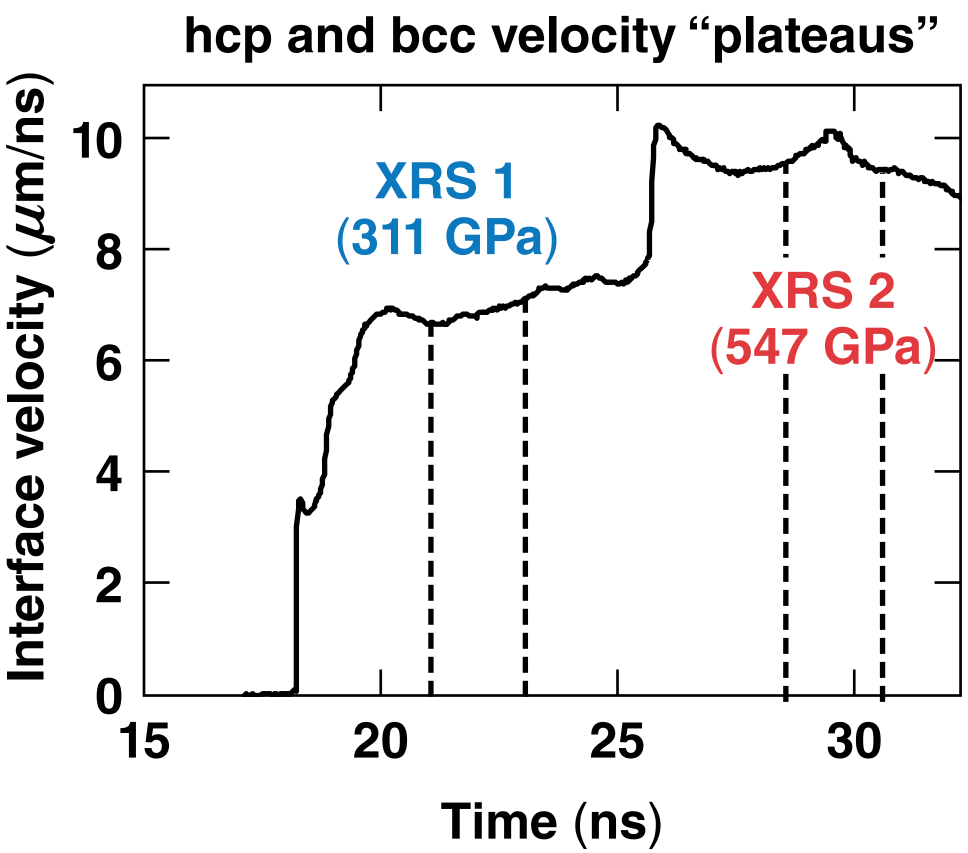
Outline

- OMEGA diffraction experiments
- NIF experiment
  - – dual backlighter
- Texture evolution

A 30-ns ramp pulse held the pressure in the Al constant for over 2 ns at two different pressures where the hcp and bcc phases were observed on OMEGA

