LLNL-CONF-490363

Ramp-Compression Experiments on Tantalum at the NIF and Omega Lasers

J. H. Eggert

July 7, 2011

JOWOG37
Aldermasten, United Kingdom
July 11, 2011 through July 15, 2011

Disclaimer

HEDP
high energy density physics

The National Ignition Facility

Ramp-Compression Experiments on Tantalum at the NIF and Omega Lasers

JOWOG 37, AWE

July 11, 2011

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This work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Just a few years ago, ultra-high pressure phase diagrams for materials were very simple

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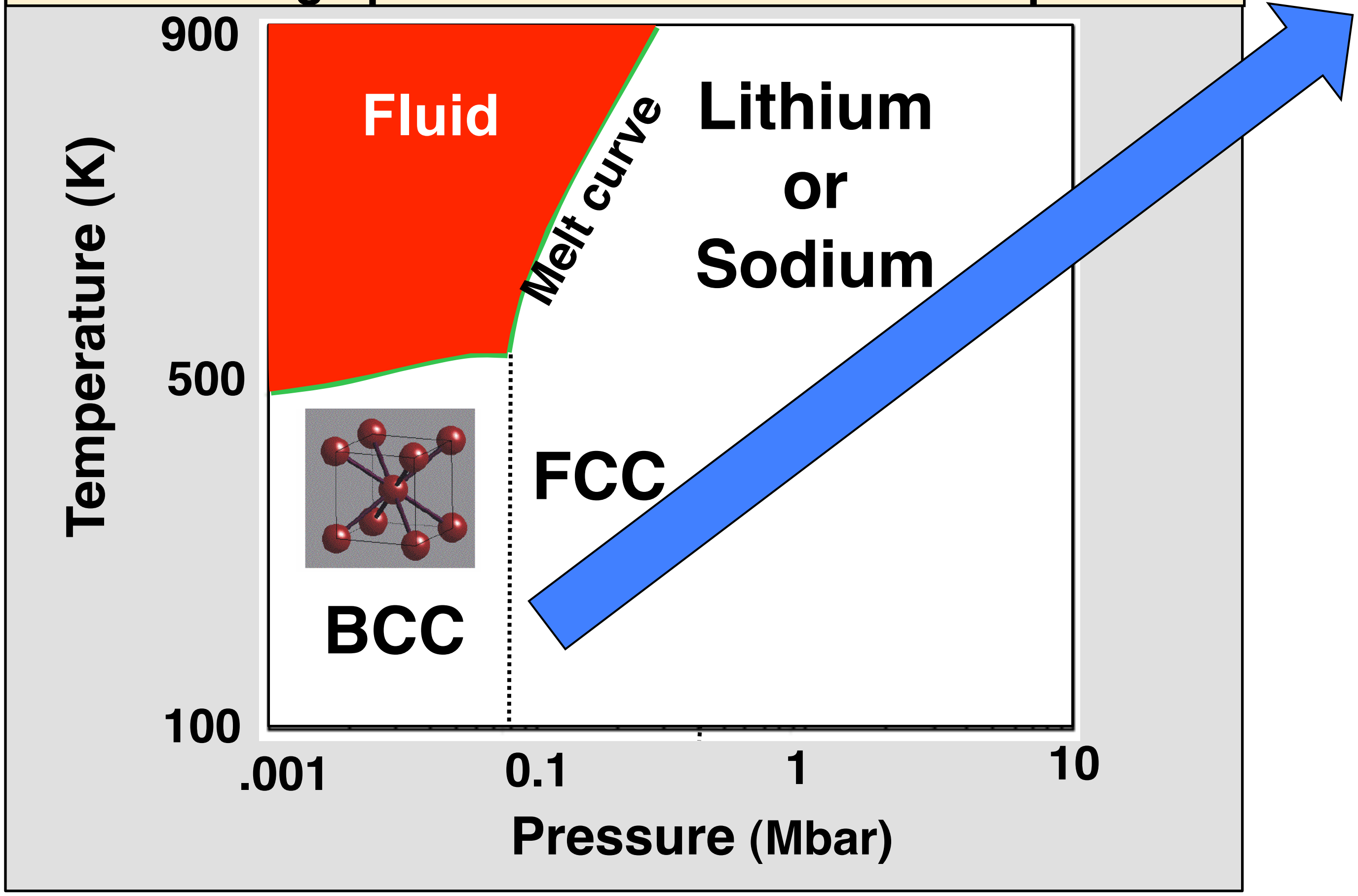
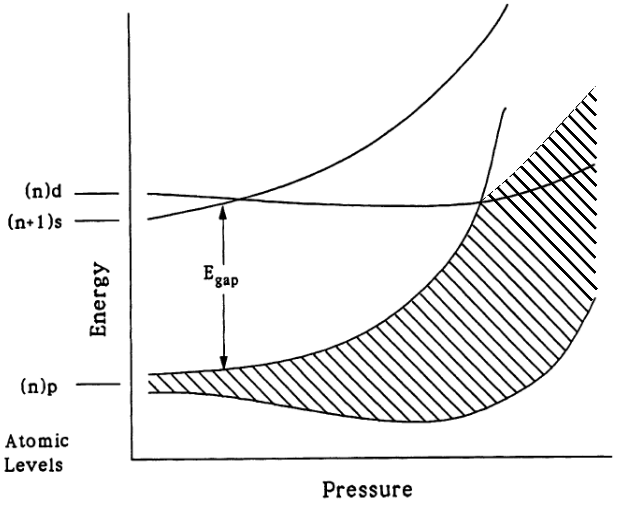
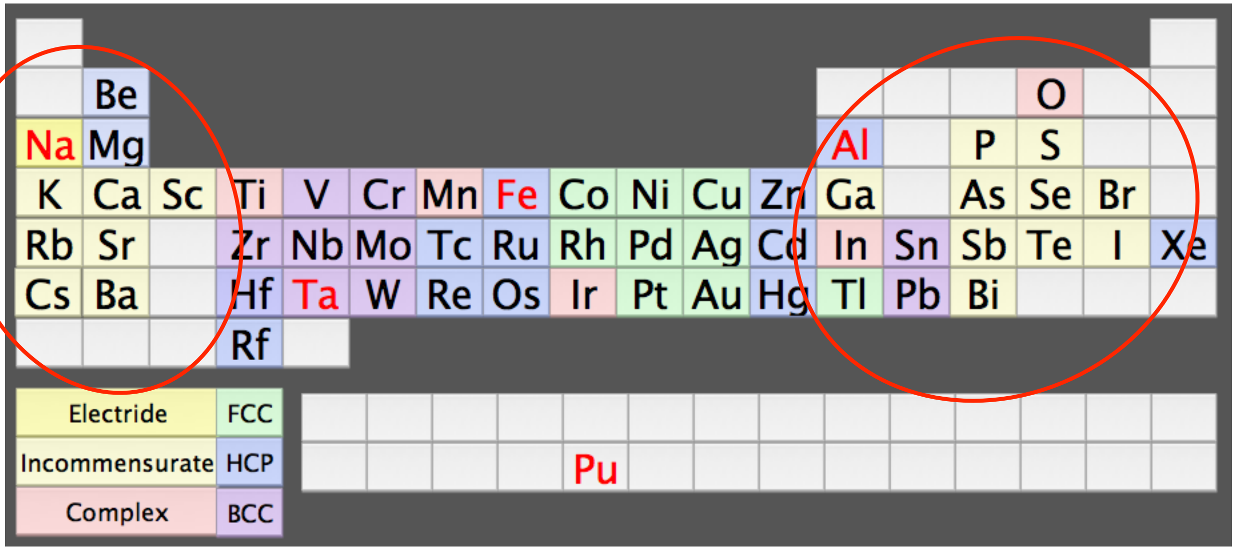
Melt curves typically followed a Lindeman law and high pressure structures were simple



Physics Gets Simple!

Traditional view is not universally borne out



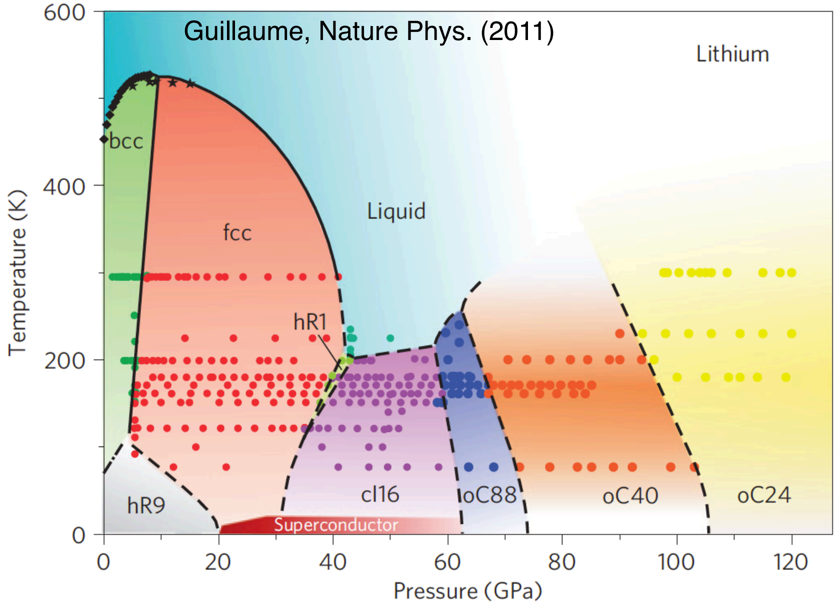


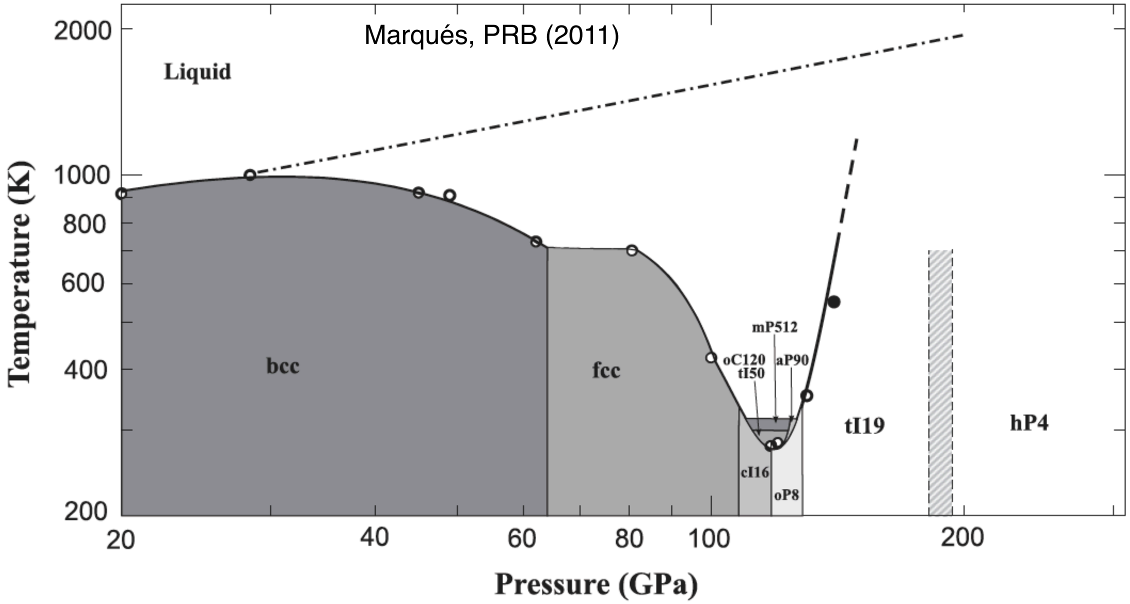
Structures observed at maximum pressure

--McMahon, Nelmes, CSR, 2006

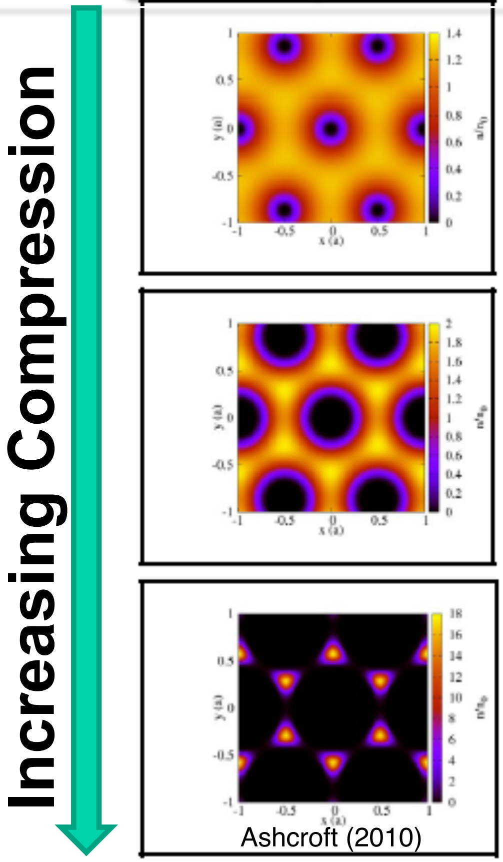
Recent high-pressure crystallography suggests that the expected simple metallic crystal structures are not always observed.

A few recent observations and calculations suggest suggest very complex high-pressure behavior


Guillaume, Nature Phys. (2011)


Marqués, PRB (2011)

Simulations predict electronic localization through compression



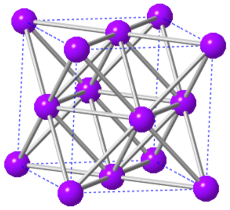
Ashcroft (2010)

Driven by orthogonalization and Pauli Exclusion to interstitial regions

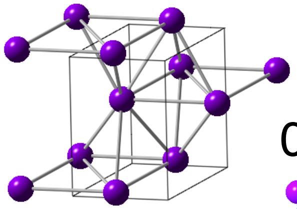
High pressures phases of aluminum are also predicted to be complex

Pickard and Needs, Nature Materials (2010).

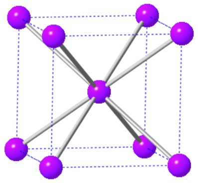
FCC



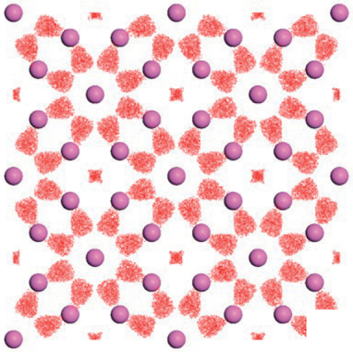
HCP
0.217 TPa



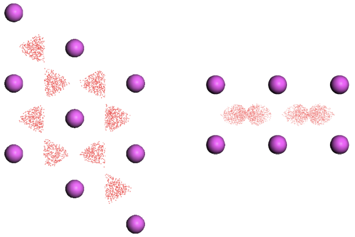
BCC
0.38 TPa



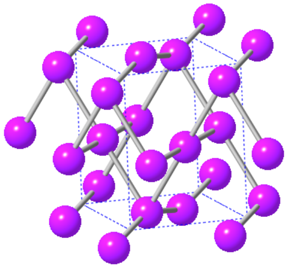
Host-Guest structure
of Ba-IVa
(Incommensurate
Electride)
3.2-8.8 TPa



Simple Hexagonal
Electride
8.8 – 10 TPa



CMMA
Electride
> 10 TPa



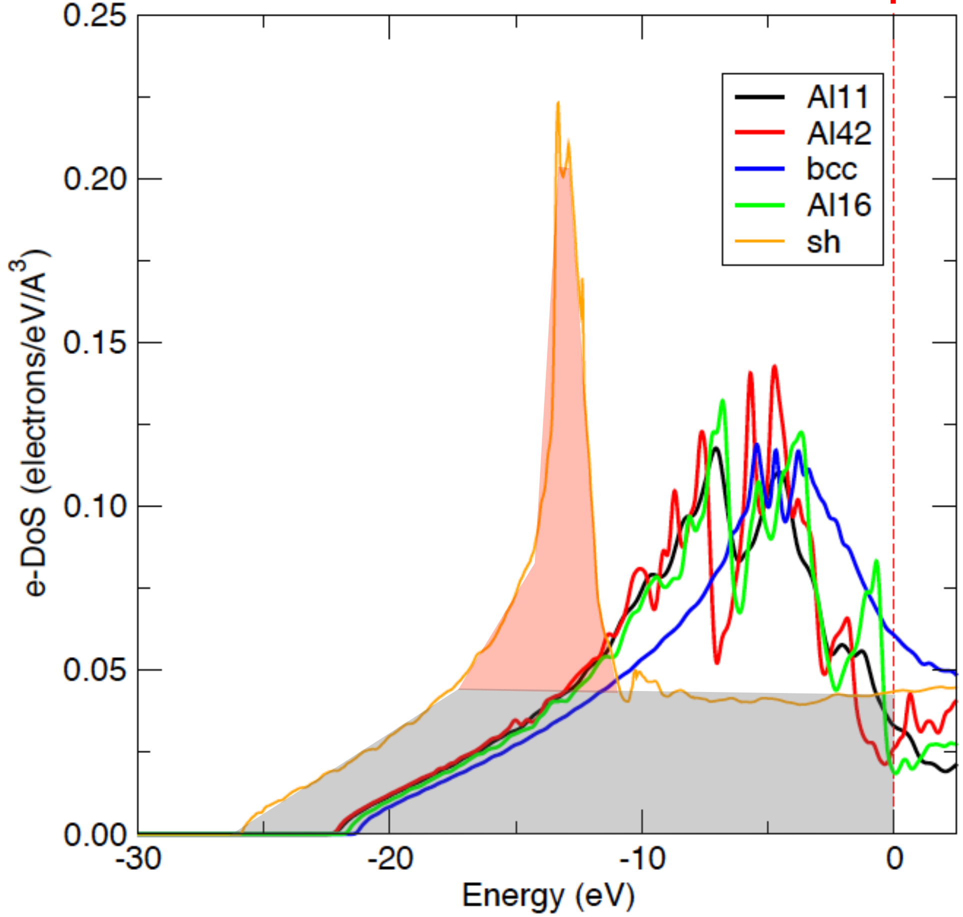
Electrides predicted to form above about 3.2 TPa

“all structures near 30 TPa
are far from close packed”

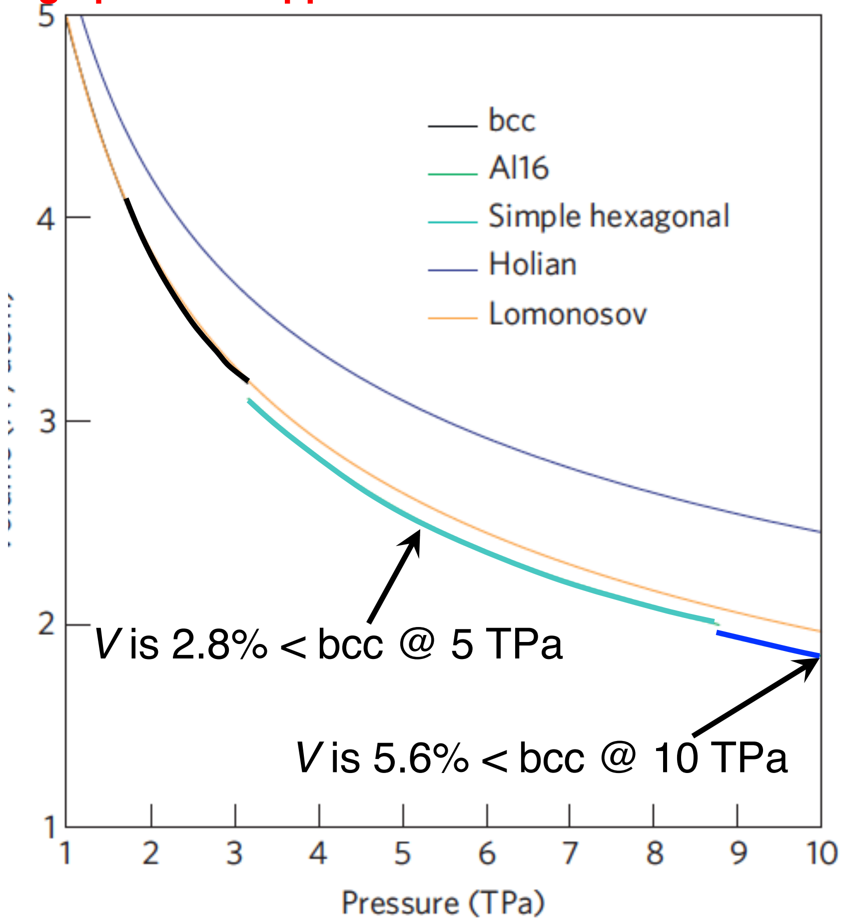
The energies involved in these transitions are enormous!

Pickard and Needs, Nature Materials (2010).

Traditional view: All materials become simple at high pressure appears to be incorrect!



Up to 10 TPa aluminum is still metallic, but the electronic structure changes are enormous!



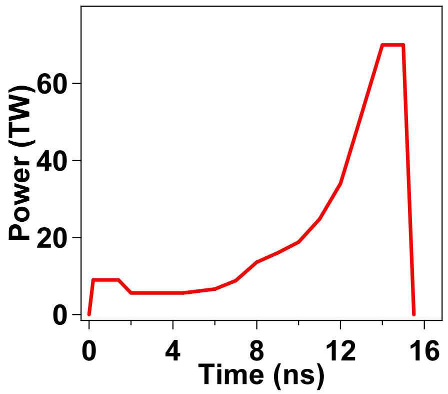
V is 2.8% < bcc @ 5 TPa

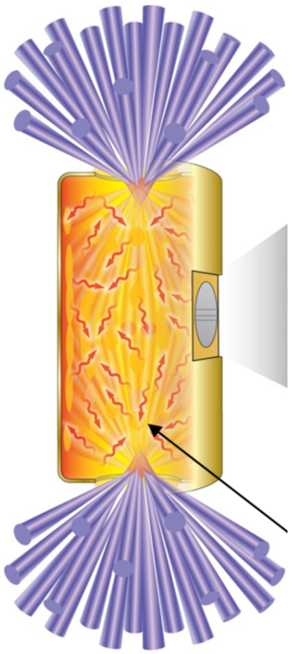
V is 5.6% < bcc @ 10 TPa

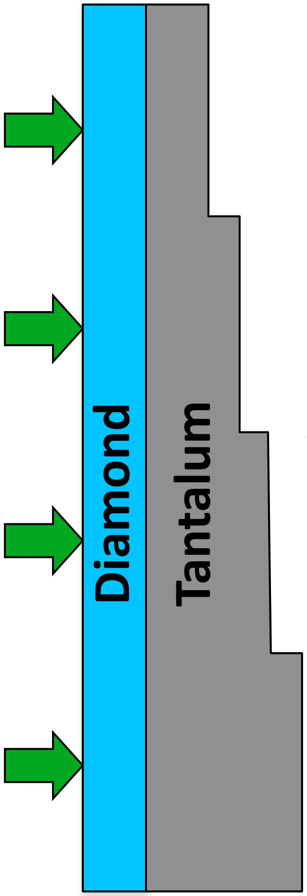
Figure 3 | Equation of state of Al. The volume–pressure relationship calculated in this work and from the EoSs of Lomonosov[4,5] and Holian[18].

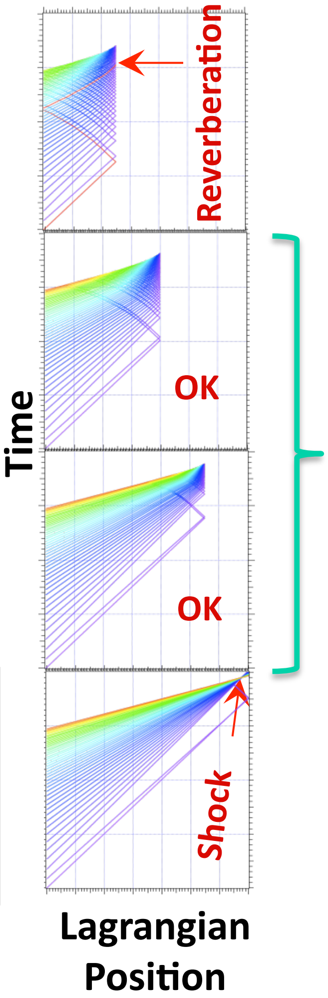
Laser-driven ramp-compression experiments

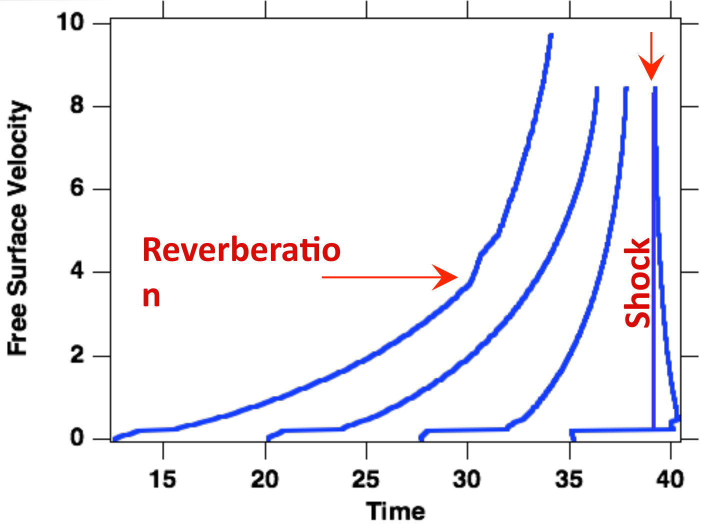
Under ramp loading, EOS (stress-density) can be determined from free-surface velocity measurements











Design constraints:

No reverberation and no shock

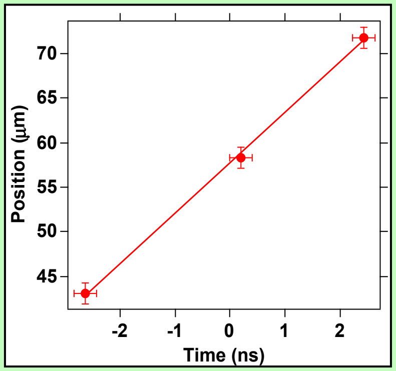
Iterative Analysis: Correction for free-surface wave interactions. Rothman, et al. J. Phys. D (2005)

EOS, $C_L(U_{FS})$

Reverse propagate $U_{FS,j}(t)$ to find drive pressure, $P_j(t)$, for all steps, *j*

Forward propagate $P_j(t)$, *with no interface* to the step thickness d_j for all steps, *j*

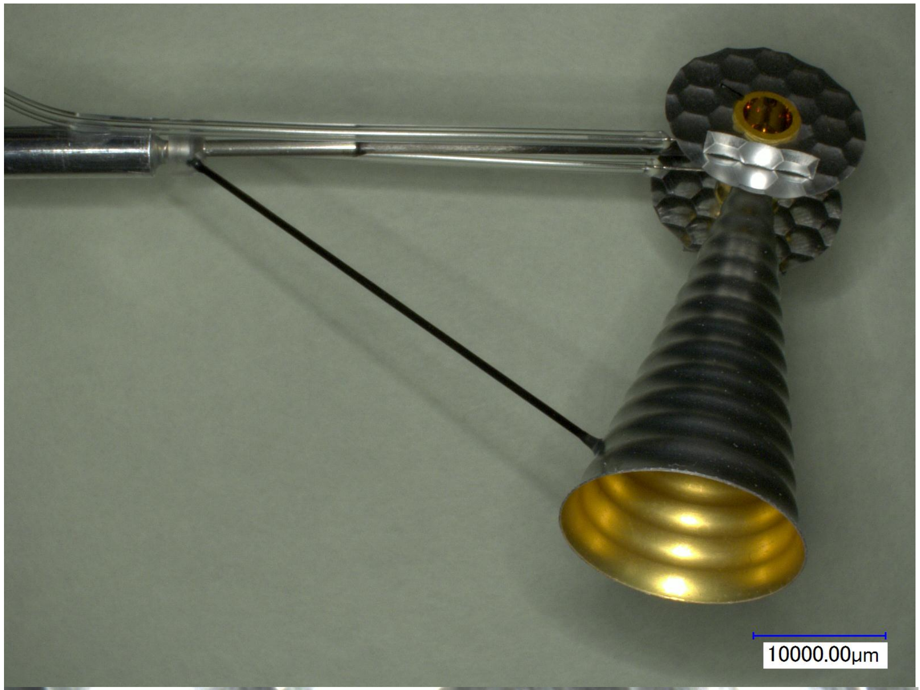
Update $C_L(U_{FS})$ by linearly fitting d_j vs. $t_{FS,j}$

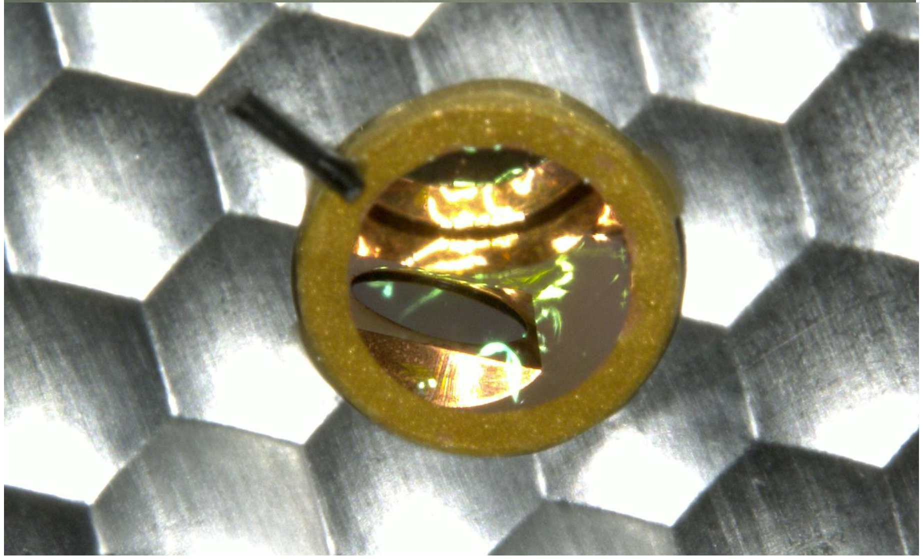


Iterate to convergence

Method requires *both* reverse and forward propagation steps

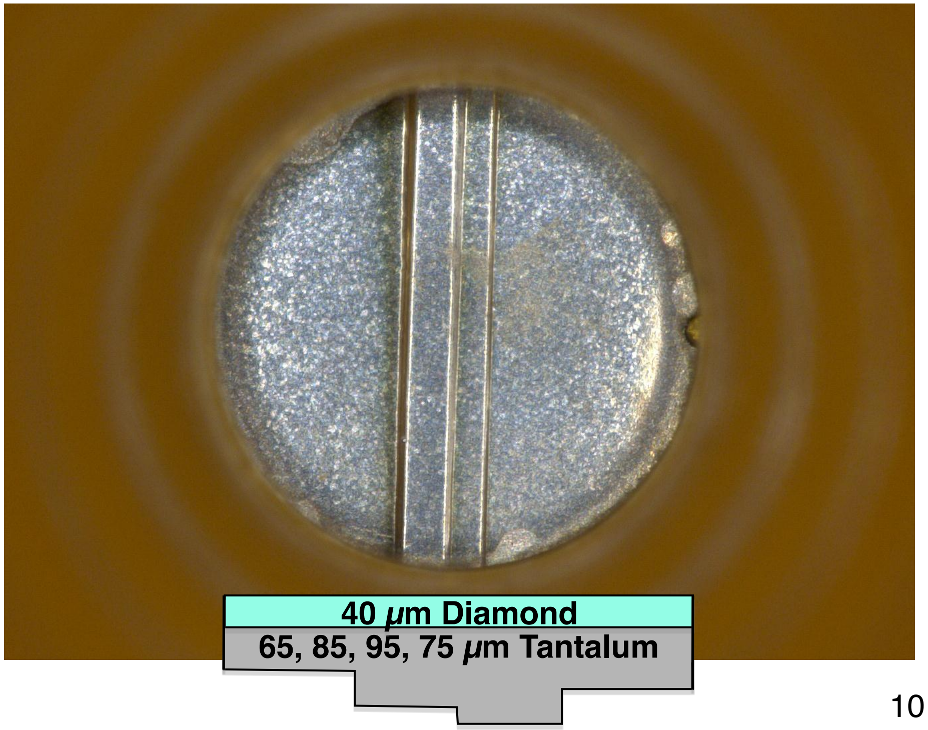
NIF: Materials EOS Drive targets





Gas-filled, room-temperature, stepped target mounted on side of Hohlraum with VISAR cone.

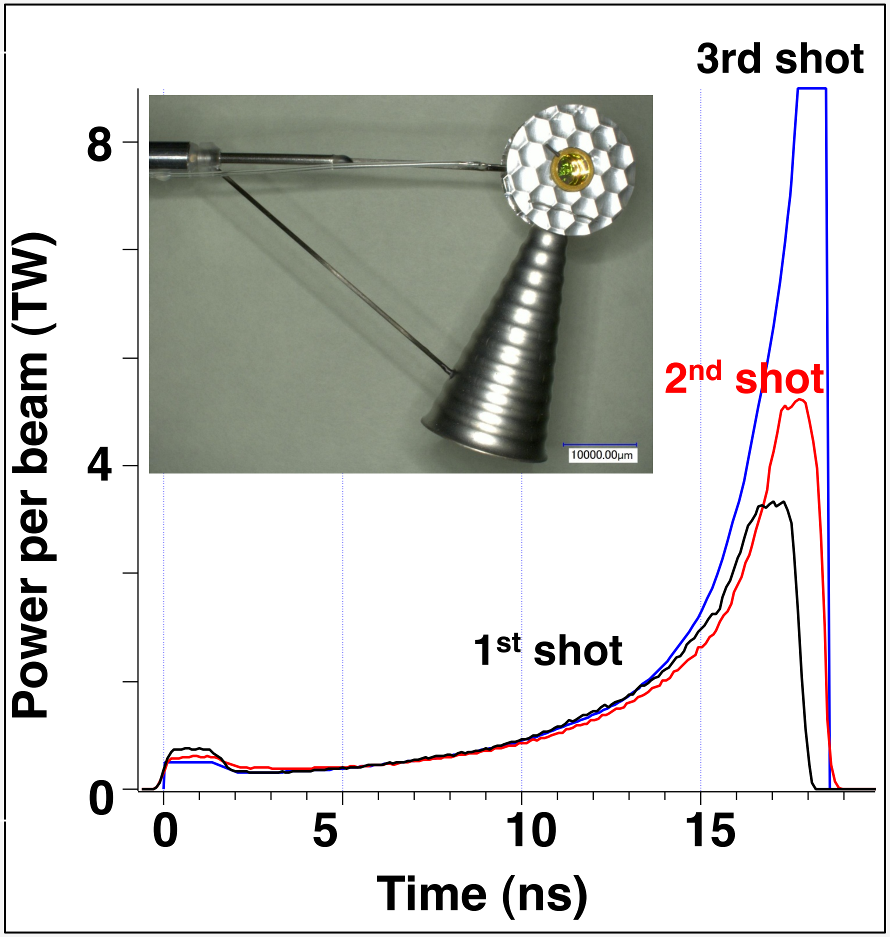
- 0.2 atm. Neopentane gas fill
- *L* = 11 mm
- ϕ = 6 mm
- *LEH* = 4.5 mm.