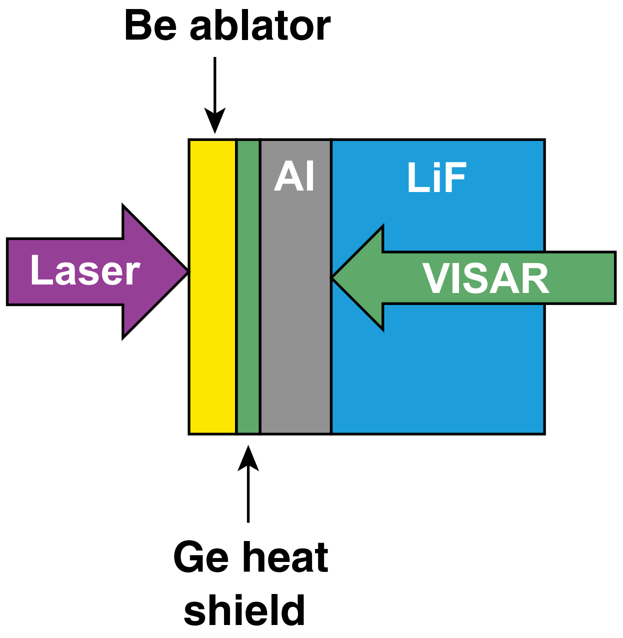


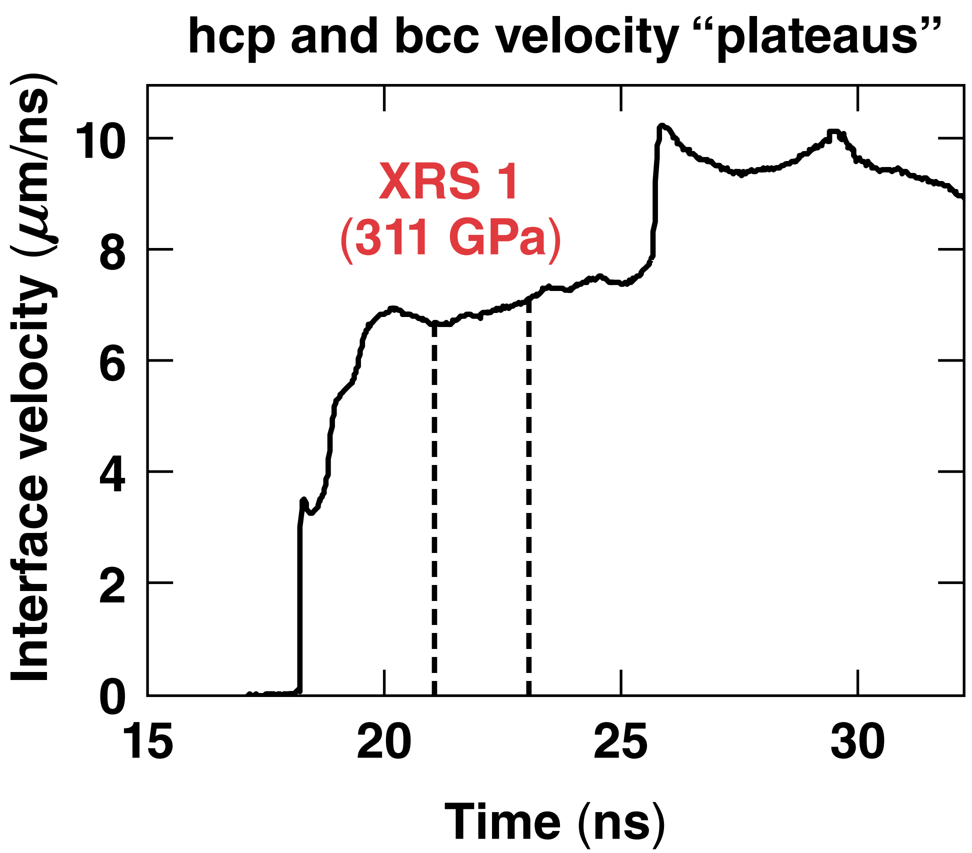


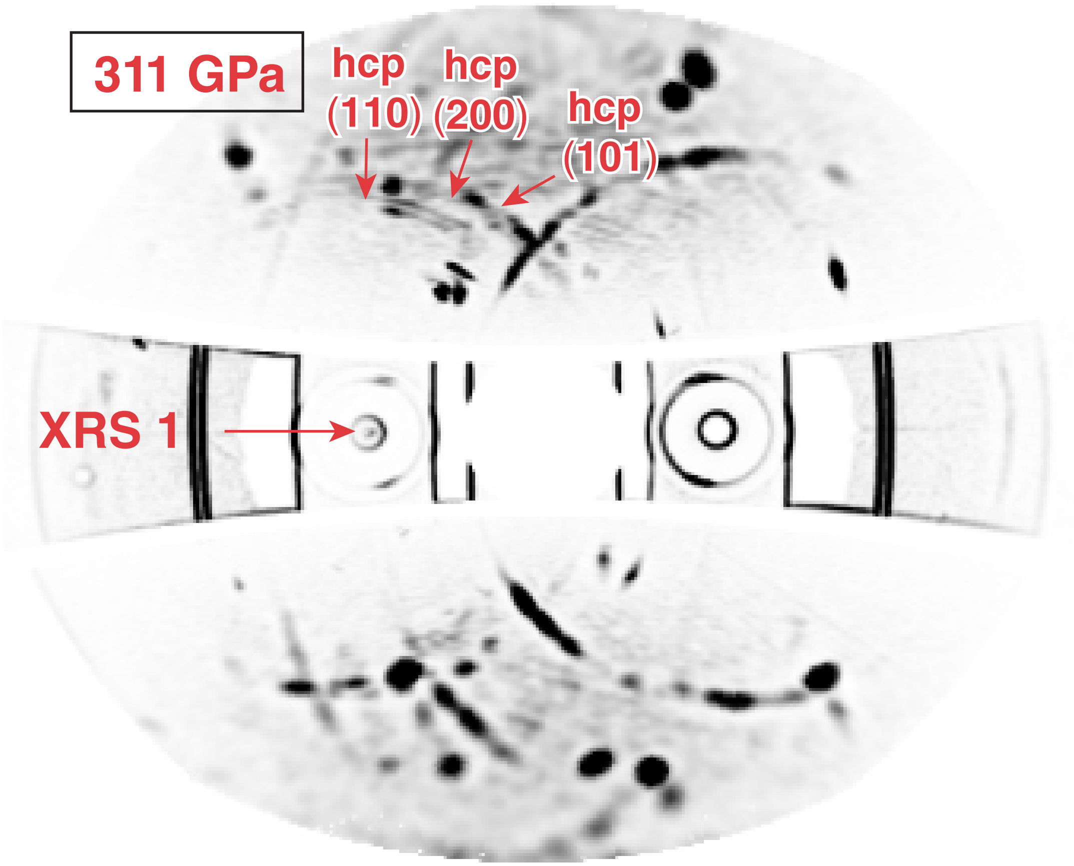


E26669

The hcp phase is observed at 311 GPa

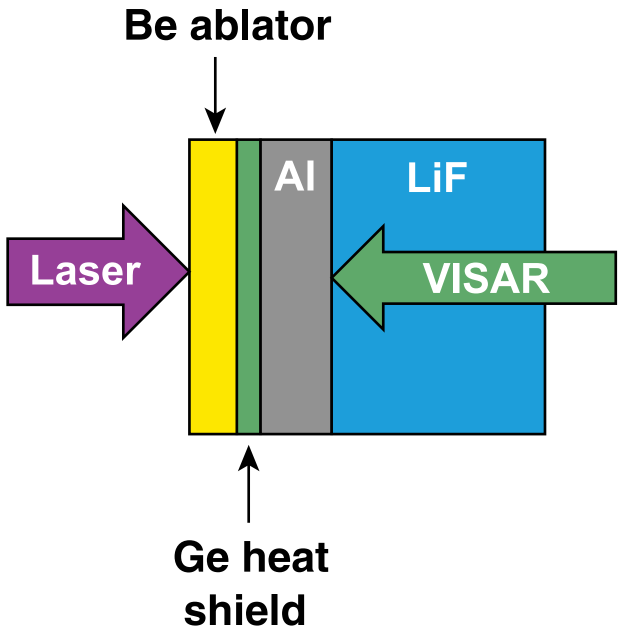


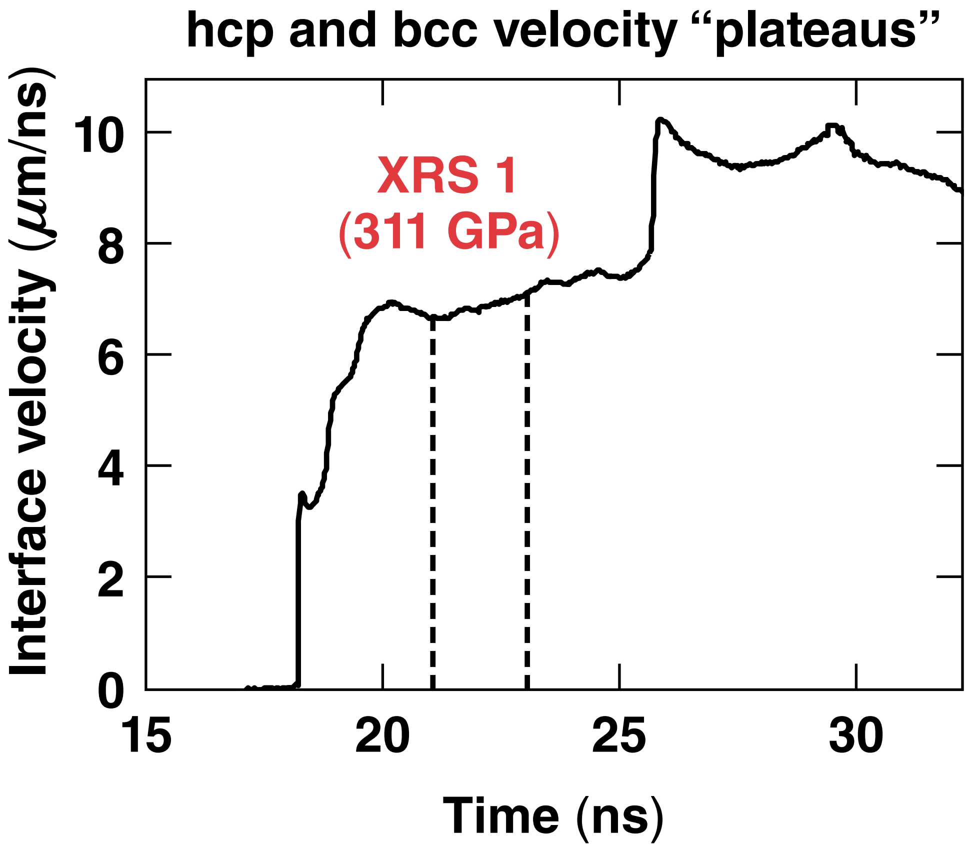


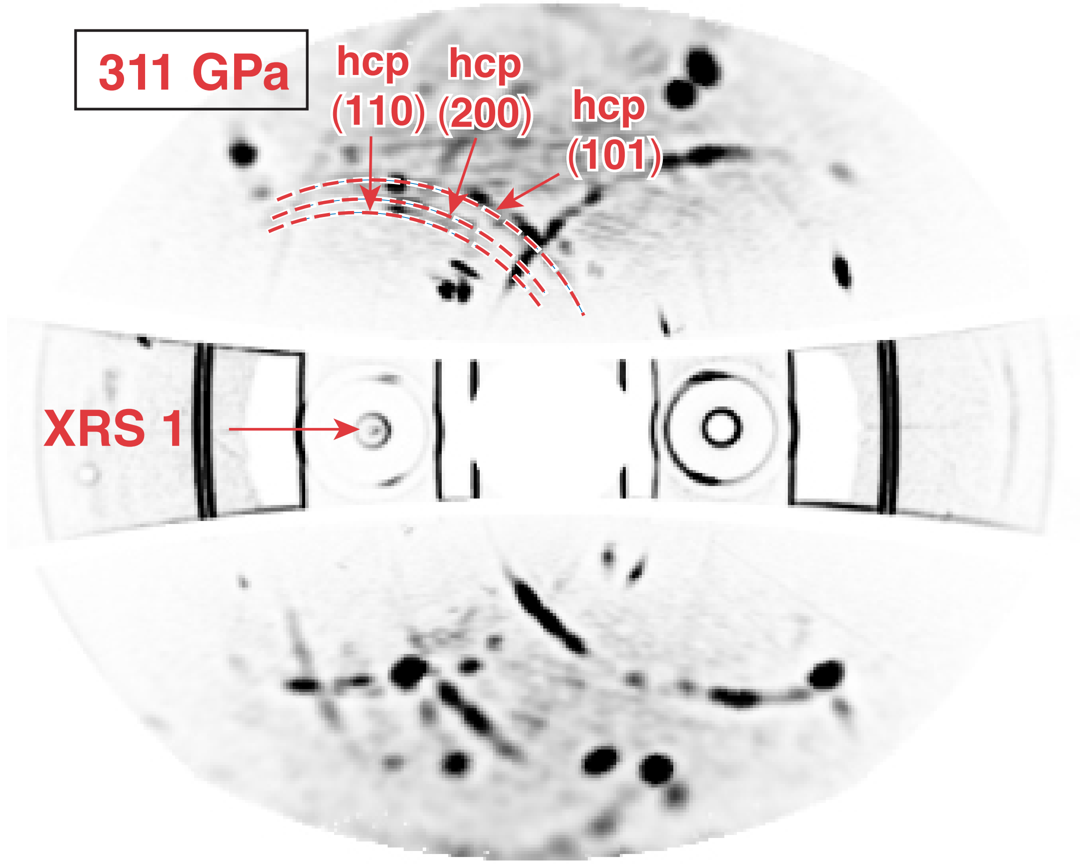


E26670a

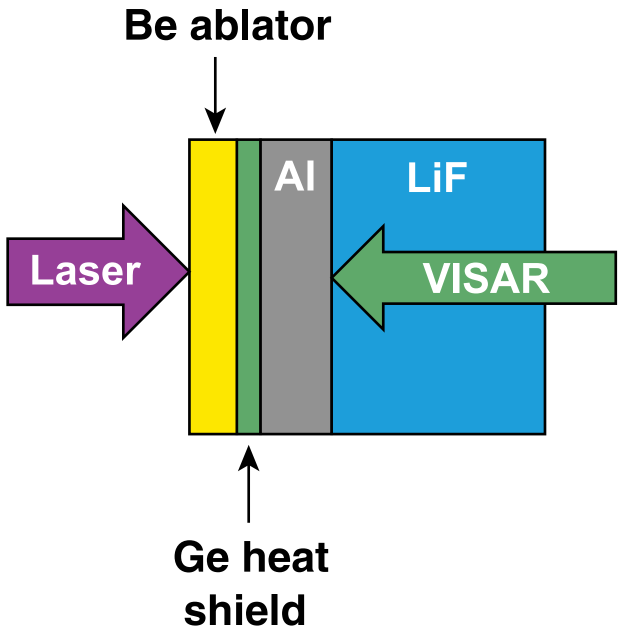
The hcp phase is observed at 311 GPa

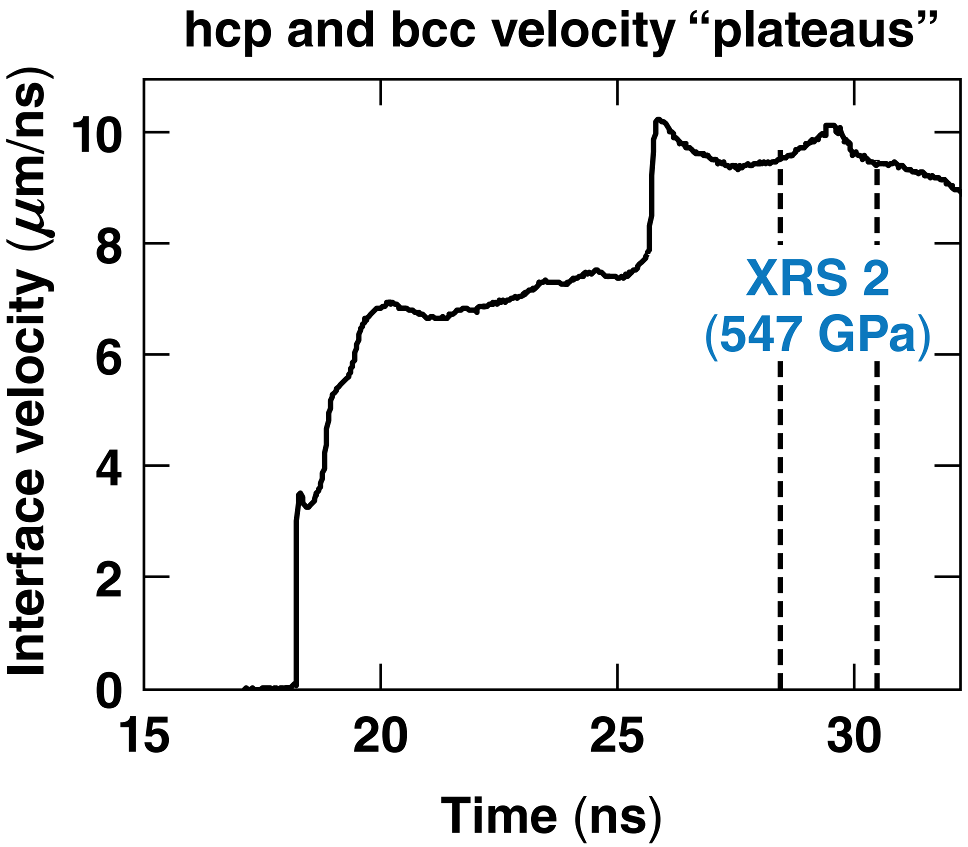


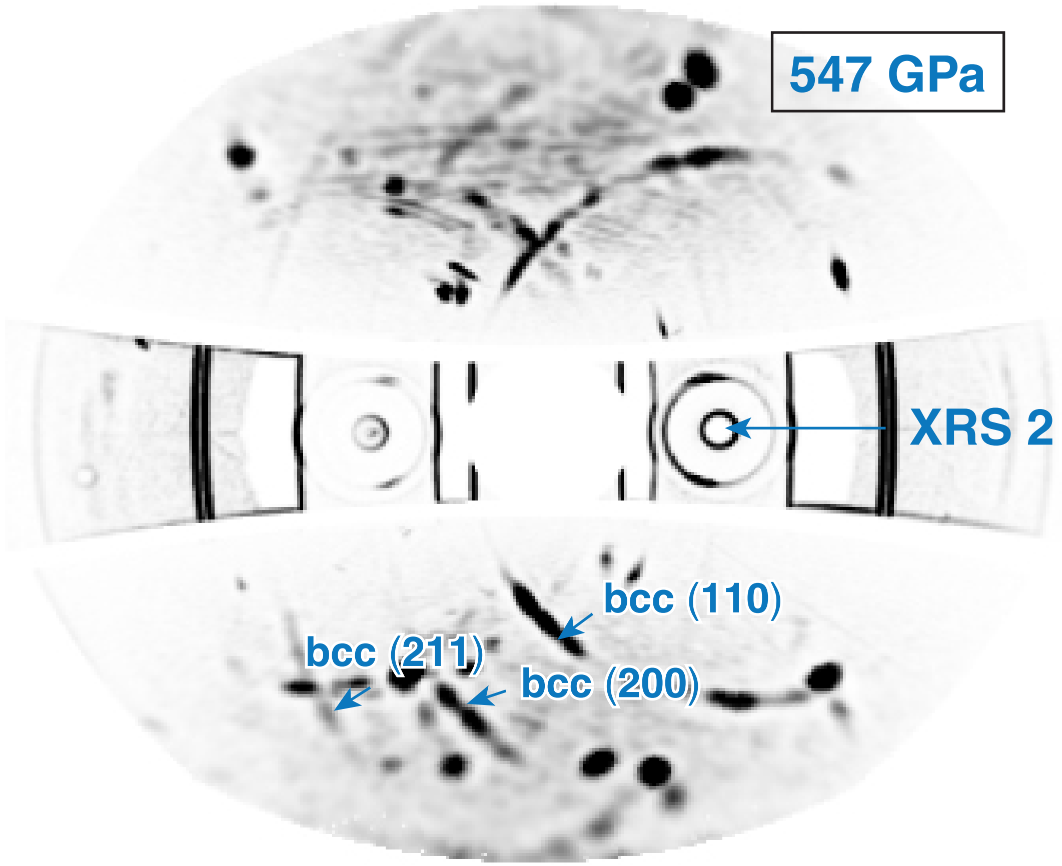




Three lines from the bcc phase are observed at 547 GPa

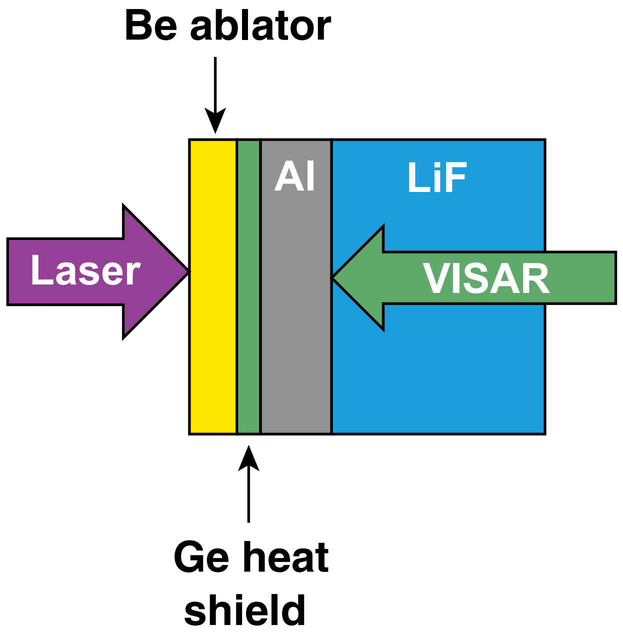