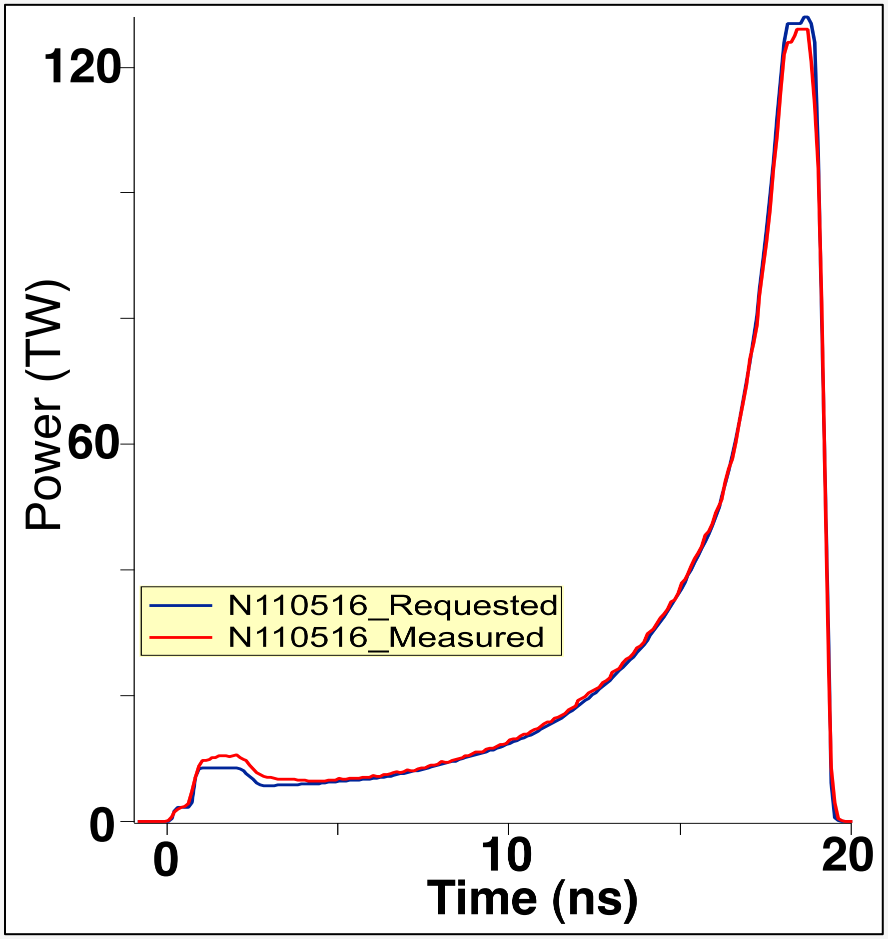
Nano-crystalline diamond EOS on NIF

In addition to the higher energy, pulse shaping was key to achieving higher pressure

Pulse Shape evolution for diamond ramp experiments



Requested vs delivered pulseshapes for ramp experiments



Ramp-compression EOS of nano-crystalline diamond to 50 Mbar.

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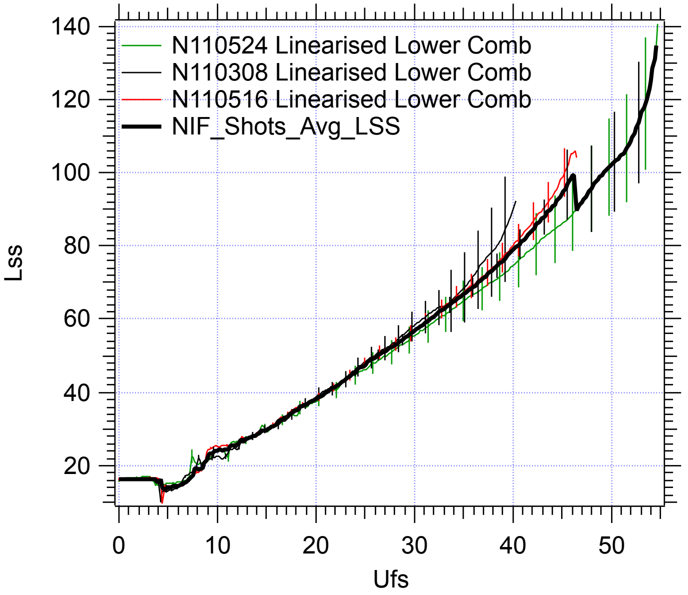
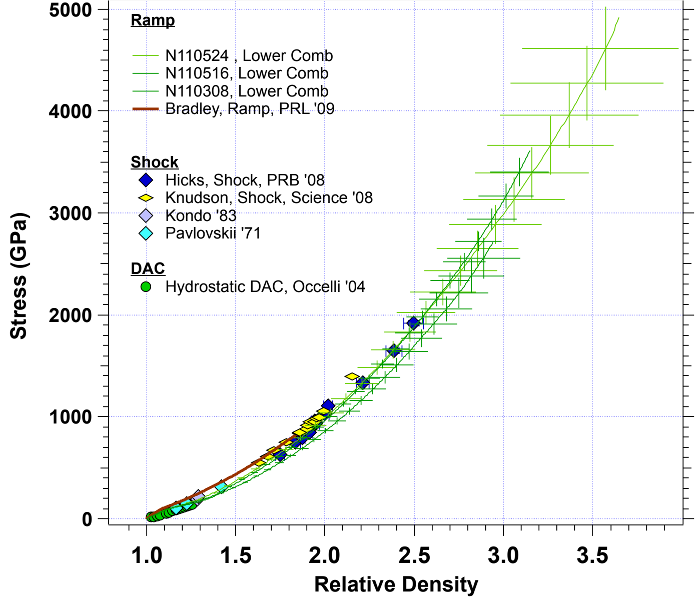
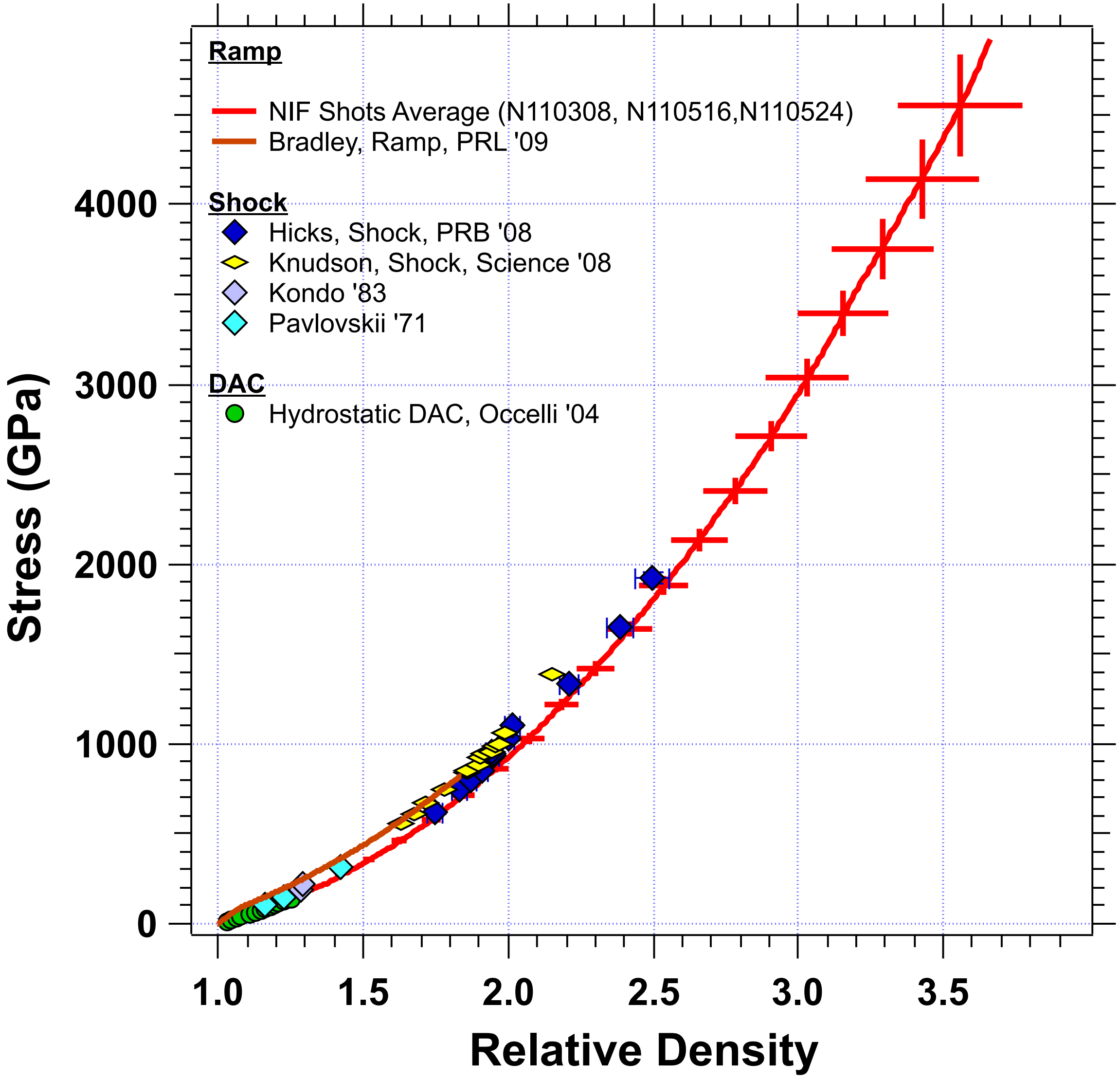


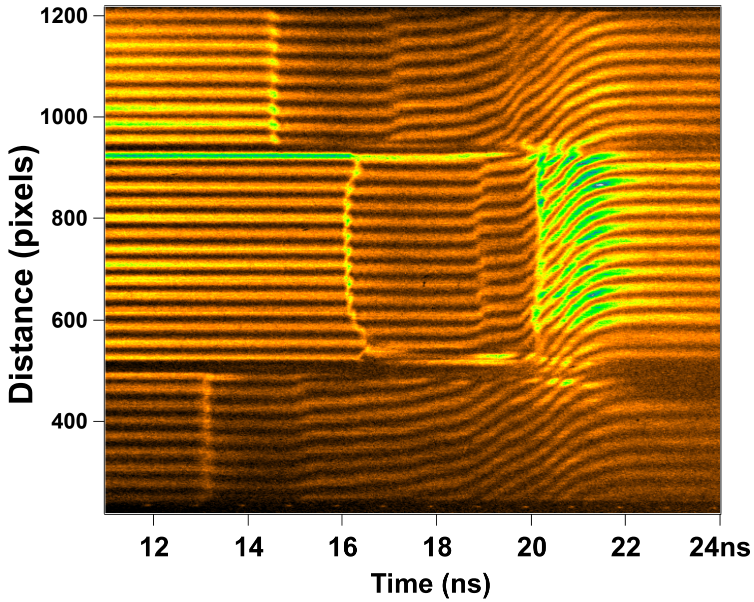


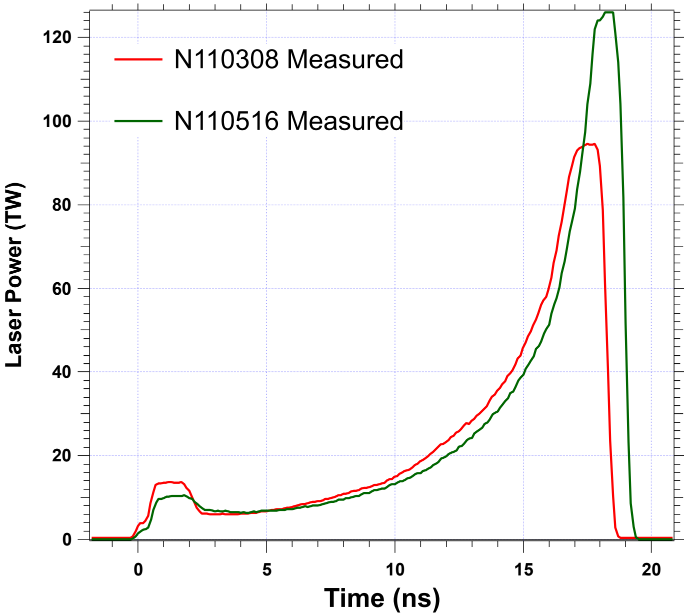


Average of three shots

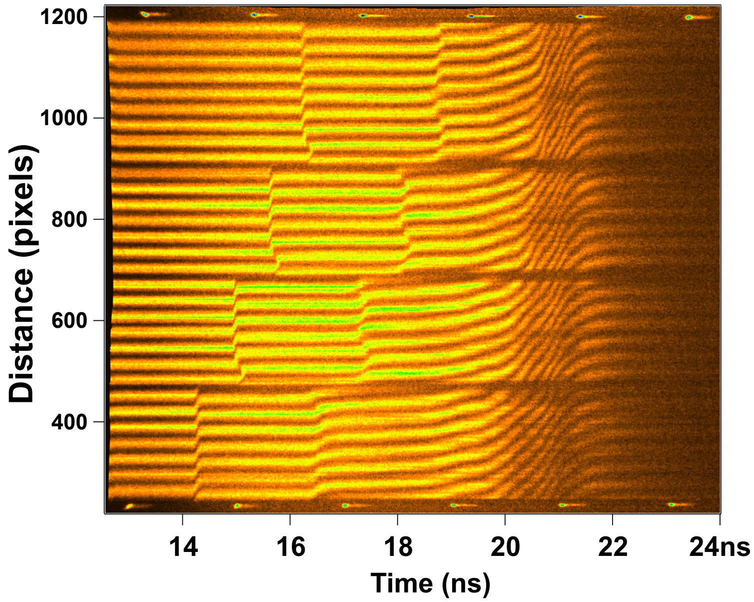
Pulse shaping required very small adjustments to laser-power drive: First two data shots.

27 Mbar
N110308



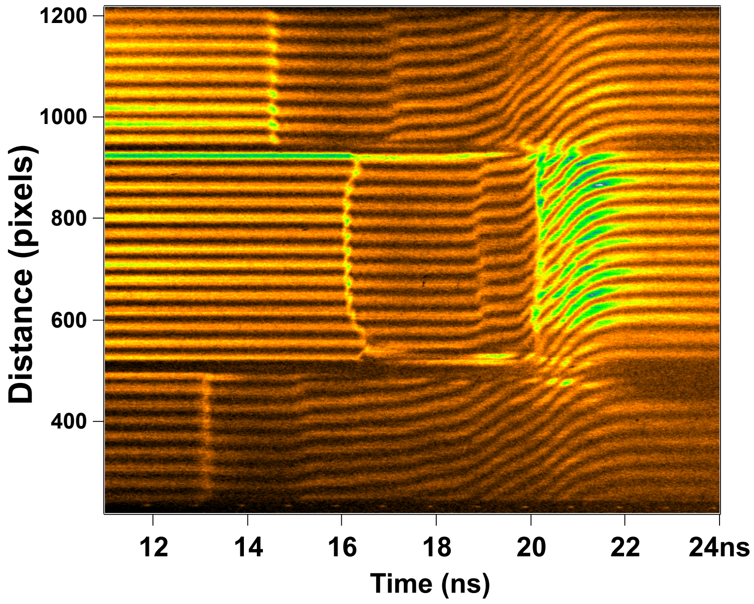


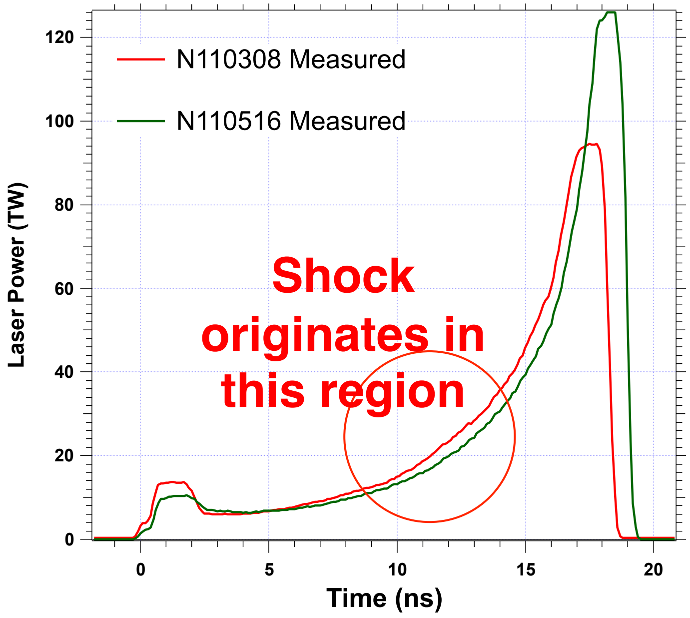
37 Mbar
N110516



We were able to identify and correct regions responsible for growing shocks.

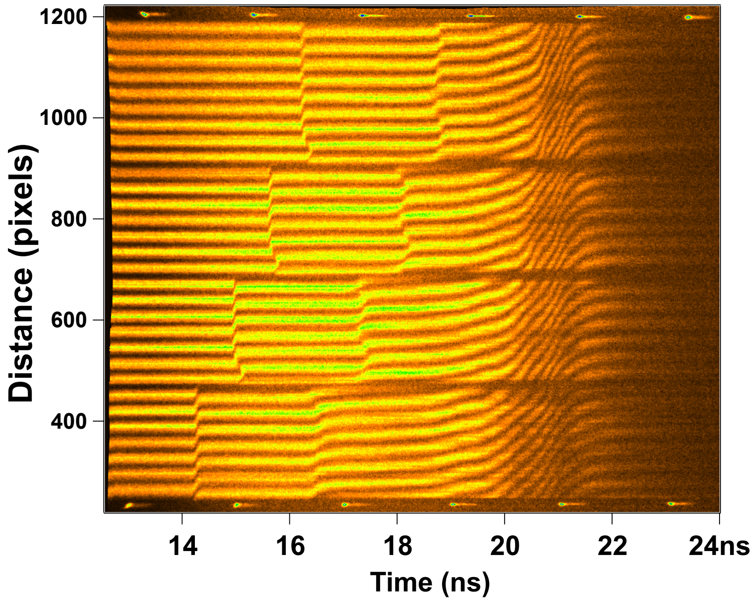
27 Mbar





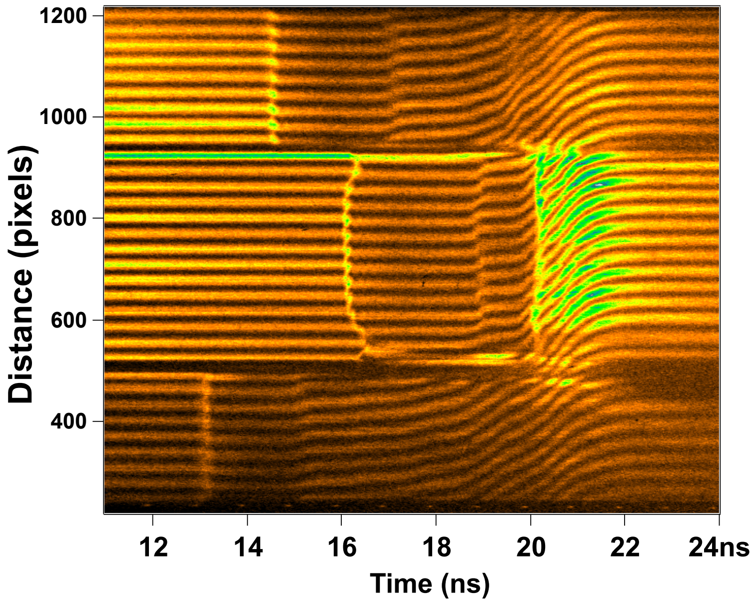
Shock originates in this region

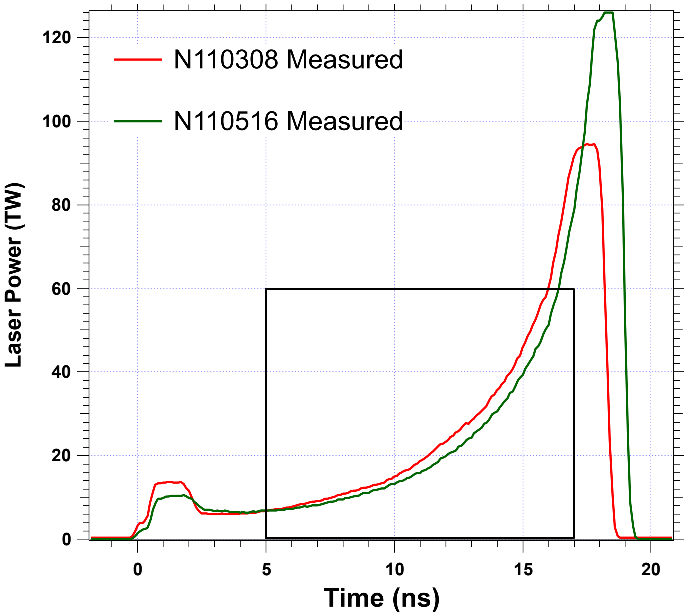
37 Mbar



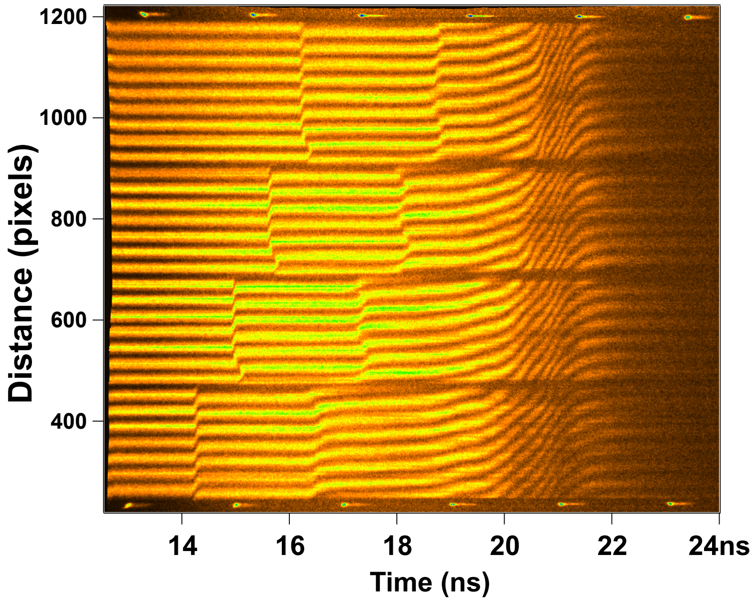
Pulse-shape correction worked extremely well.

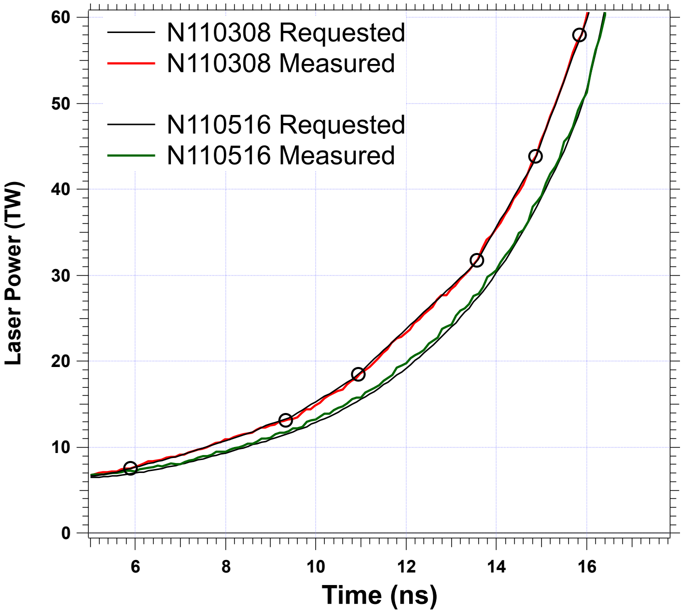
27 Mbar





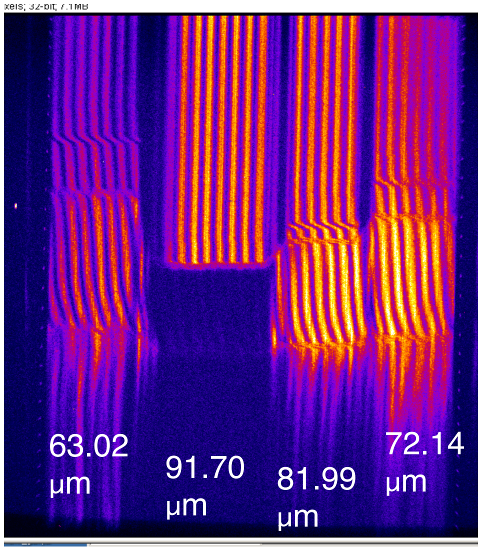
37 Mbar



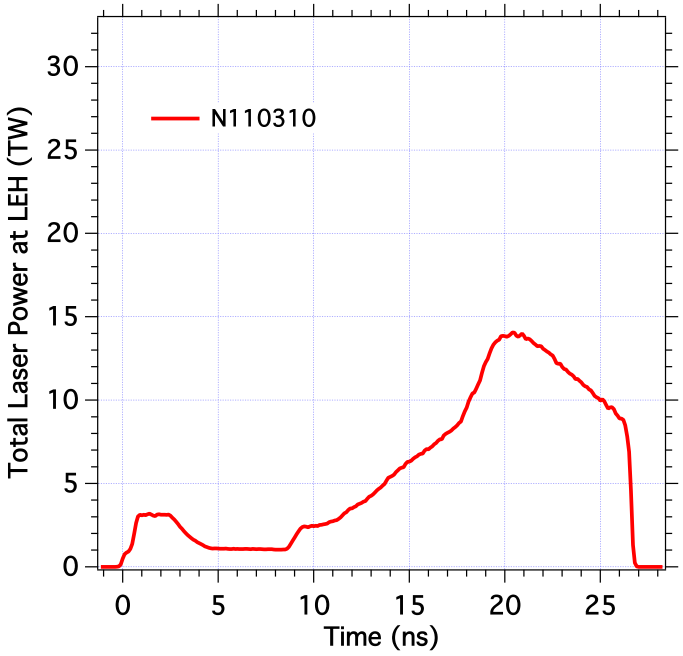


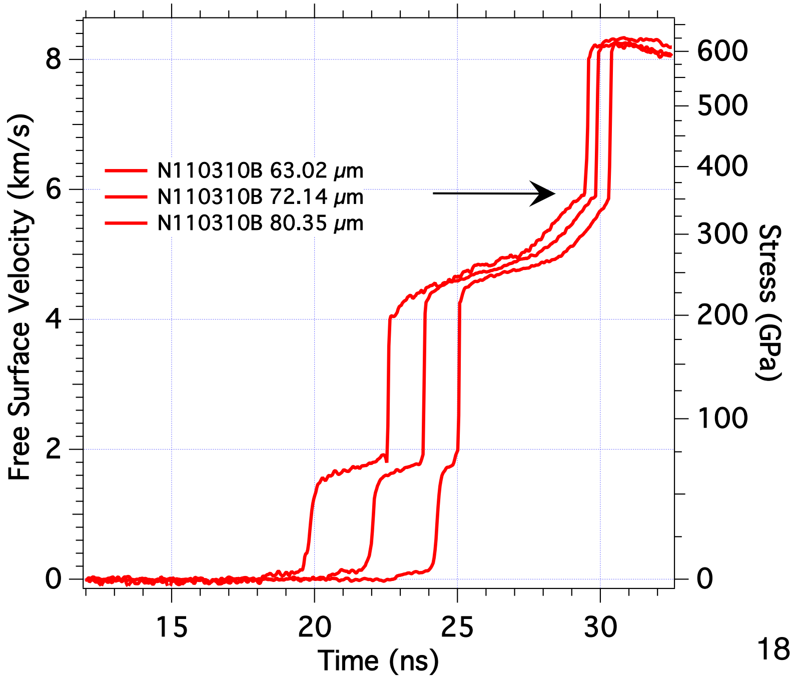
Vapor-deposited tantalum EOS on NIF

On the NIF, Tantalum shocked up independent of thickness

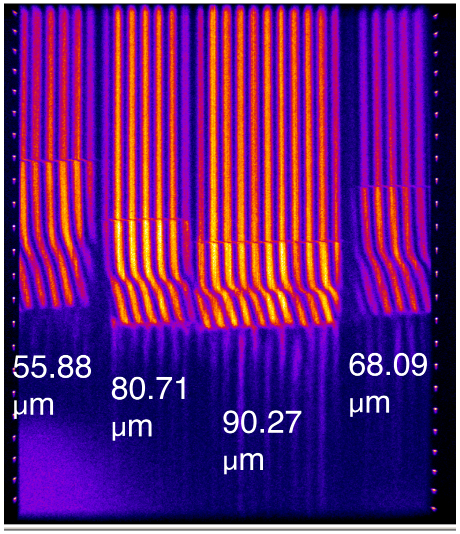


< Eliminate multiple shocks >

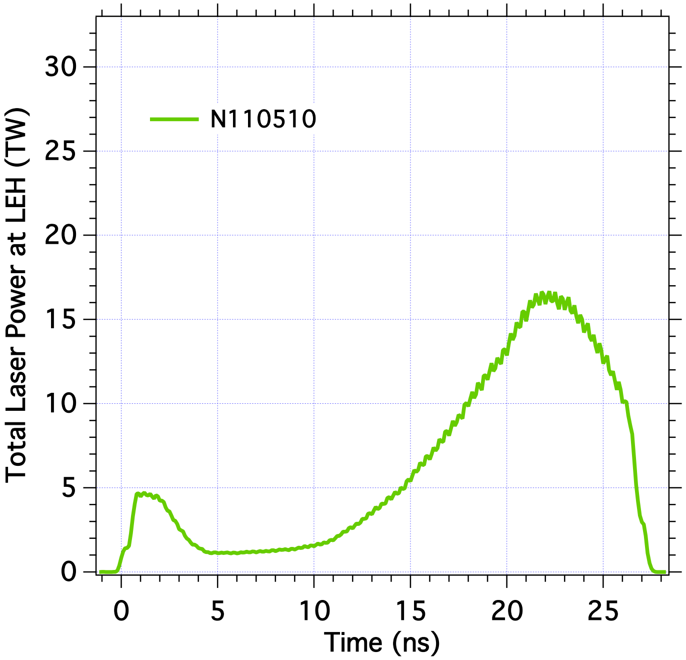


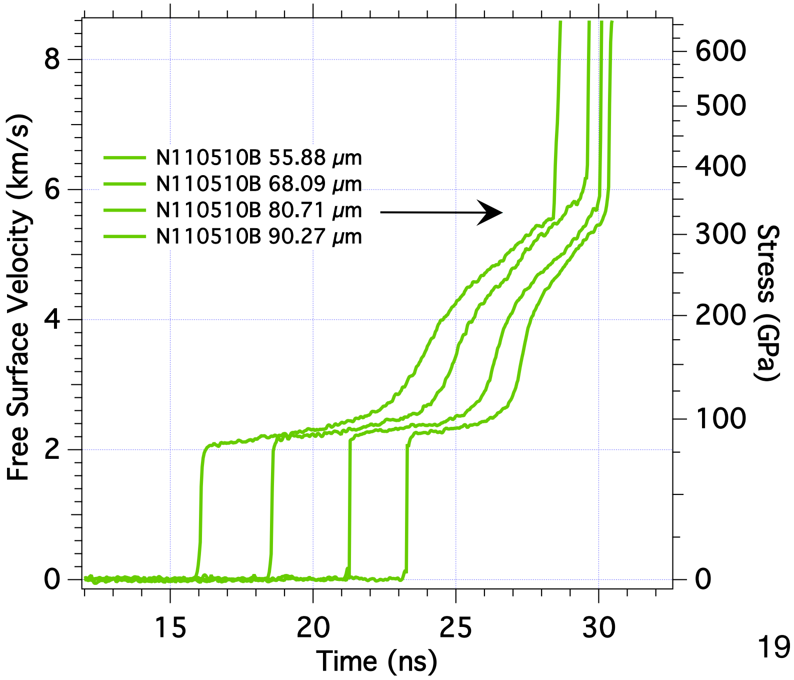


After eliminating 2nd shock, tantalum still shocked up at the same velocity on each step