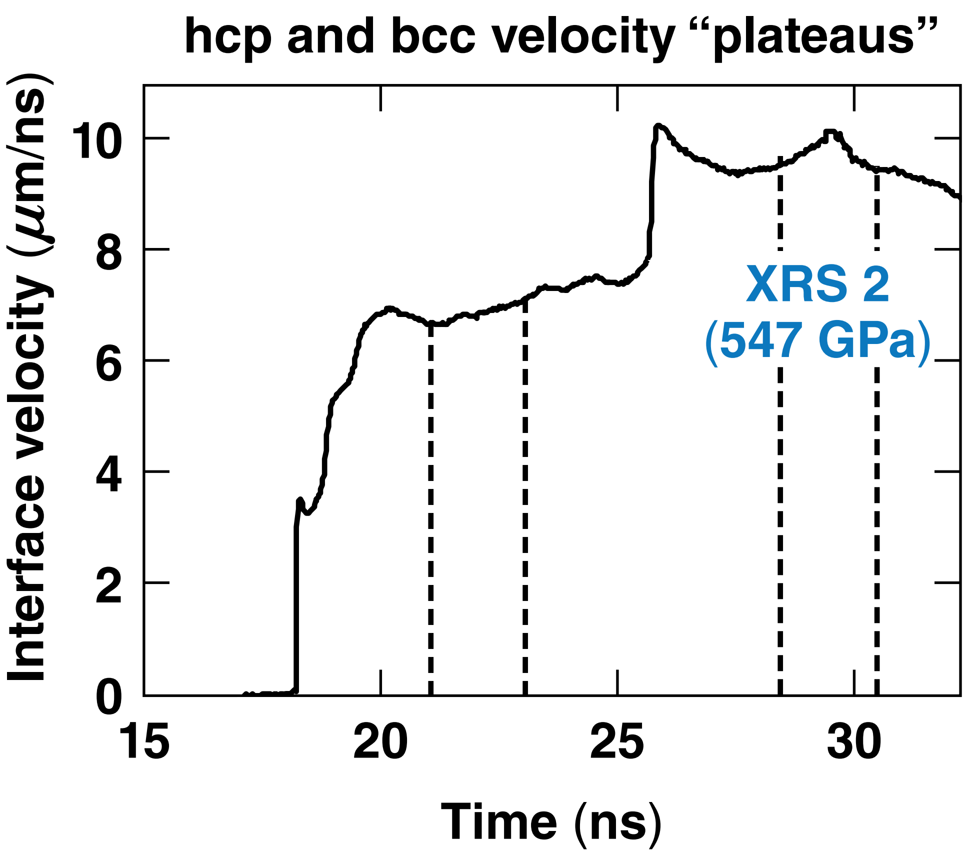


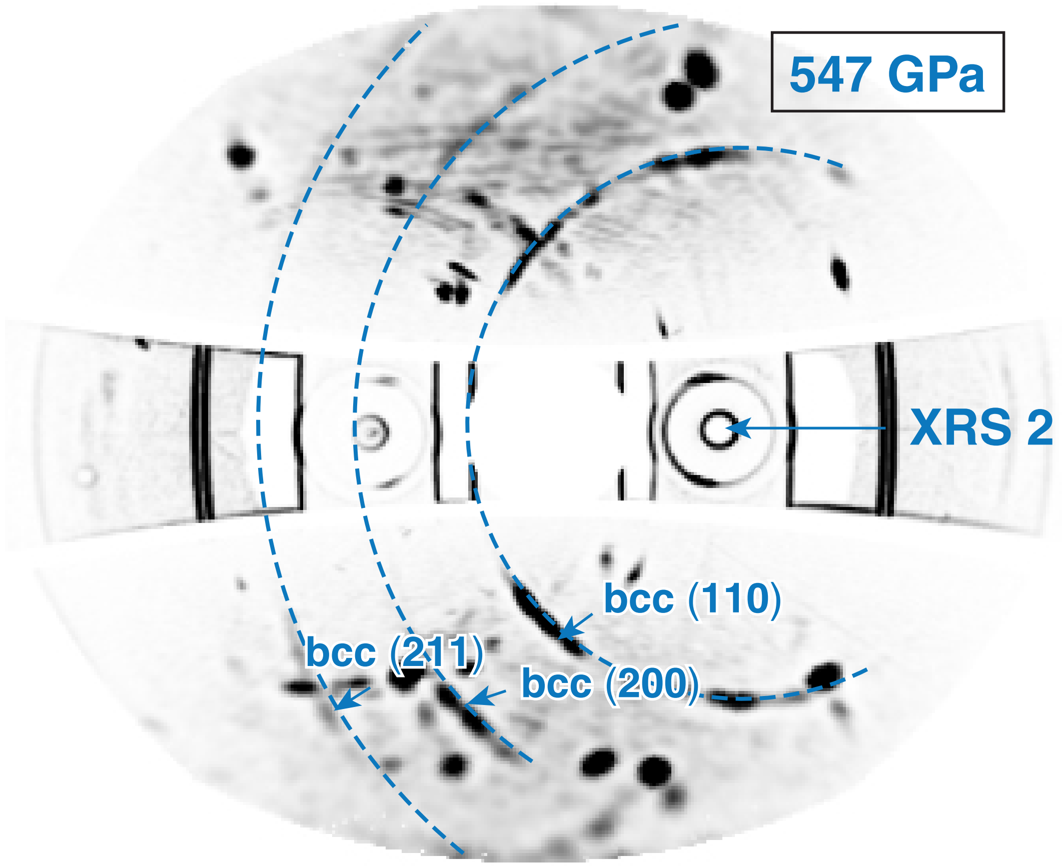


E26670c

Three lines from the bcc phase are observed at 547 GPa

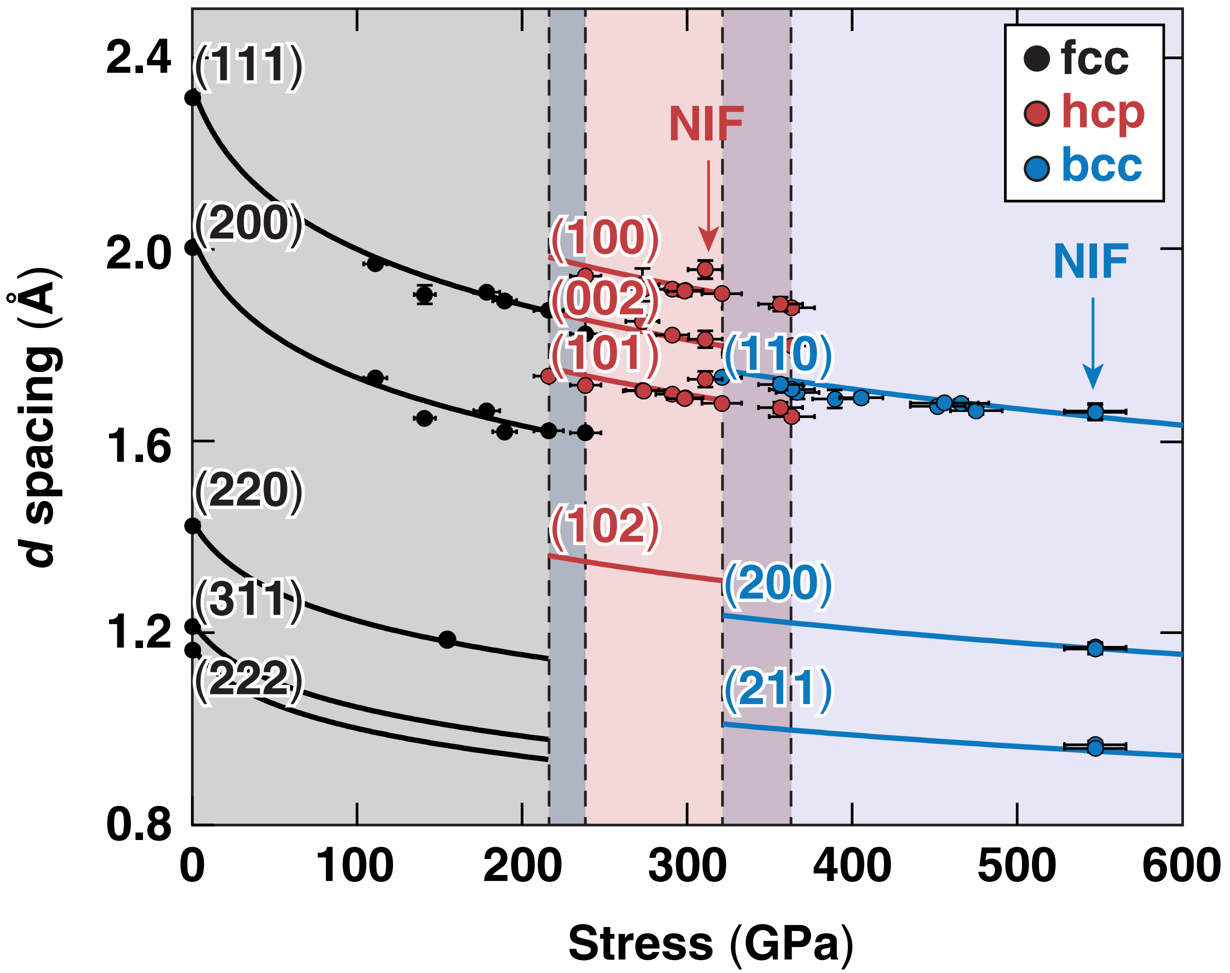


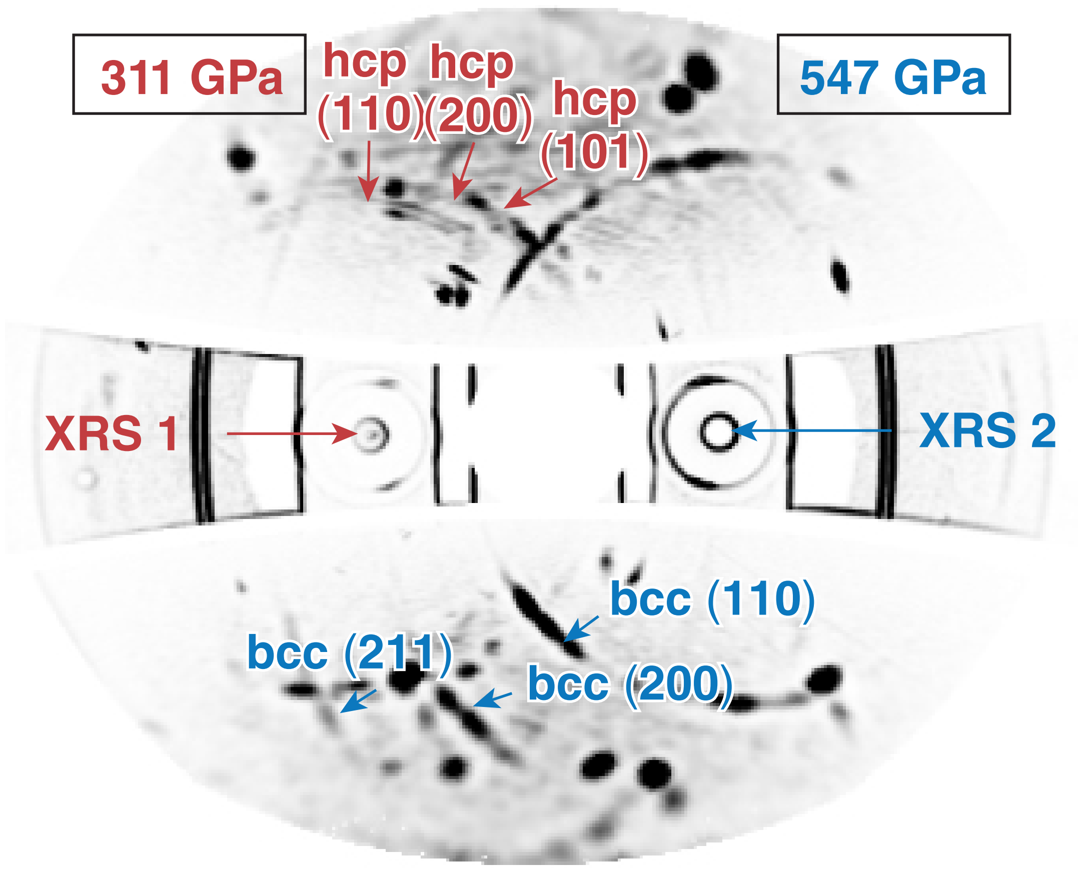




E26670d

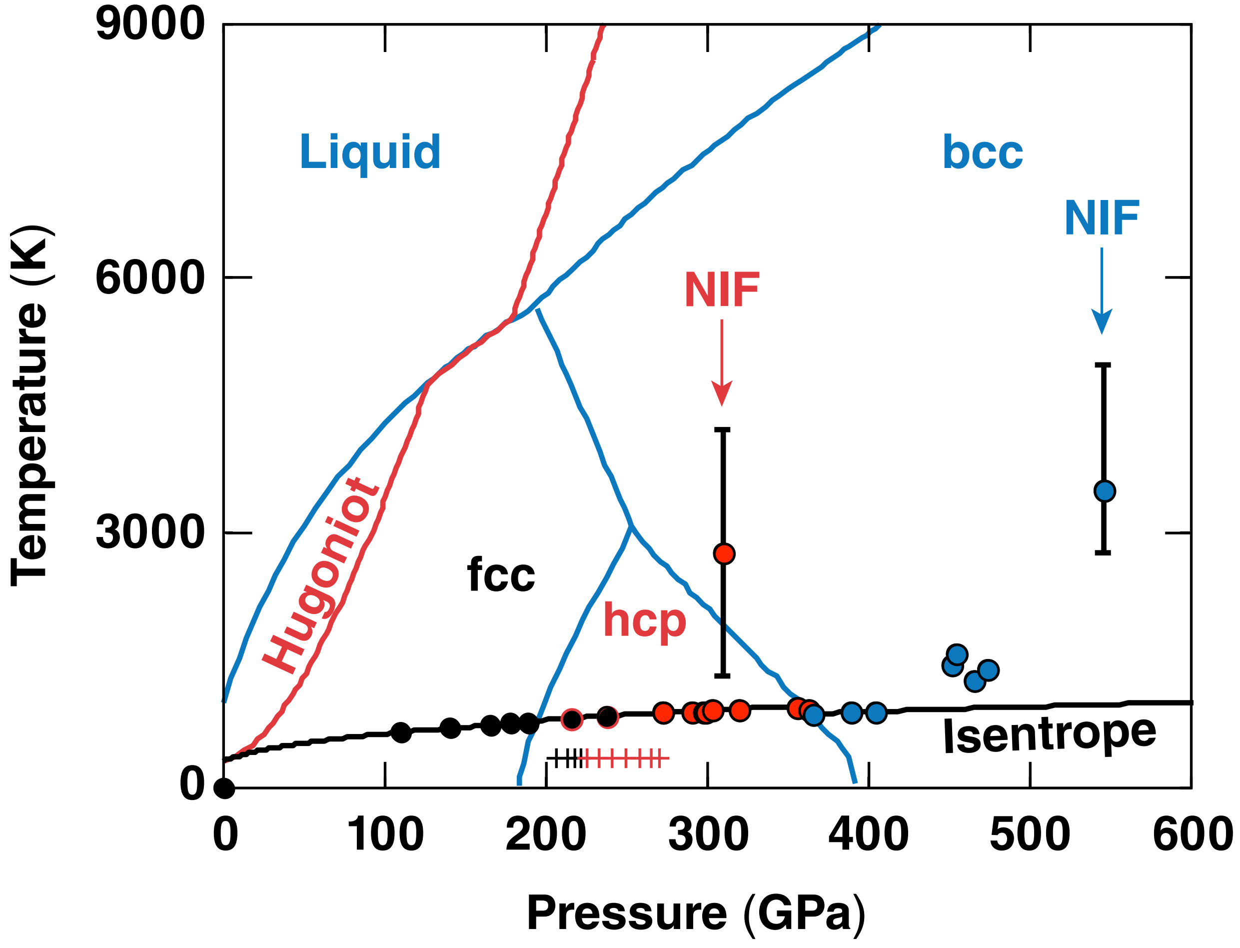