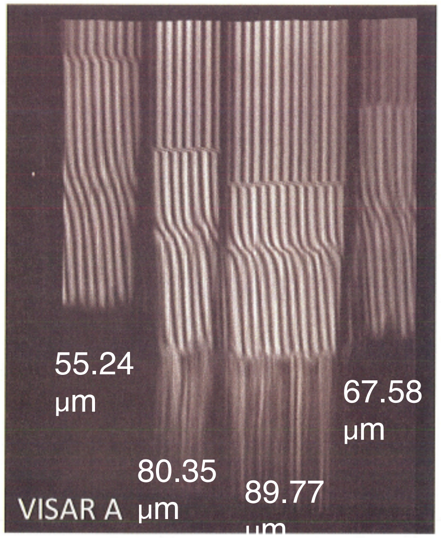
< Reduce strain rate at shock >

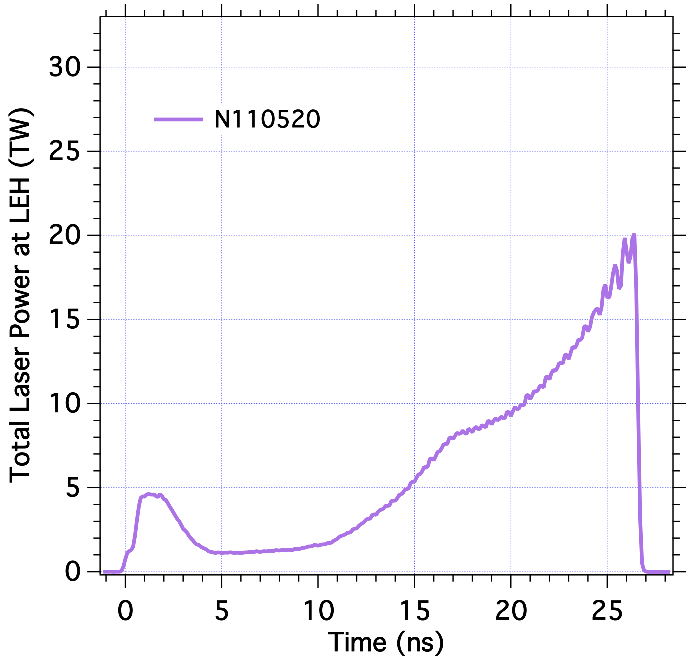


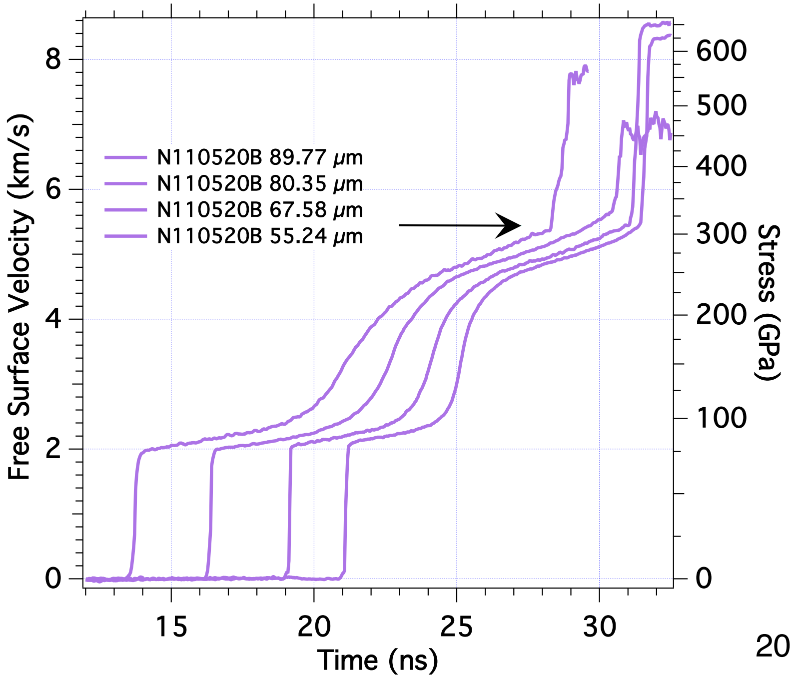


On the NIF, Tantalum shocks up at the same velocity on each step

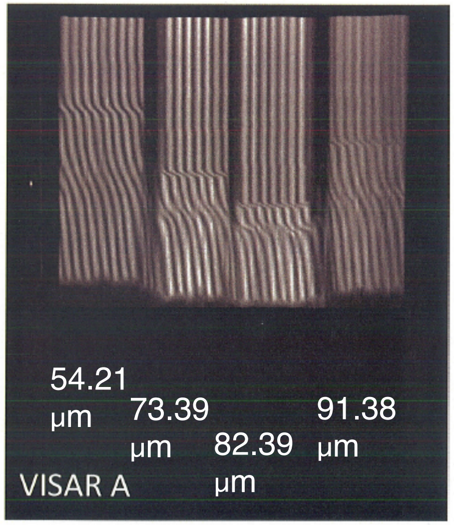
< Increase final pressure >



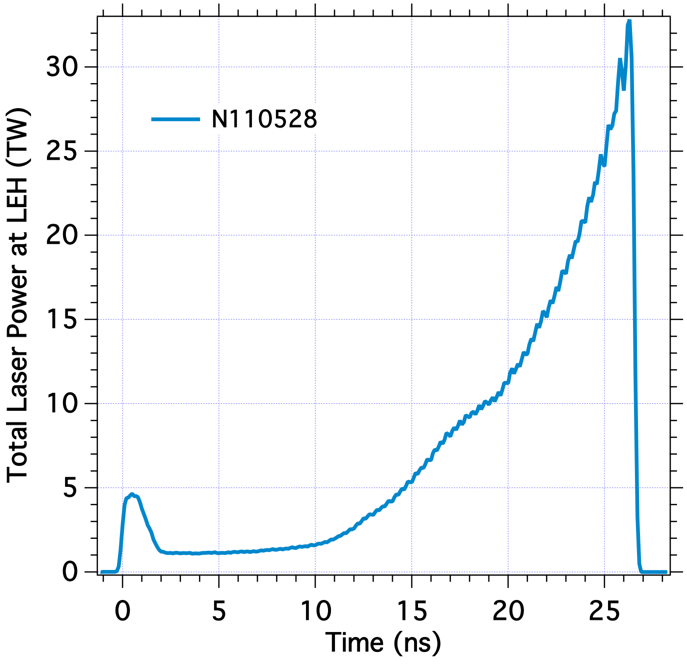


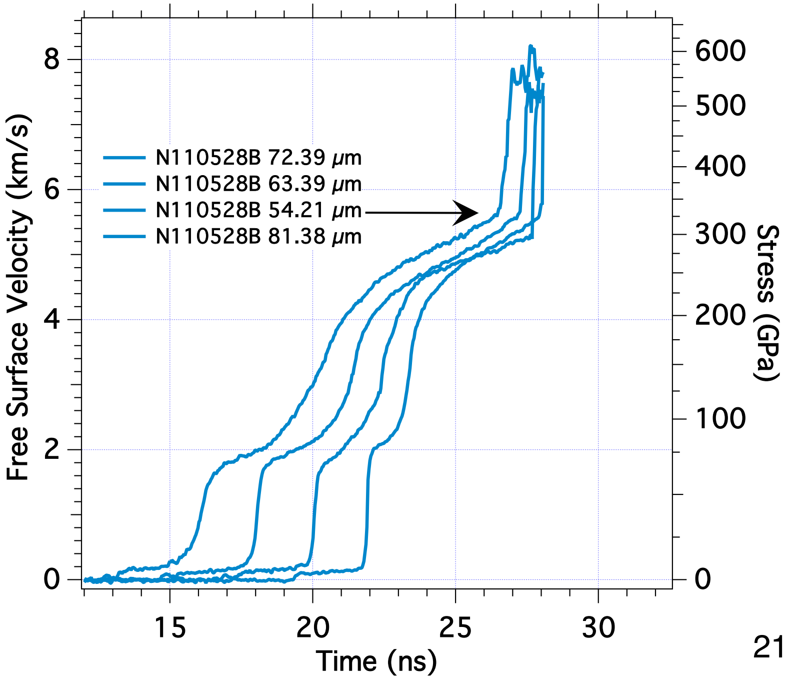


On the NIF, Tantalum shocks up at the same velocity on each step

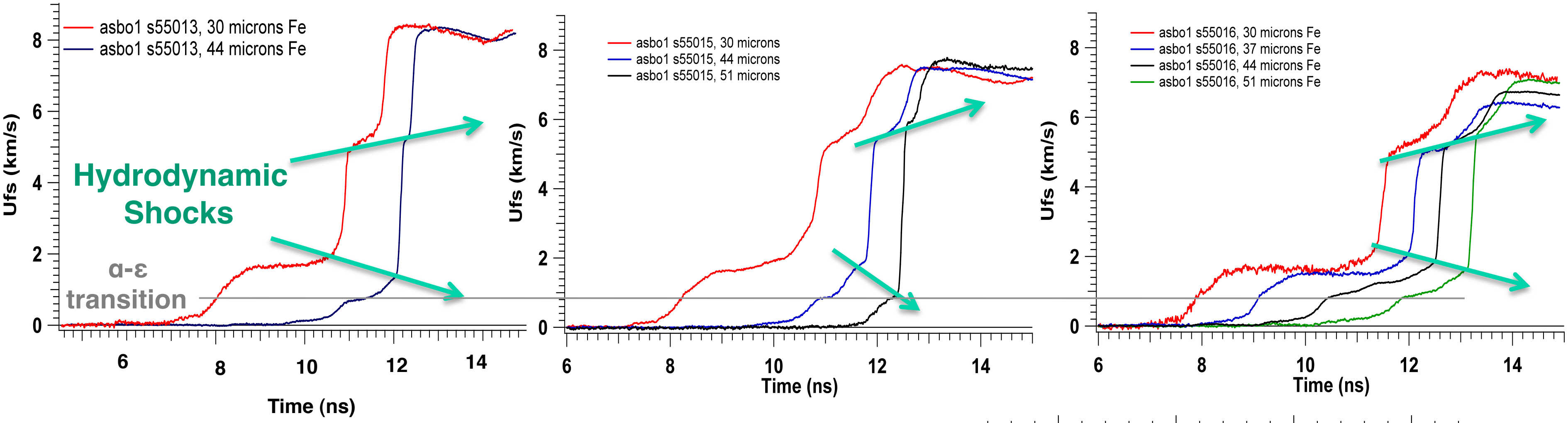


Shock initiation at ~ 3.4 Mbar repeatedly with minor dependence on sample thickness or drive profile.

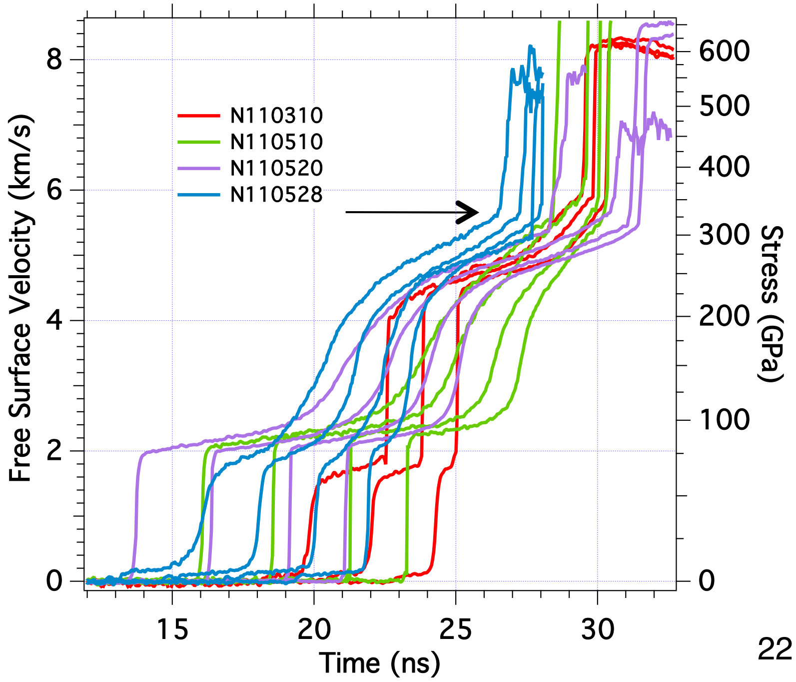




Hydrodynamic shocks in iron experiments at Omega



- •Hydrodynamic shocks grow with thickness at both upper and lower limit of shock.
- •Phase transition plateaus and shock initiation velocity are fixed with thickness



•On NIF, the Ta shocks do not appear to be hydrodynamic steepening in origin

For tantalum, shock initiation is very independent of pressure-drive profile

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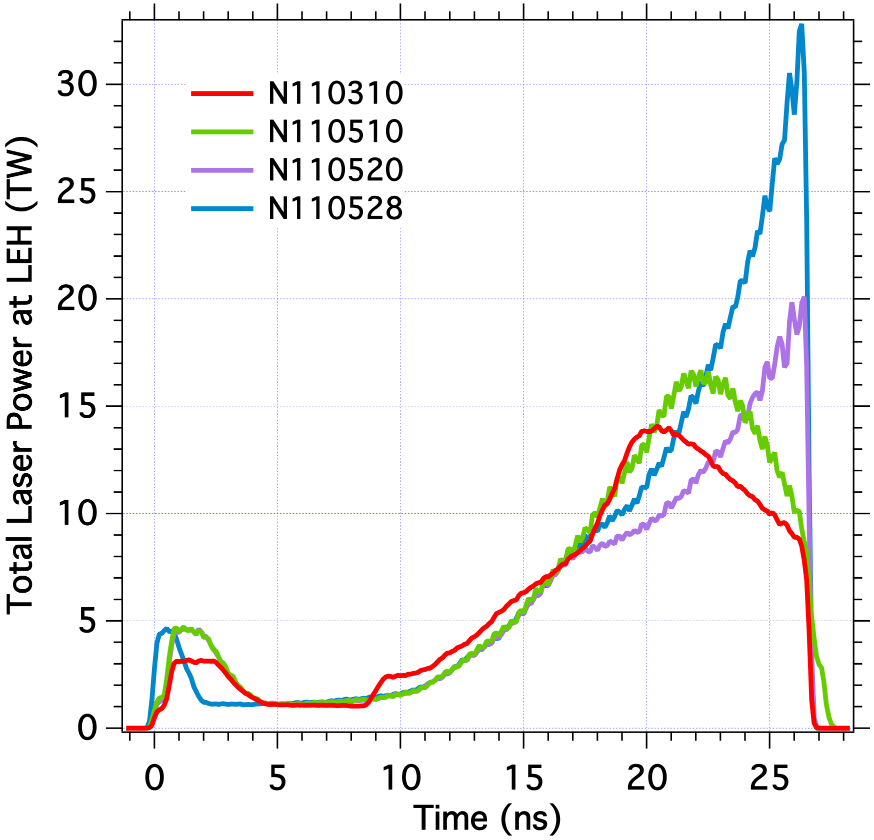
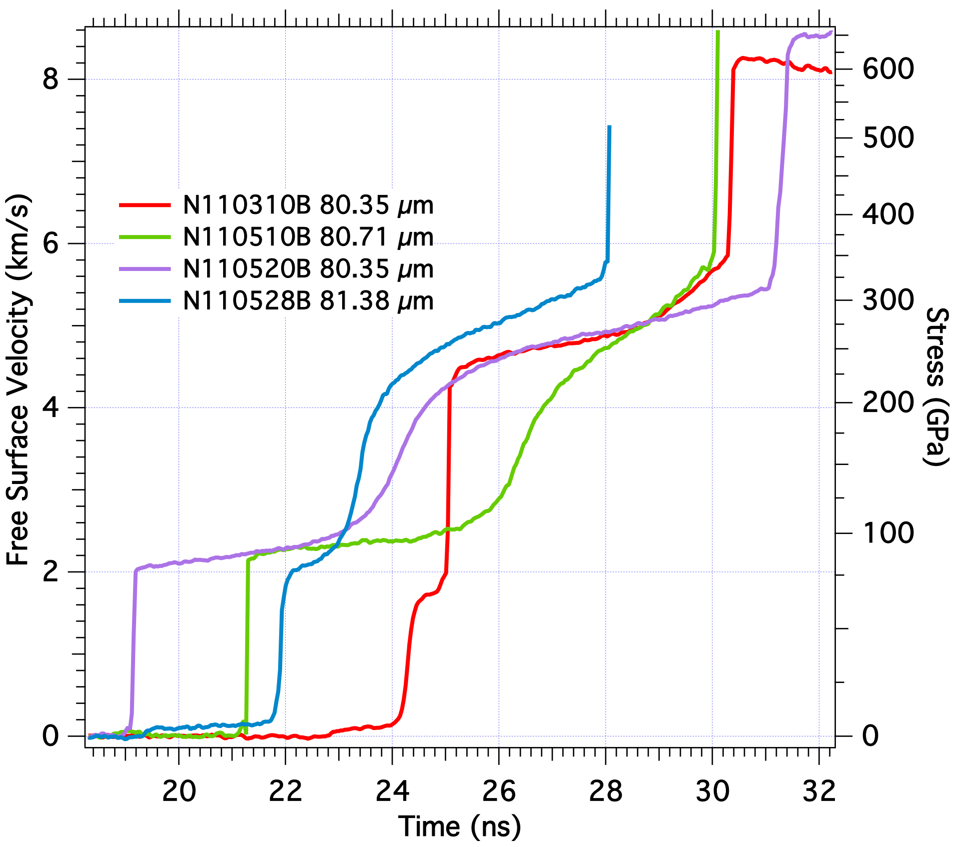
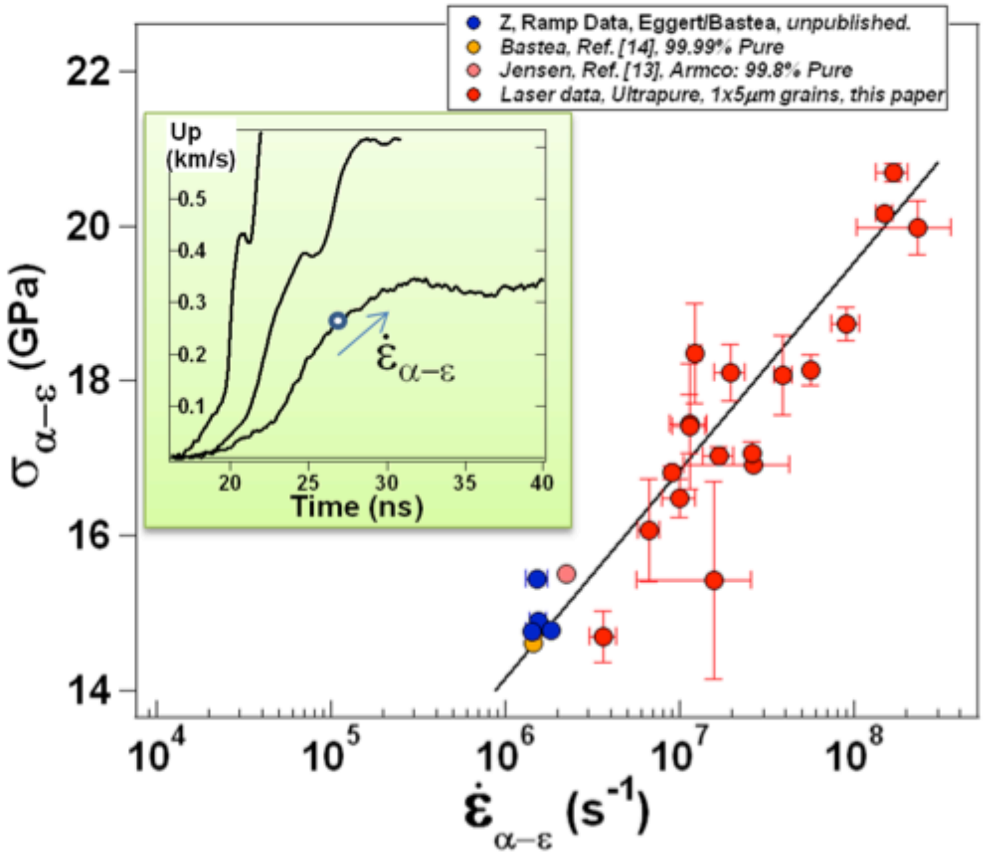
Variation of pressure drive (stress rate) is much larger than was needed for diamond. Shock does not appear due to hydrodynamic steepening.



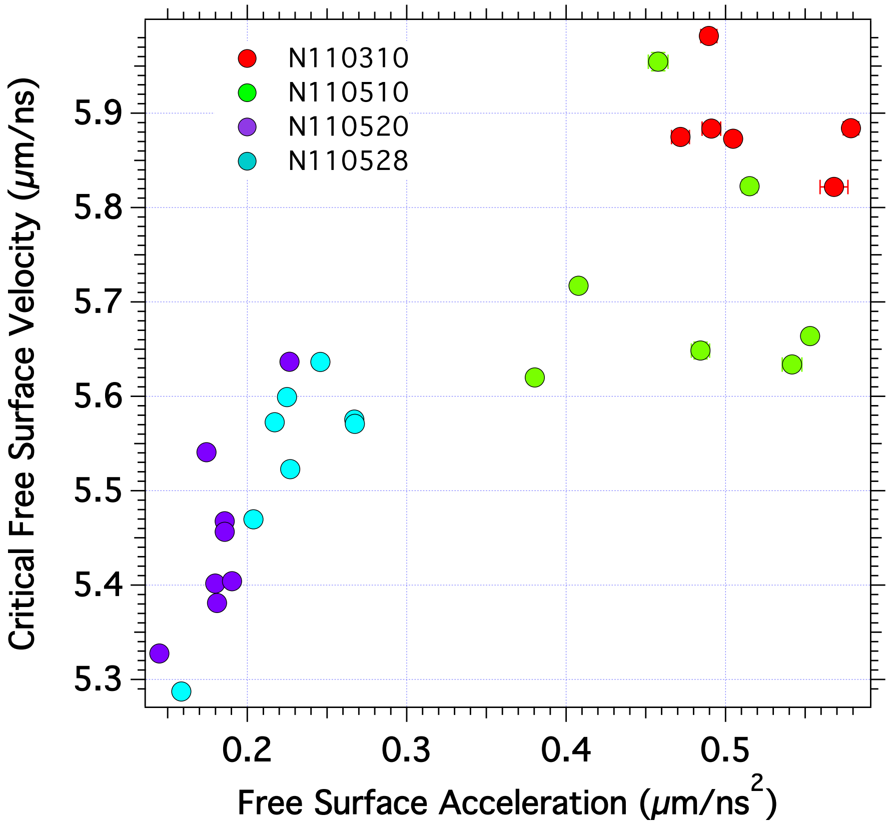


Critical stress for phase transitions increase with free-surface acceleration (strain rate)

Data for iron on Omega and Z



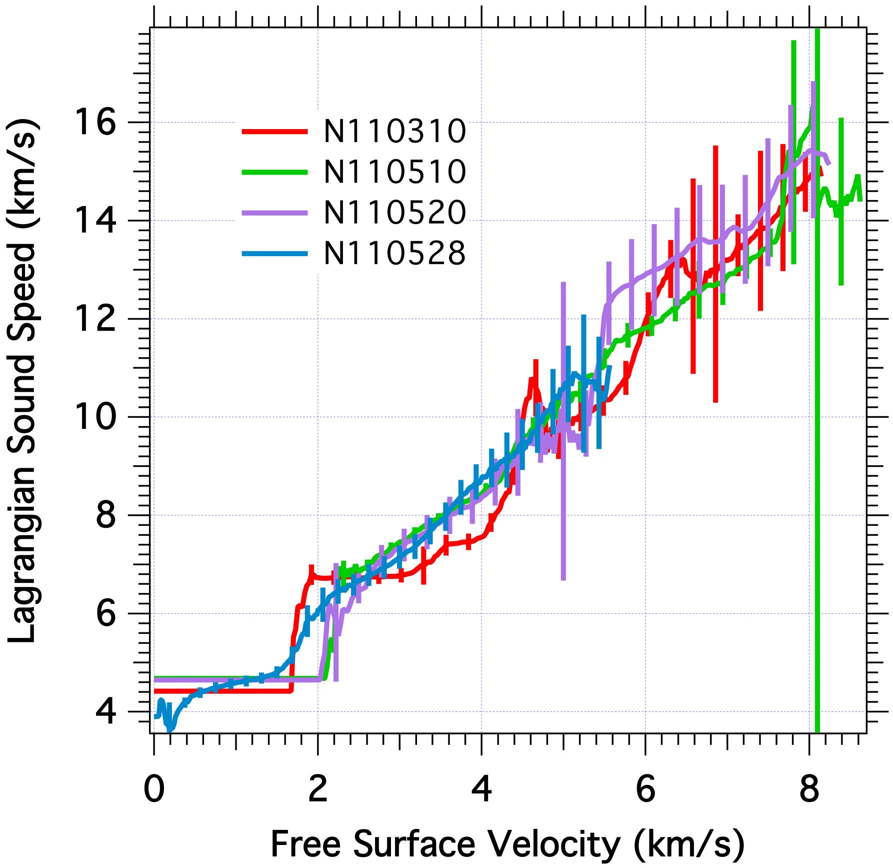
Similar results for Ta on NIF

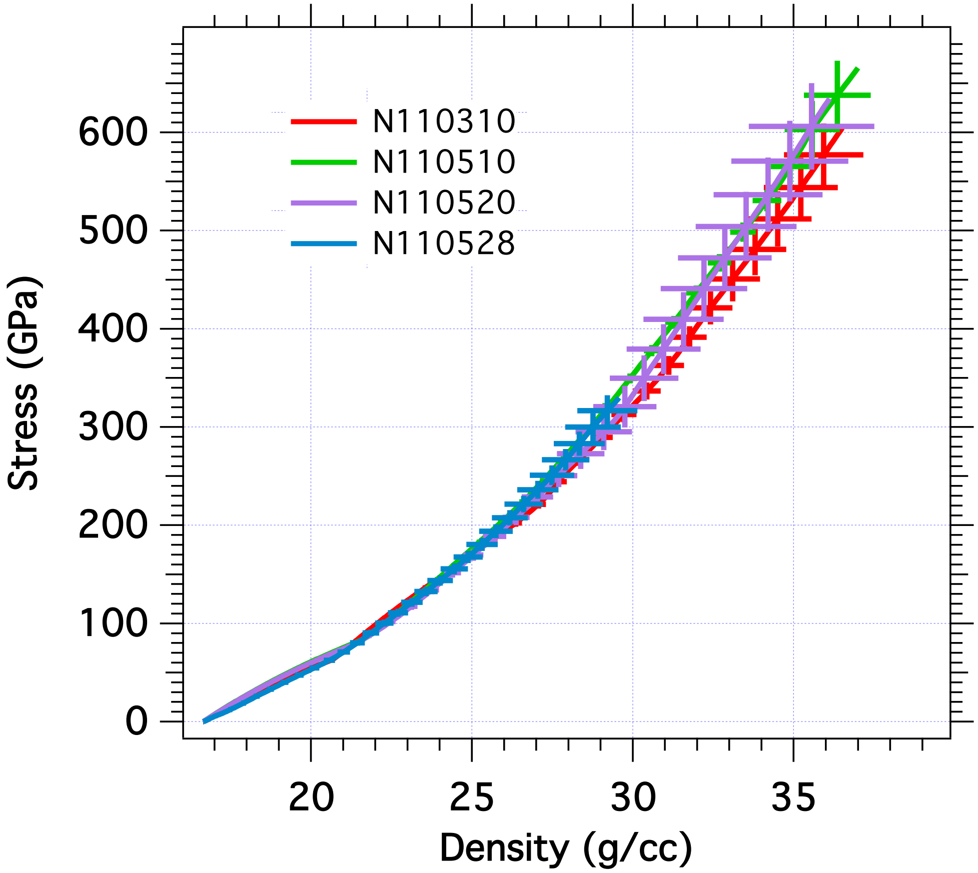


Results for tantalum on NIF appear most consistent with a phase transition

Since the shock was steady, we can extract an EOS to 6.7 Mbar

Independent analyses for each shot





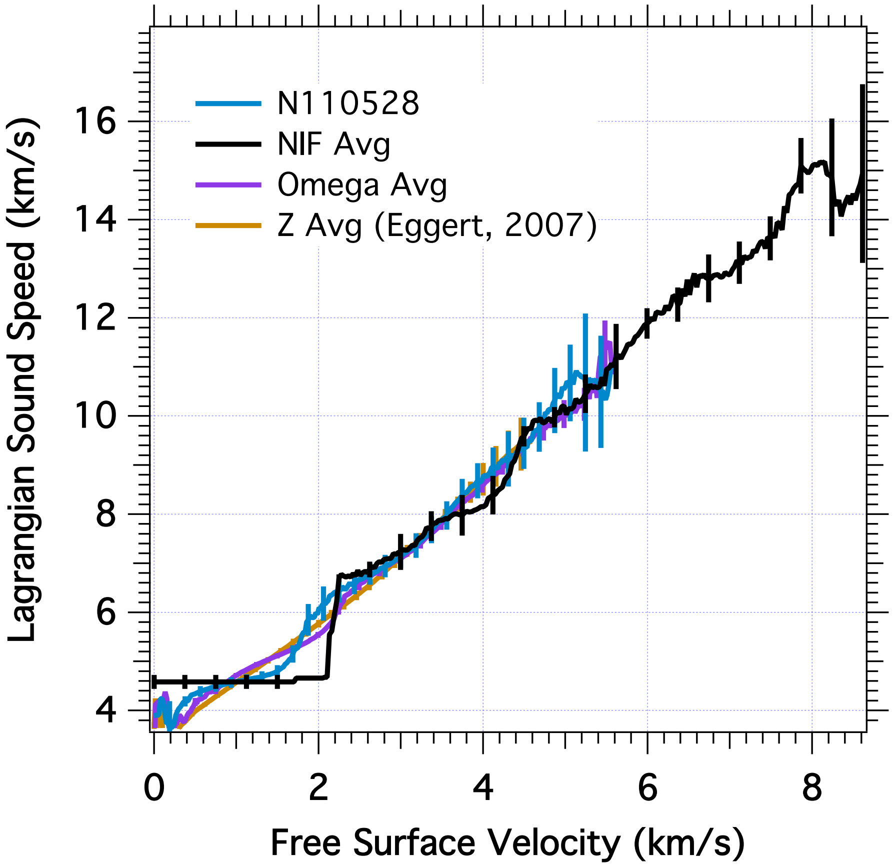
Lagrangian R-H Equations:

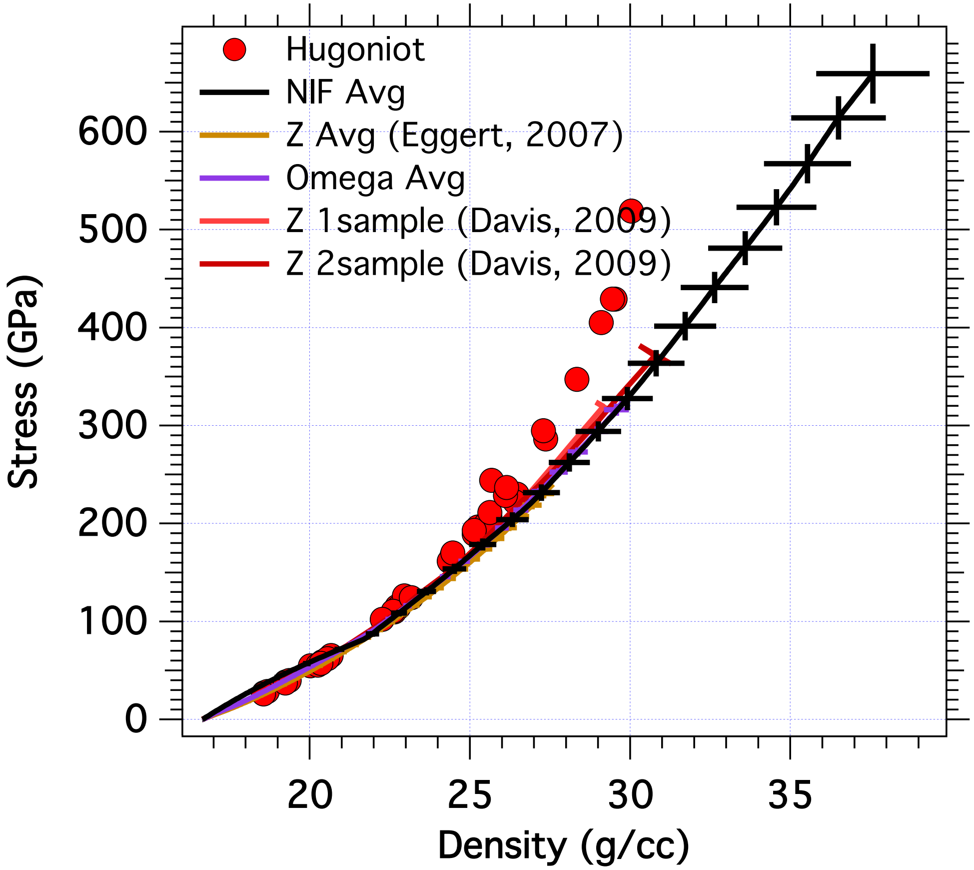
$$P_2 - P_1 = \rho_0 U_{SL}\left(U_{p2} - U_{p1}\right)$$

$$\rho_0 U_s = \rho_2\left(\frac{\rho_0}{\rho_1}U_s - \left(U_{p2} - U_{p1}\right)\right)$$

We average the sound speed for multiple shots

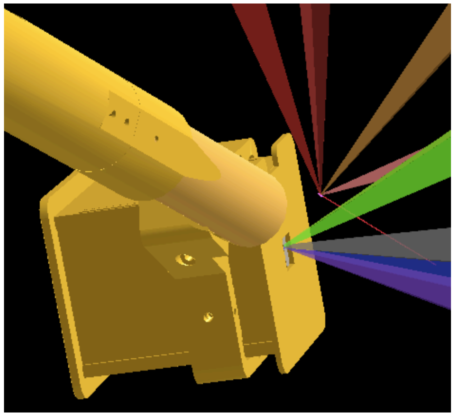
Excellent agreement with previous data from Z and Omega

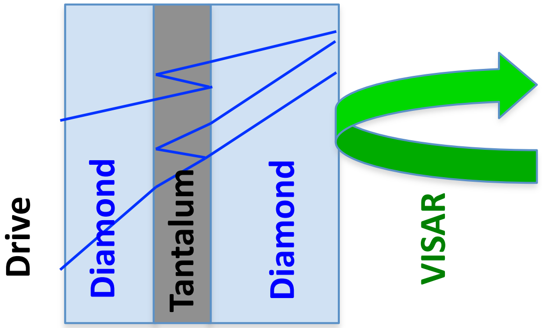


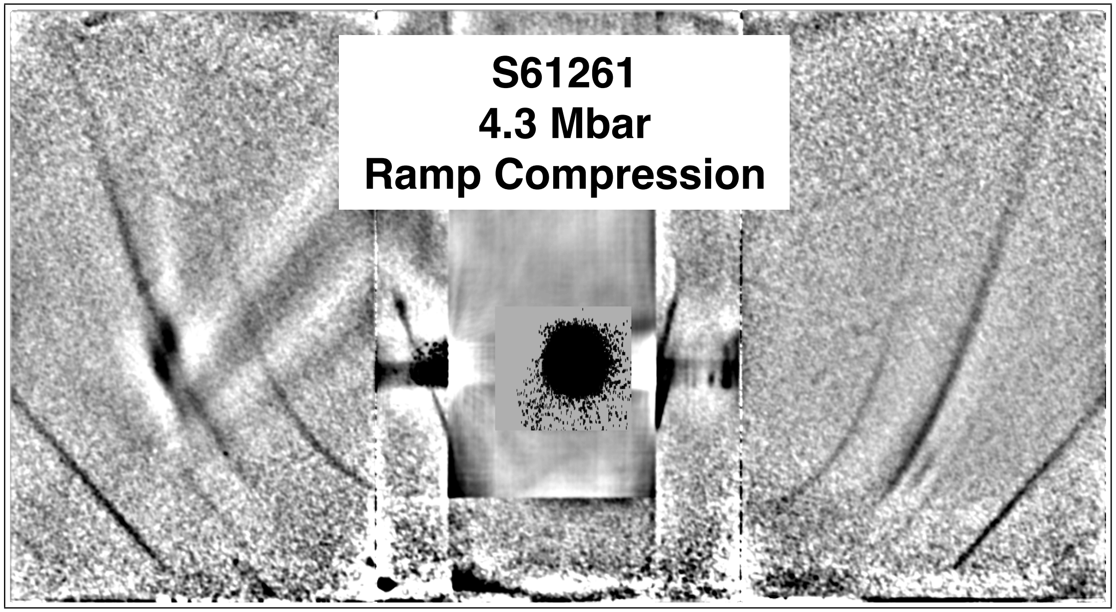


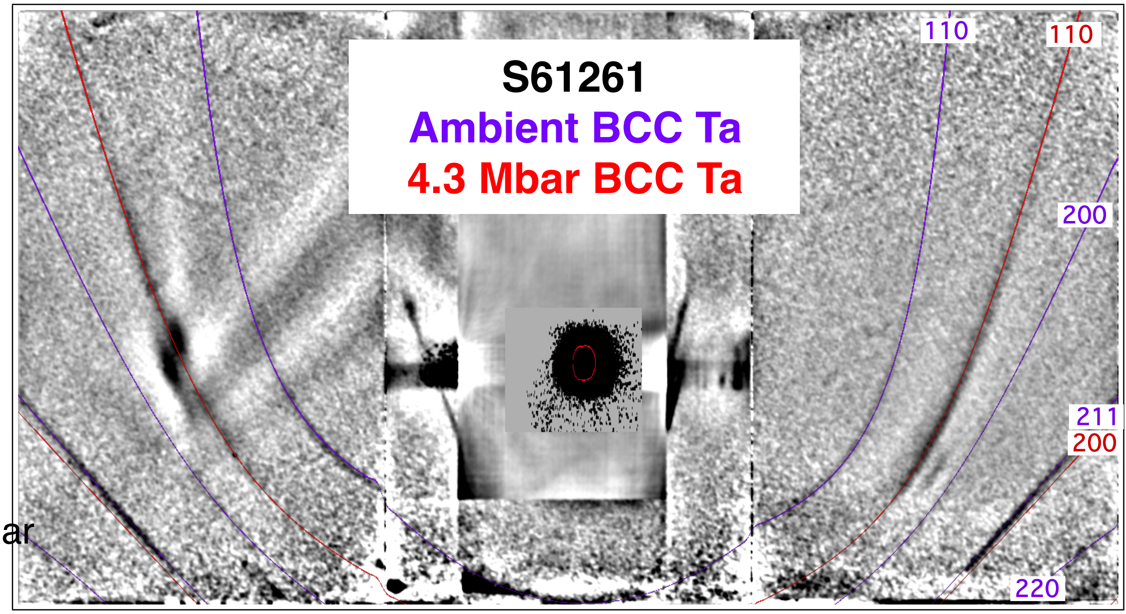
Powder x-ray diffraction of rolled tantalum on Omega