NIF experiments probe two high-pressure phases in a single shot and confirm the bcc phase in OMEGA data



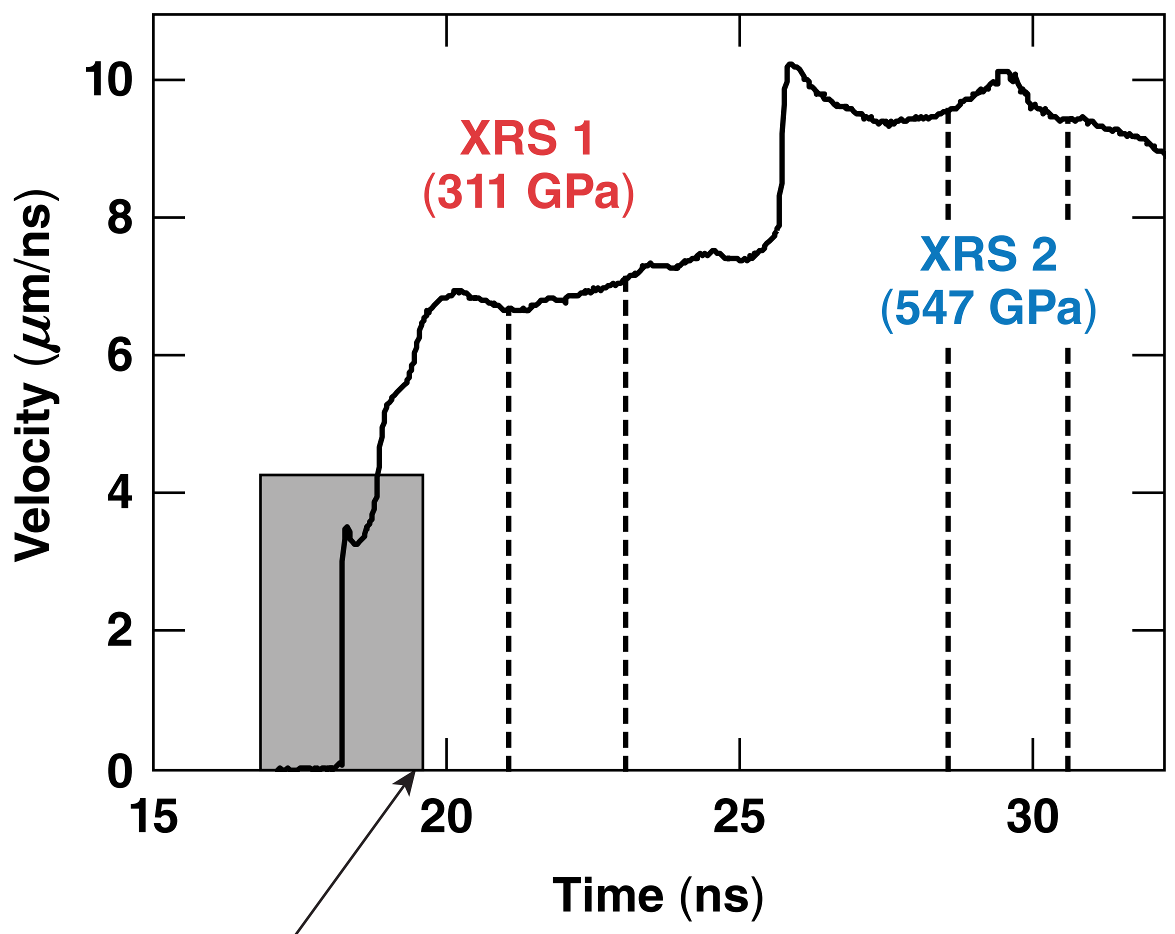


E26785

A calculated shock-ramp–compression path for the NIF experiment suggests the hcp phase is stable at higher temperatures than calculated by DFT



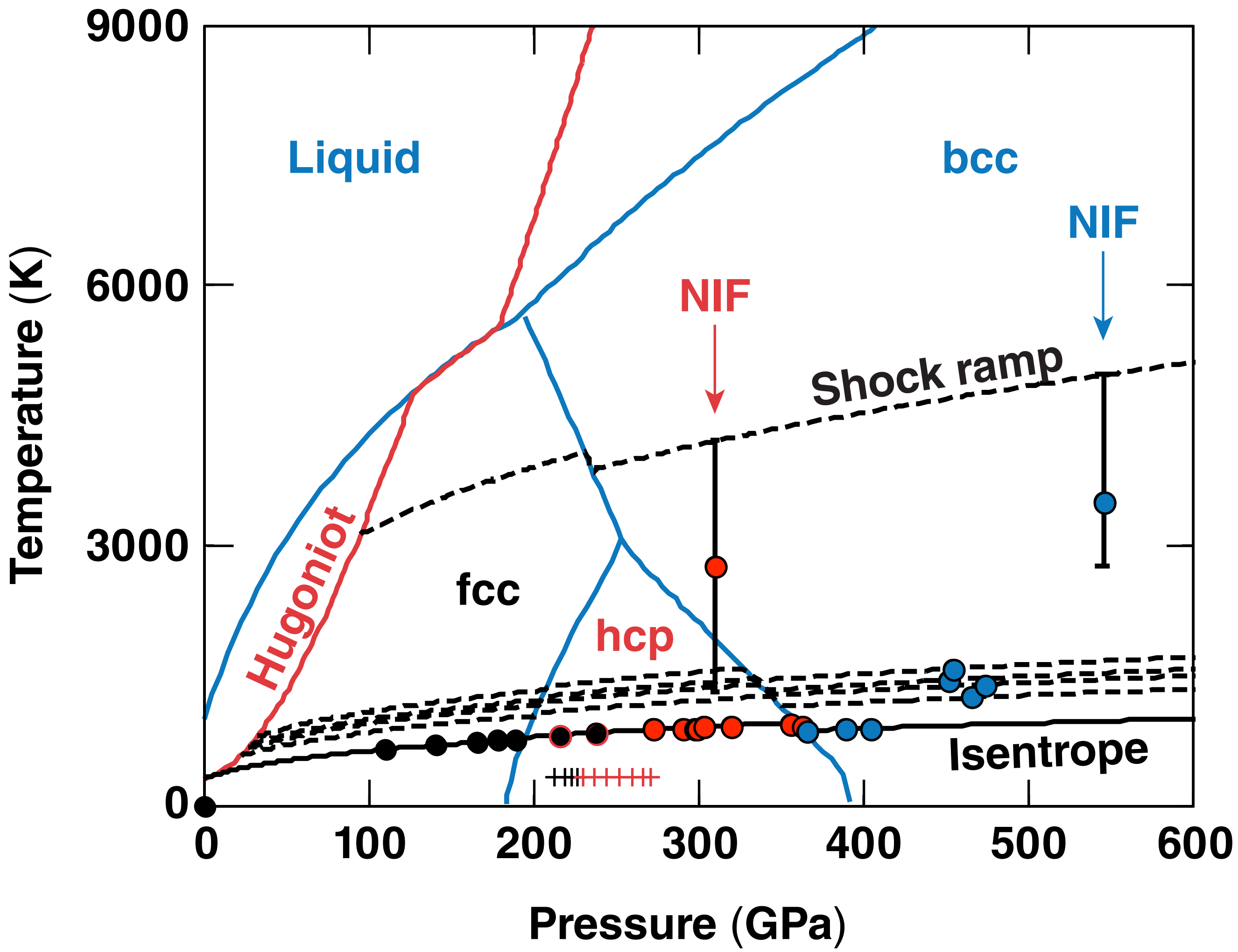
hcp and bcc velocity "plateaus"



Shock observed at Al–LiF interface (100 GPa, 3100 K).

E26672

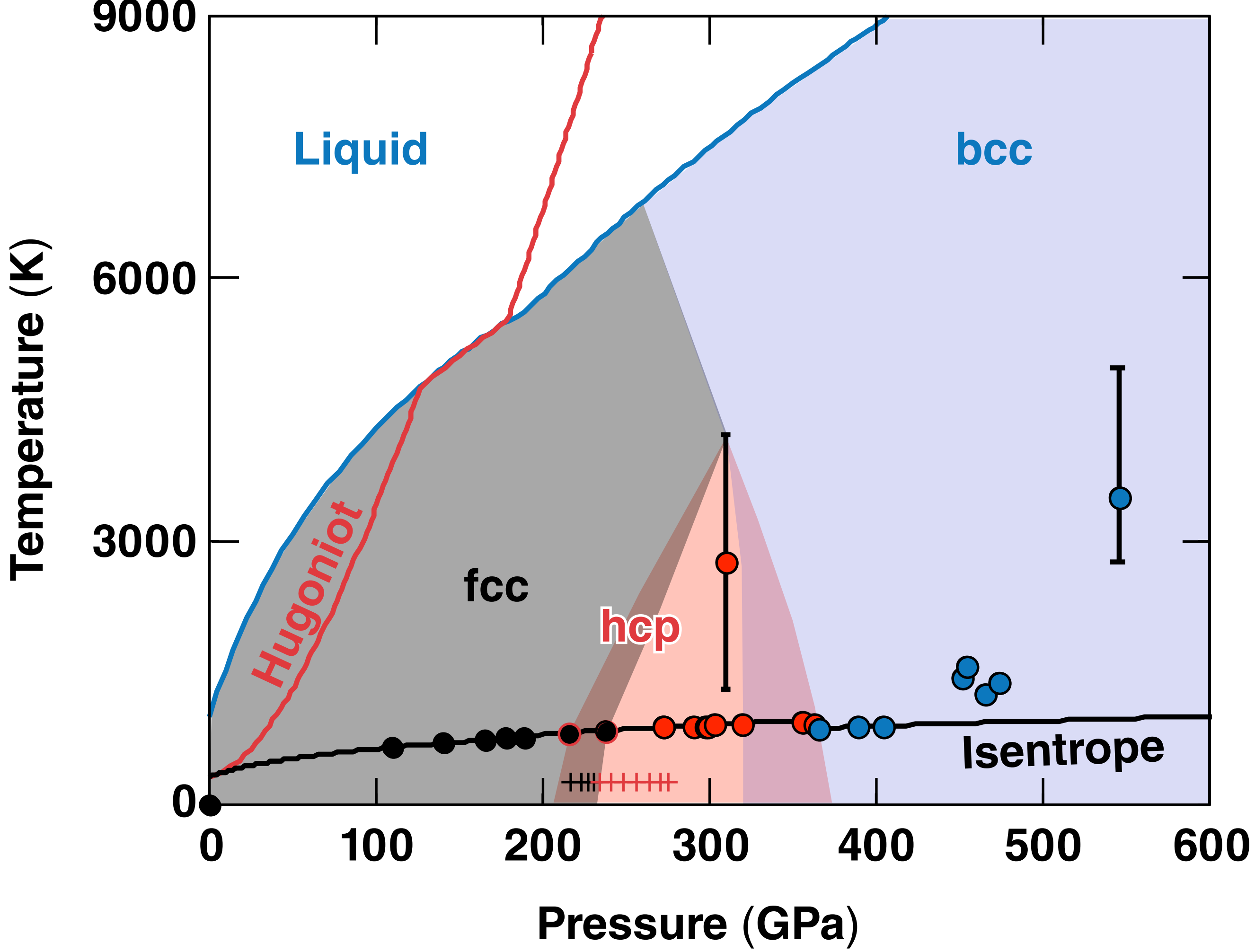
A calculated shock-ramp–compression path for the NIF experiment suggests the hcp phase is more stable at higher temperatures than calculated by DFT



The Al in the NIF data is at an elevated temperature state compared to the Al in the OMEGA data as a resut of shock heating.

A calculated shock-ramp–compression path for the NIF experiment suggests the hcp phase is more stable at higher temperatures than calculated by DFT

Notional phase diagram



These data provide key experimental benchmarks for DFT calculations.