We have also performed high-pressure x-ray diffraction on tantalum at the Omega laser









RampDiff-11B (Ta, ramp5)

Shot **61261,** OMEGA 2011-0223

Target: C[17]Ta[3]C[40], **BL: Fe**

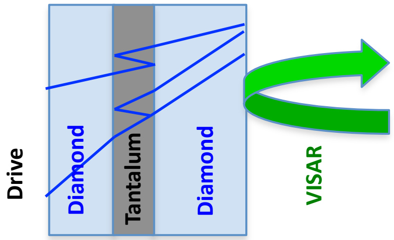
Ramp drive: 246 J (t_{BL} = 4.6 ns)

$P_{expected}$: 5.0 Mbar, $P_{max\_exp} = 4.34 \pm 0.09$ Mbar

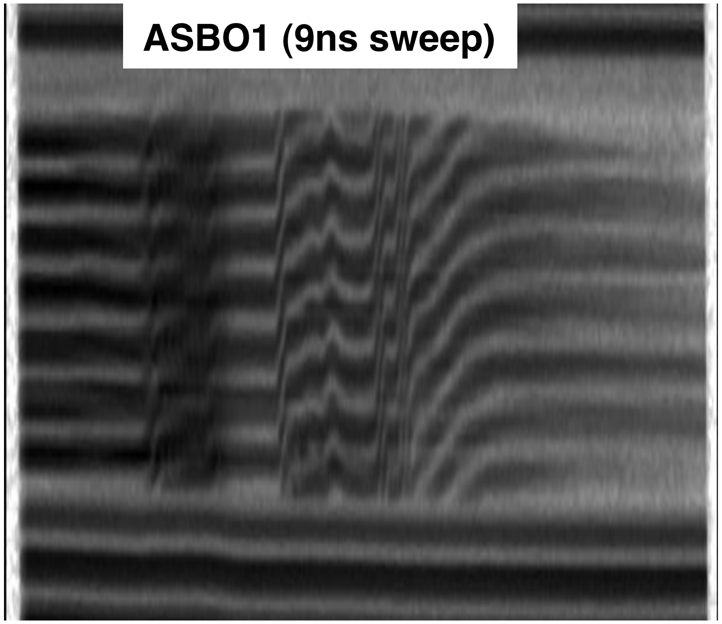
We determine stress by backward integration of diamond free-surface velocity

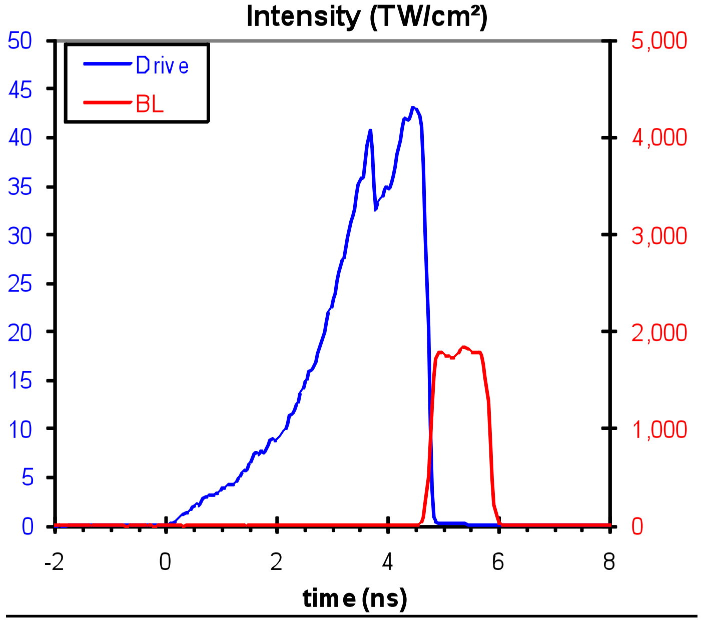
Shot **61261,**
OMEGA 2011-0223

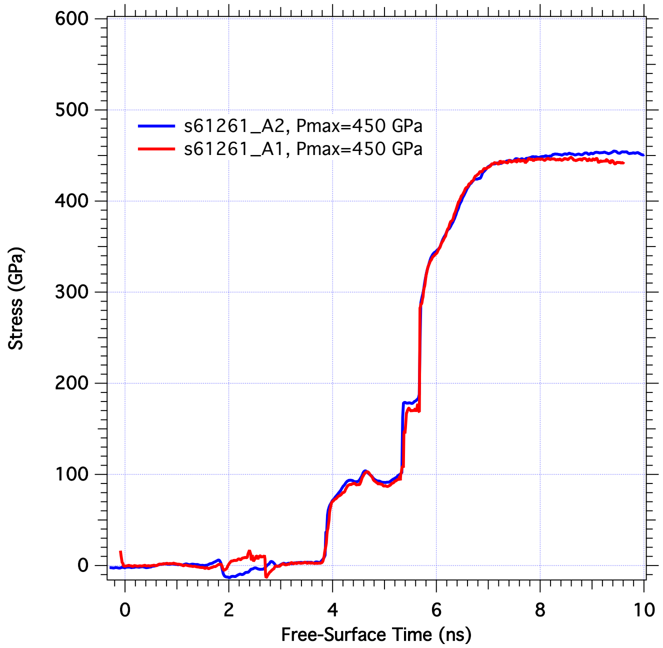
Target: C[17]**Ta**[3]C [40], **BL: Fe**

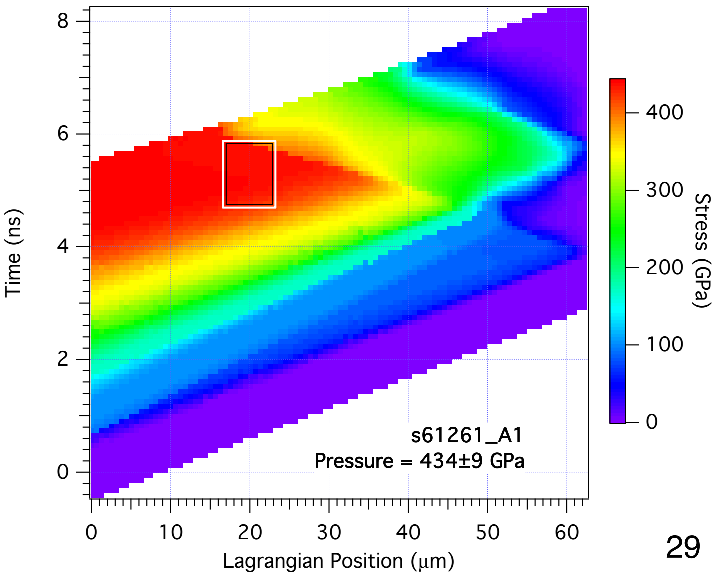


Ramp drive: 246 J
(t_{BL} = 4.6 ns)
P = 4.34±0.09 Mbar

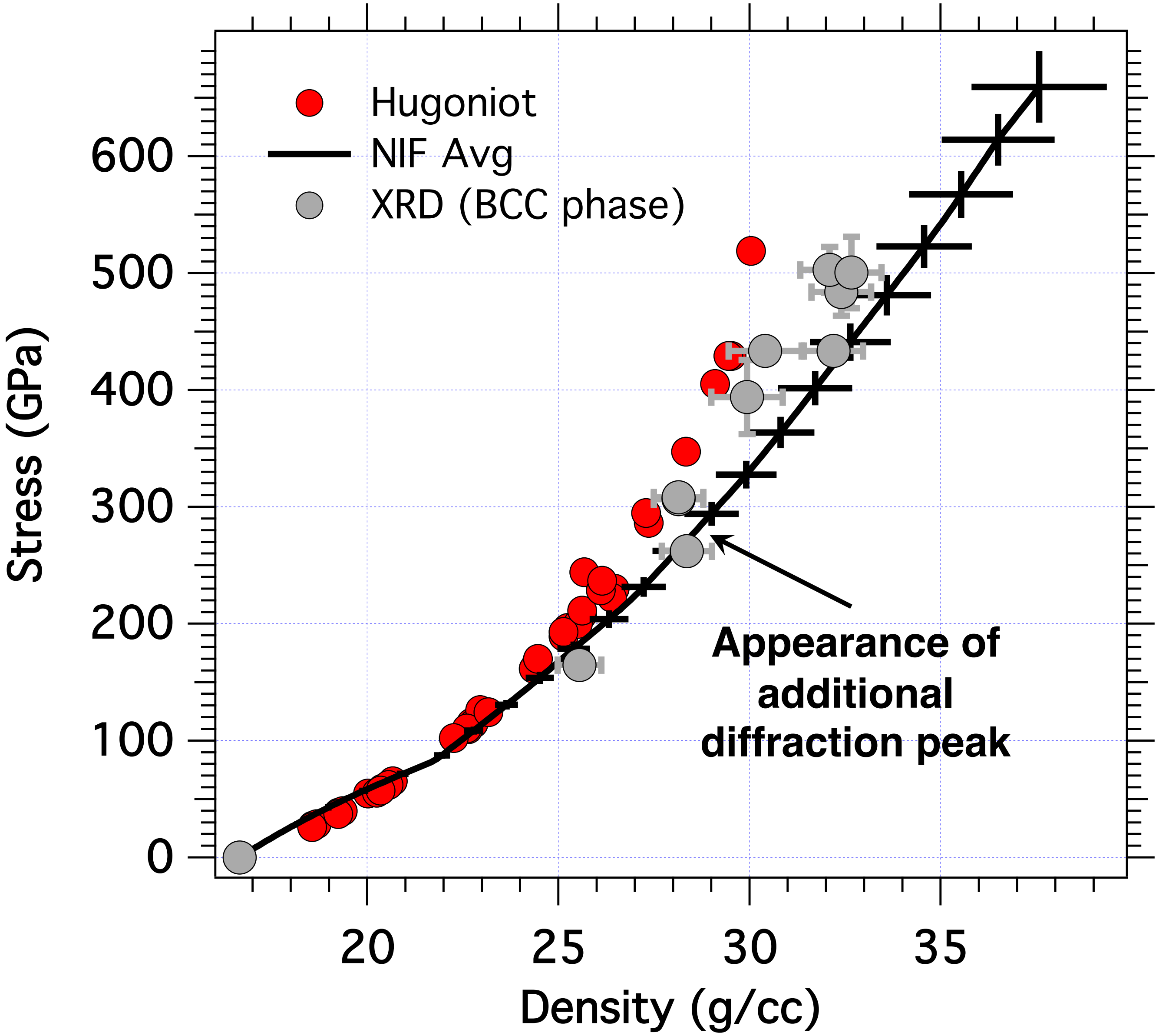




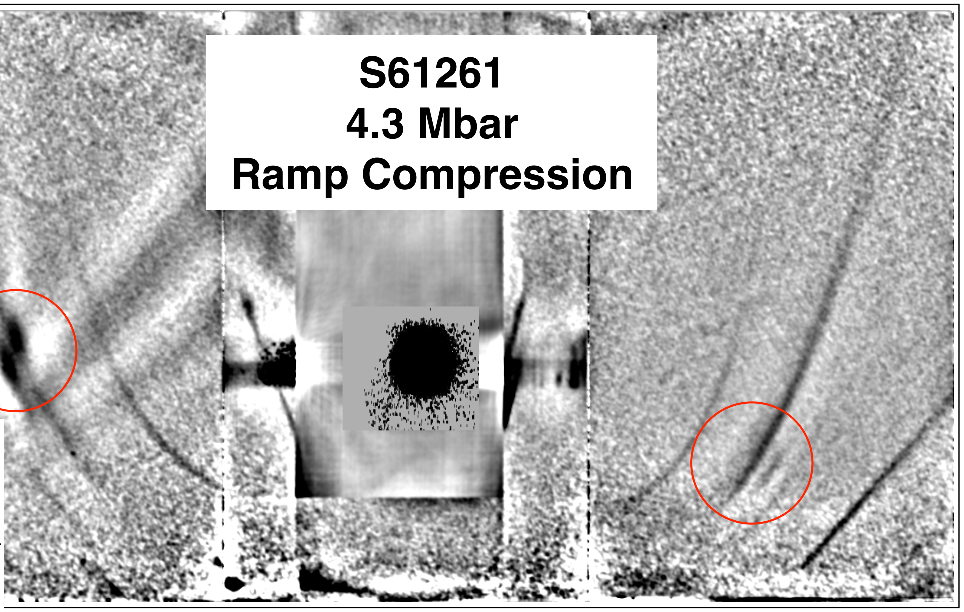


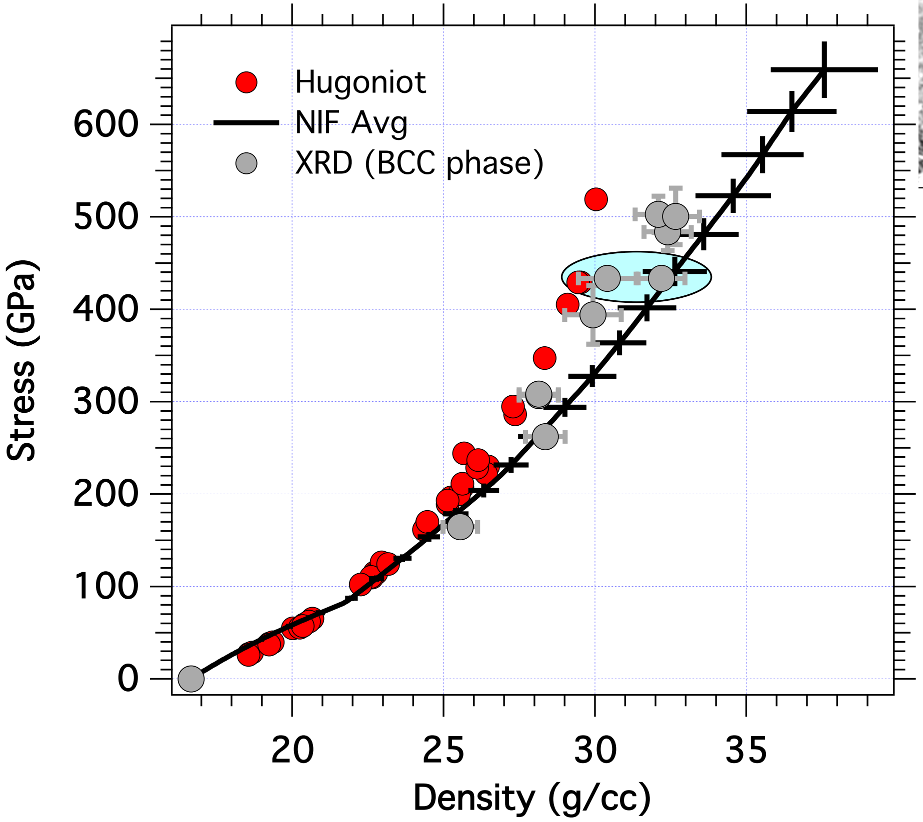


We have measured the (assumed) BCC density for 8 shots.



Diffraction for S61261 can be interpreted as two phase coexistence





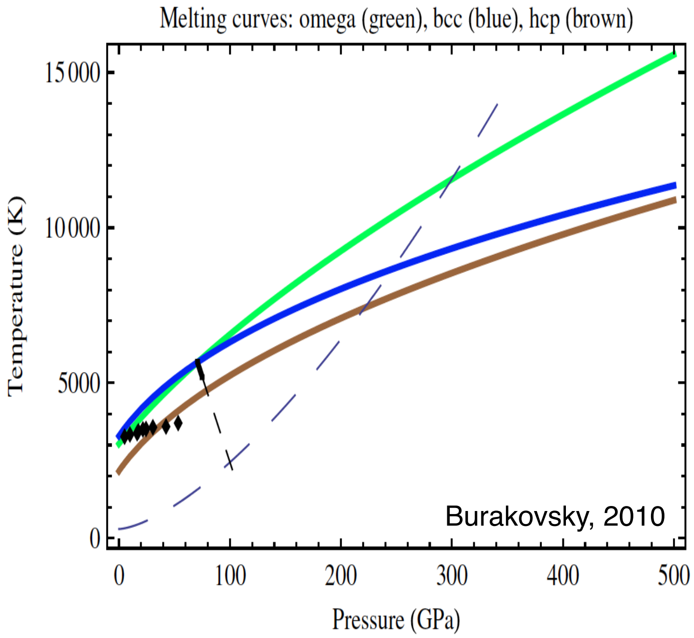
A consistent understanding of both the NIF EOS and the Omega diffraction data can be had by positing a Ta phase transition near 3.4 Mbar.