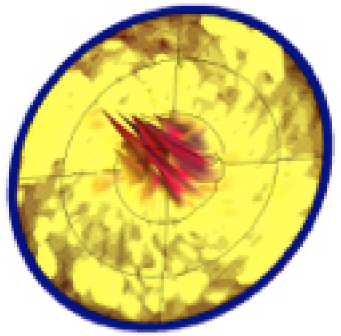
E26673

Outline

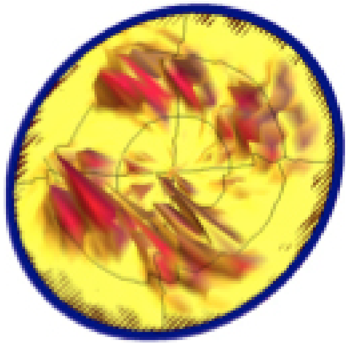
- OMEGA diffraction experiments
- NIF experiment
  - dual backlighter
- **Texture evolution**

The rolled foils were characterized on a diffractometer beforehand and show (200) plane normals are nearly parallel to the pressure loading axis

Al (200) pole figure

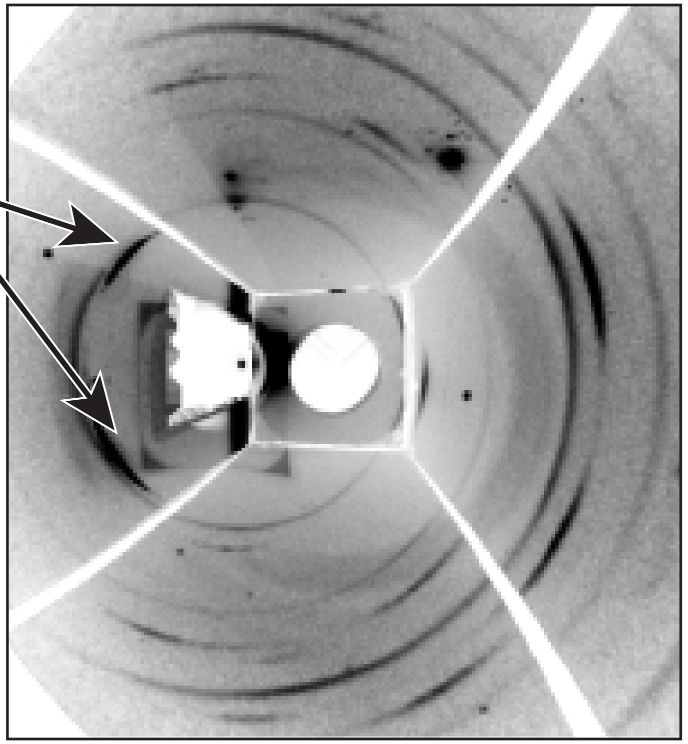


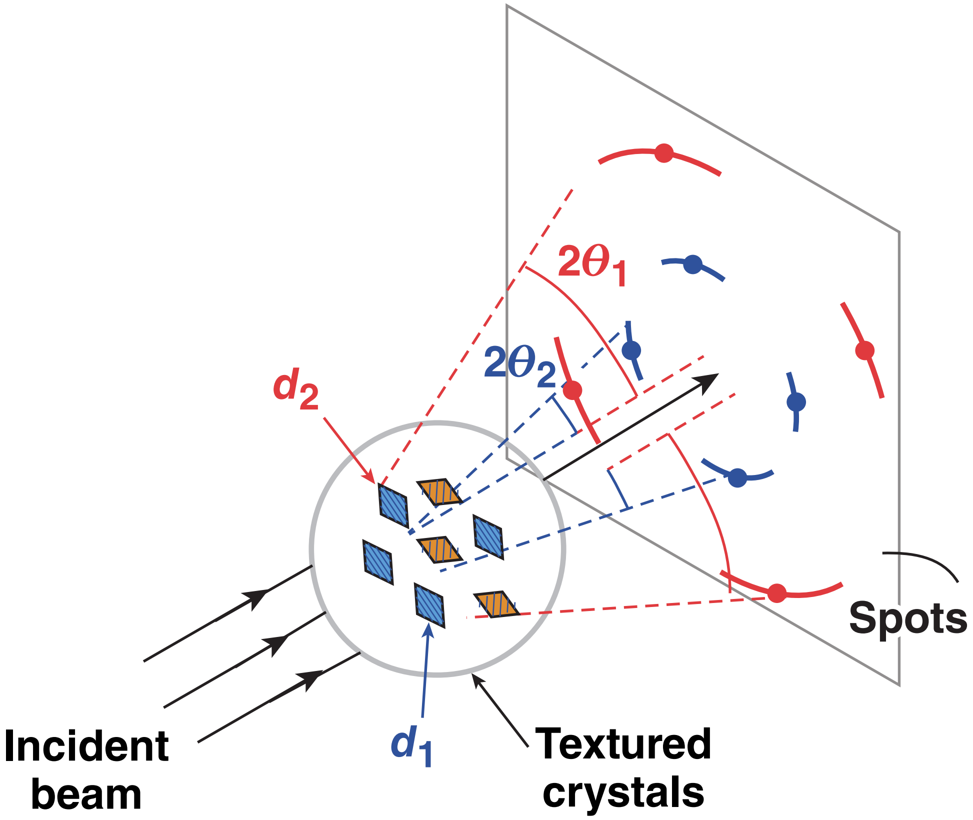
Al (111) pole figure



Rolled Al foil

Al (111) "spots"

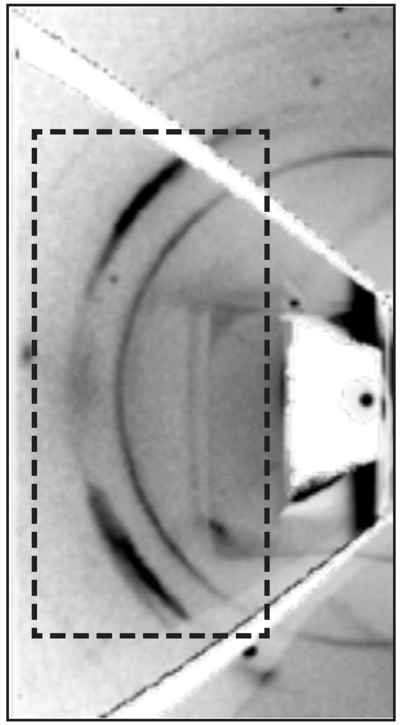




Crystallographic texture is the distribution of grain orientations in a polycrystalline sample. Textured foils diffract into spots rather than continuous rings.

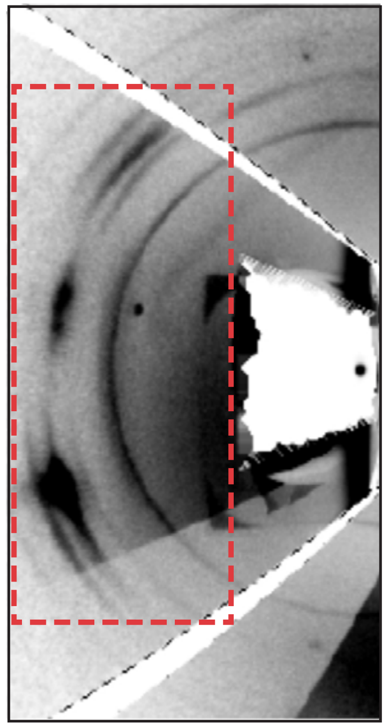
The initial texture of the rolled foils is maintained through the fcc—hcp and hcp—bcc phase transitions

fcc (111) 216 GPa



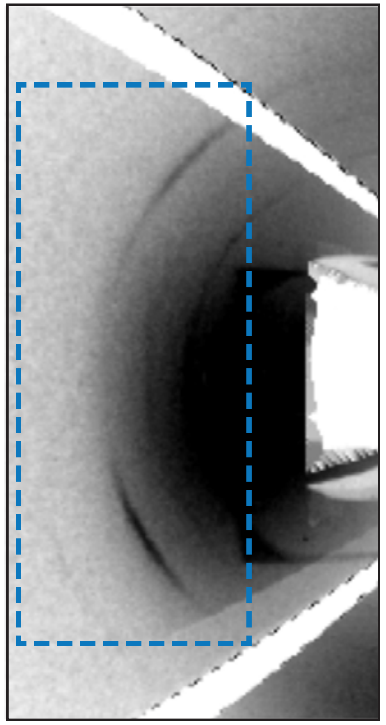
Shot 23765

hcp (002) 291 GPa



Shot 24289

bcc (110) 456 GPa



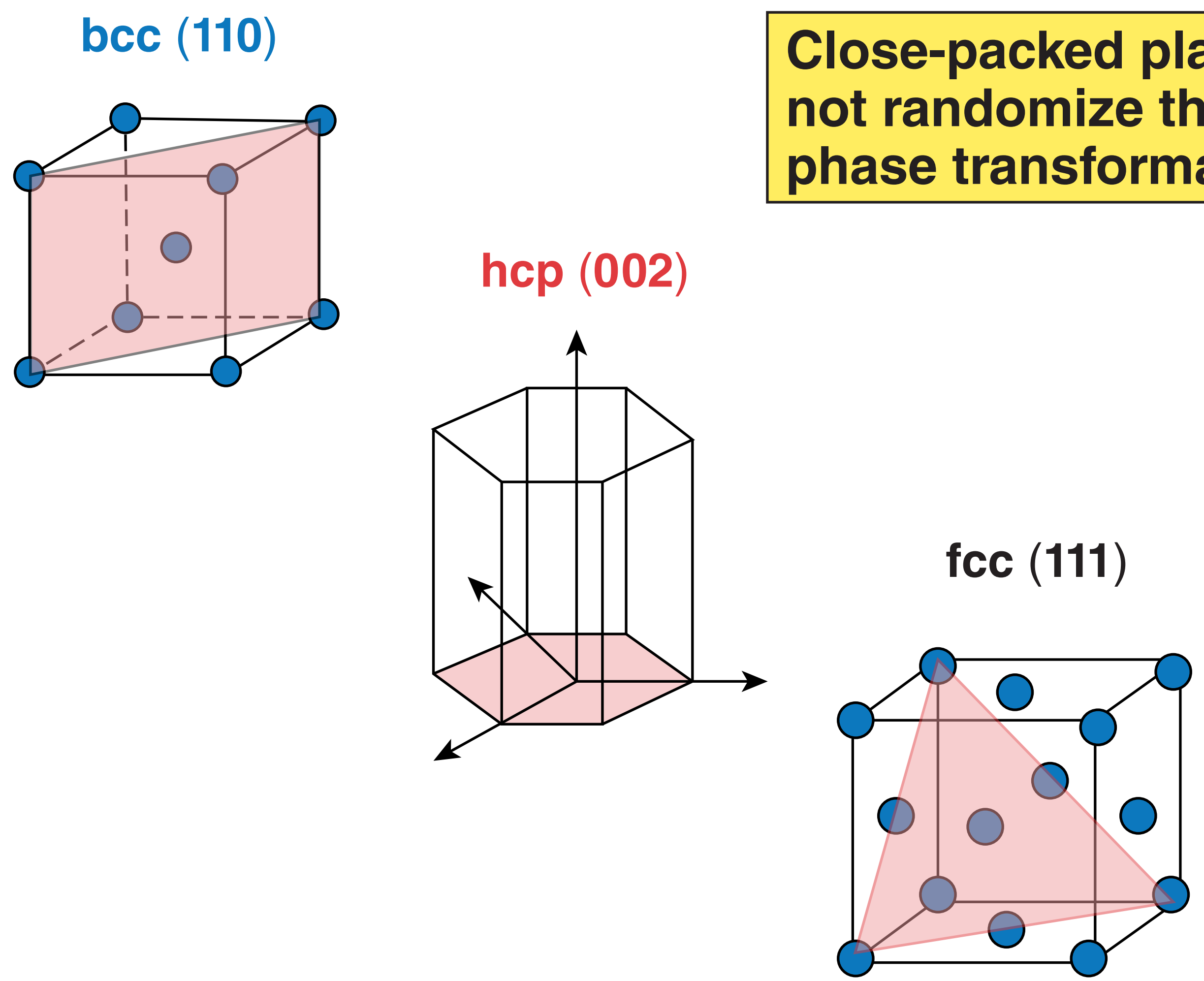
Shot 24556

The preferred orientation in "textured" rolled foils can provide insight into the atomic pathways.

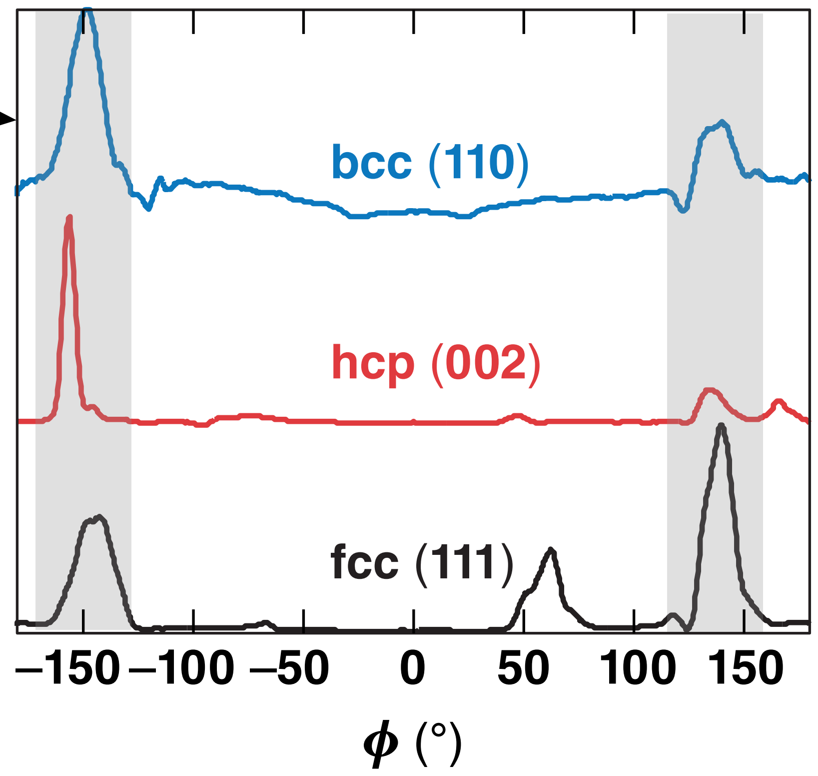
E26677

J. A. Hawreliak *et al.*, Phys. Rev. B 83, 144114 (2011).

We expect diffraction lines should become more powder-like through phase transformations as atoms rearrange



Close-packed planes do not randomize through the phase transformations.



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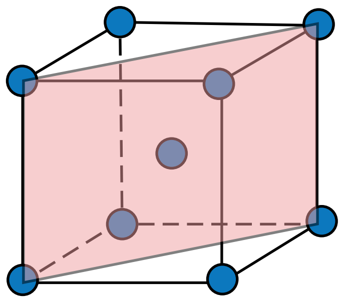
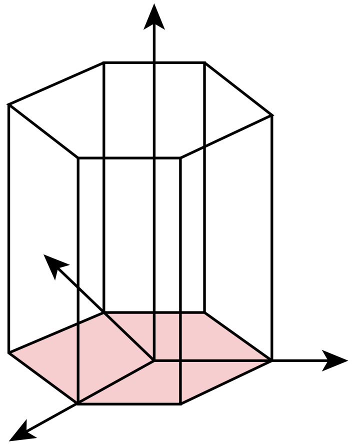
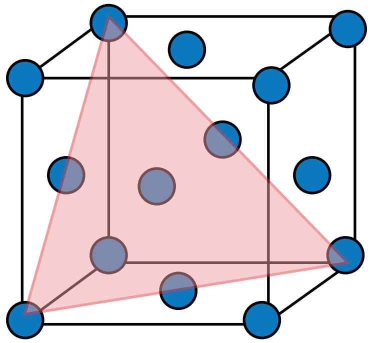
The high-pressure texture of the hcp and bcc phases suggests close-packed or nearly close-packed lattice planes remain parallel through both transformations

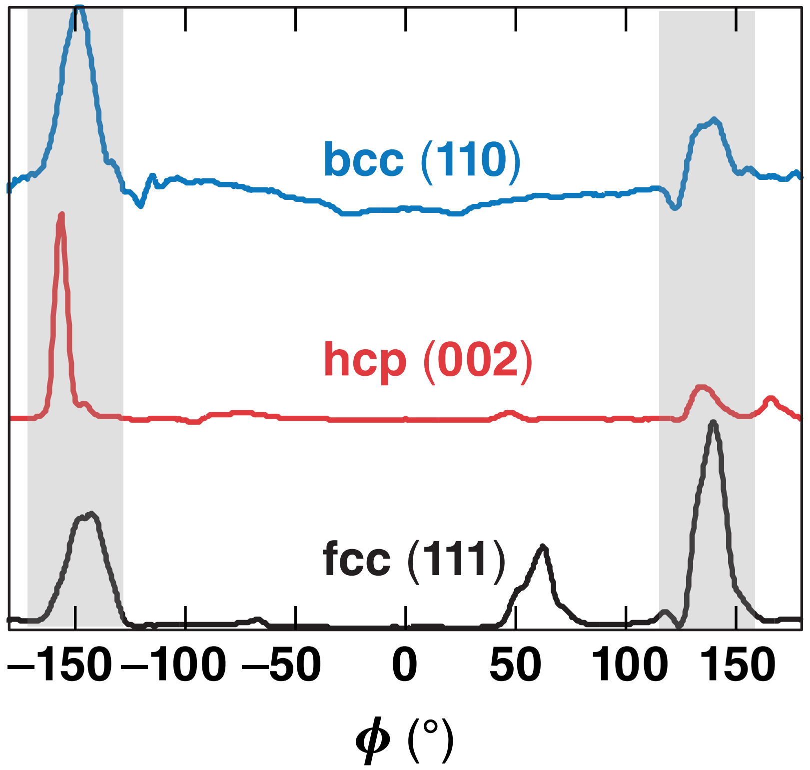




Shoji–Nishiyama OR:*
$\{111\}_{fcc}$ // $\{0001\}_{hcp}$

Burgers OR:**
$\{0001\}_{hcp}$ // $\{110\}_{bcc}$





Z. Nishiyama, *Martensitic Transformation*, edited by M. Fine *et al.*, 1st ed., Materials Science Series (Academic Press, New York, 1978); W. G. Burgers, Physica 1, 561 (1934).
*Orientation relationship

We present the first *in-situ* high-pressure observation of bcc aluminum

- Aluminum and other prototypical *sp*-bonded materials are predicted to transform into complex, open, and incommensurate structures at multiterapascal pressures
- High-power lasers ramp compressed Al and nanosecond *in-situ* x-ray diffraction (XRD) measured the crystal structure at pressures of 111 GPa to 547 GPa
- The fcc–hcp and hcp–bcc phase transformations are observed at 216±9 GPa and 321±12 GPa, respectively
- Texture evolution shows that even on nanosecond time scales, atoms can rearrange in the spaces between close-packed planes

Kinetics of phase transitions will be studied using time-resolved x-ray diffraction.*

E26644

*R. Benedetti *et al.*, YO6.00011, this conference