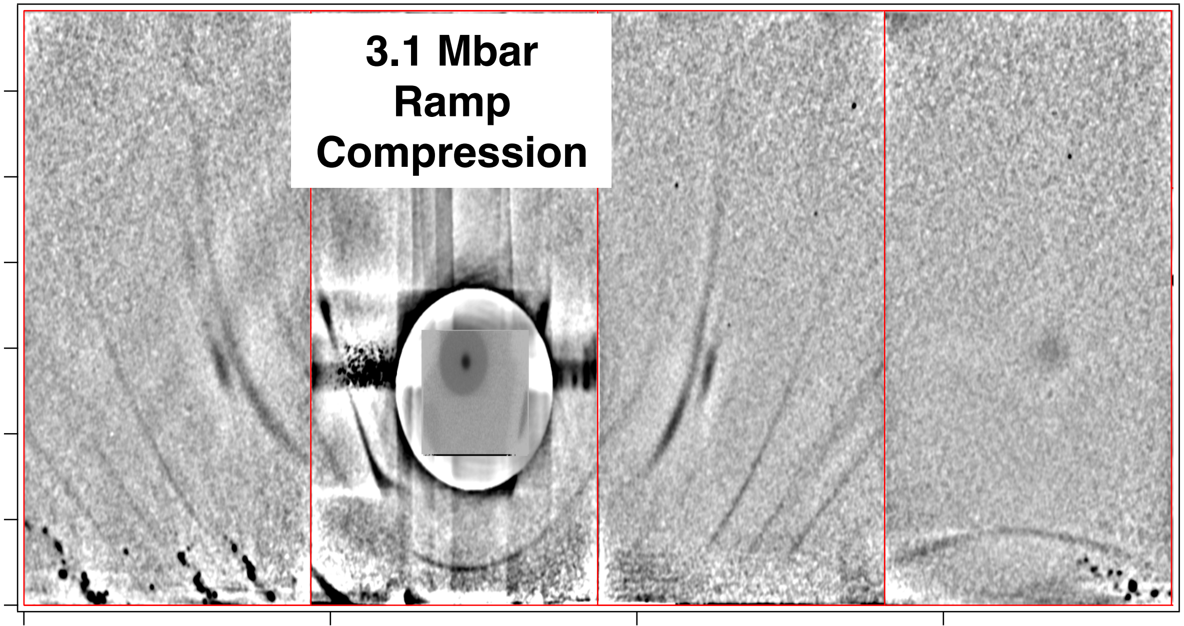
e.g. Burakovski (2010) predict ω-phase.

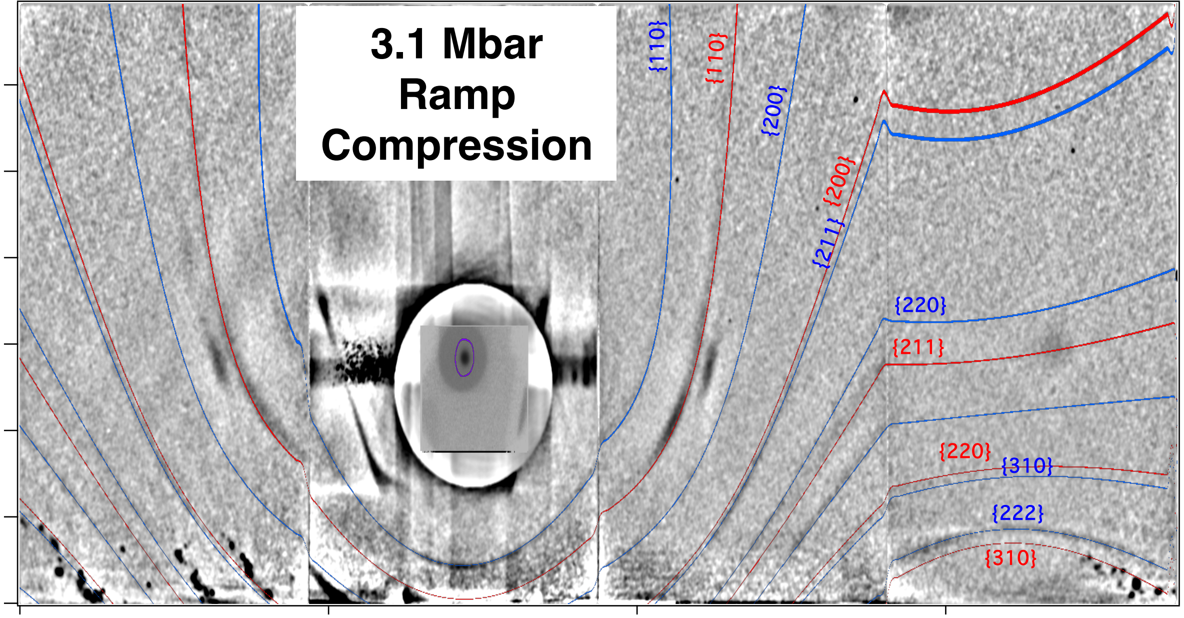
High-Pressure X-Ray Diffraction of Tantalum: Possible phase transition.

RampDiff-11B (Ta, ramp4)
Shot **61267,** OMEGA 2011-0223

Target: C[22]Ta[3]C[40], **BL: Cu**
Ramp drive: 171 J (t_{BL} = 4.7 ns)
P = 3.1 Mbar

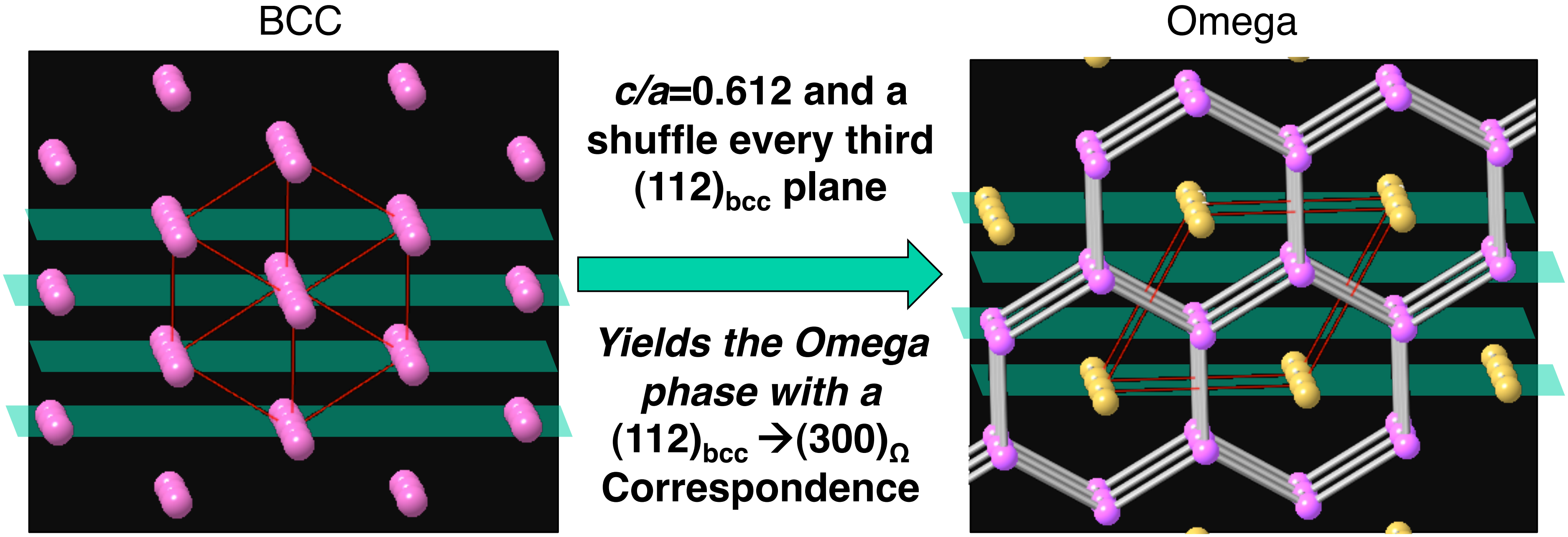






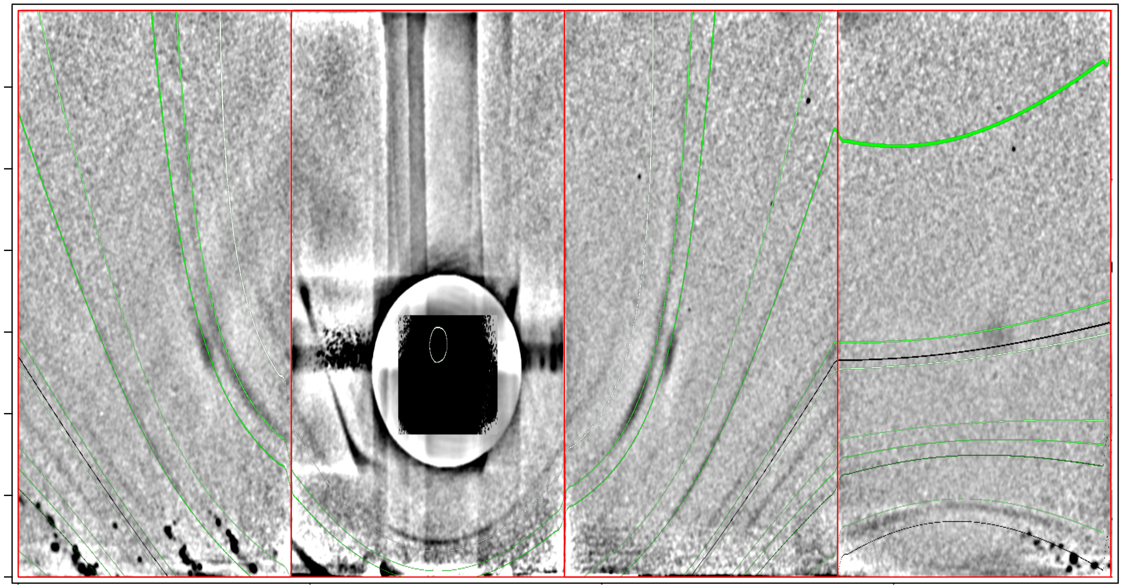
$\{211\}_{BCC}$ line is exactly 90° between plane normal and compression axis.

Burakovsky (2010) predicted Omega phase with c/a~0.572



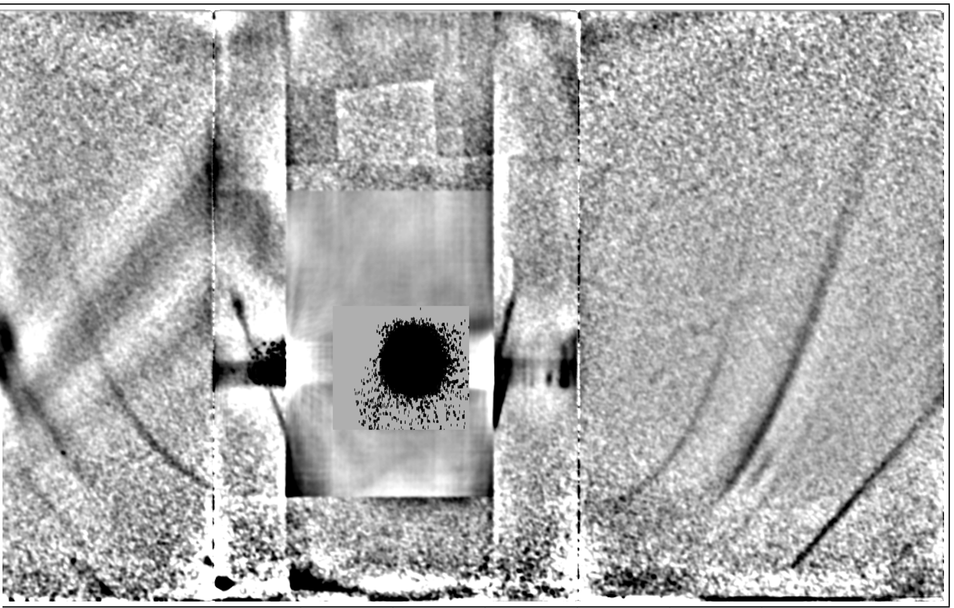
c/a=0.612 and a shuffle every third $(112)_{bcc}$ plane

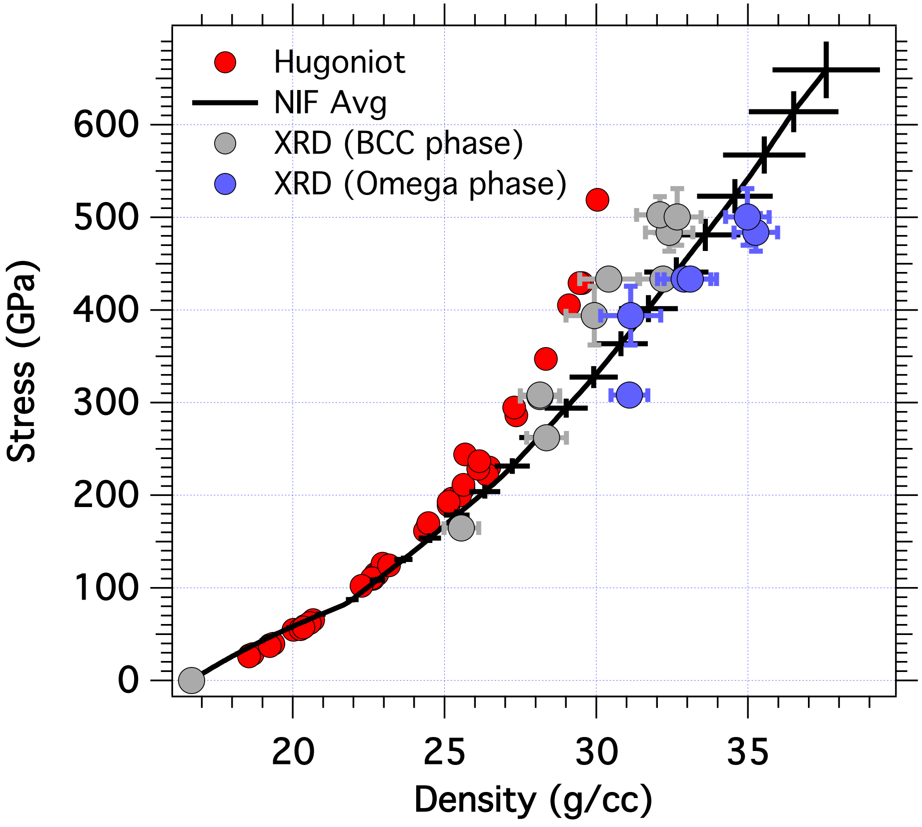
Yields the Omega phase with a $(112)_{bcc} \rightarrow (300)_{\Omega}$ **Correspondence**

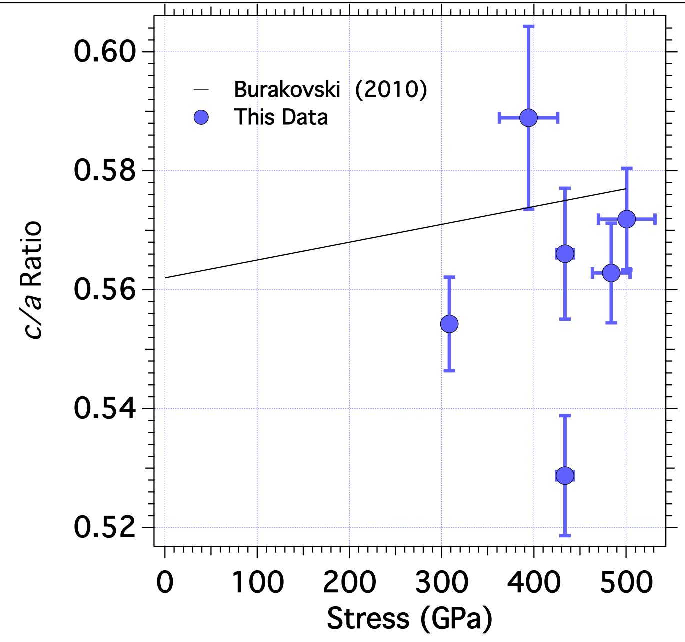


Omega best fit with *V*=29 cc, and *c/a*=0.56

We can also determine density assuming the omega phase





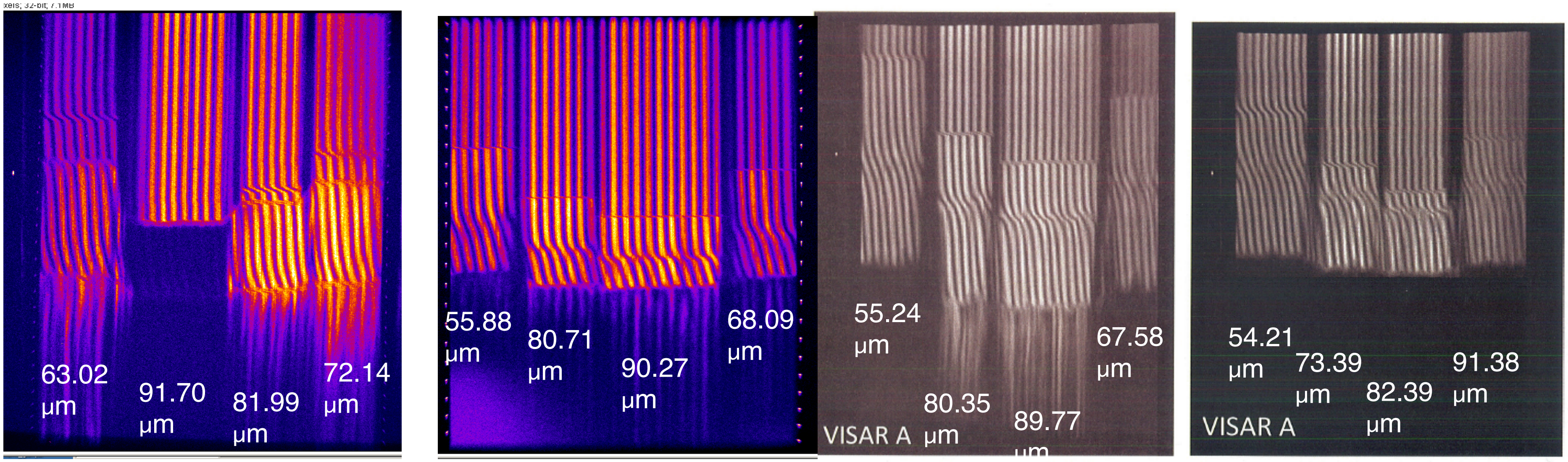


About 30% of NIF’s capacity was needed to reach 50 Mbar on ramped diamond, and about 8% of capacity to reach 9 Mbar in Ta.

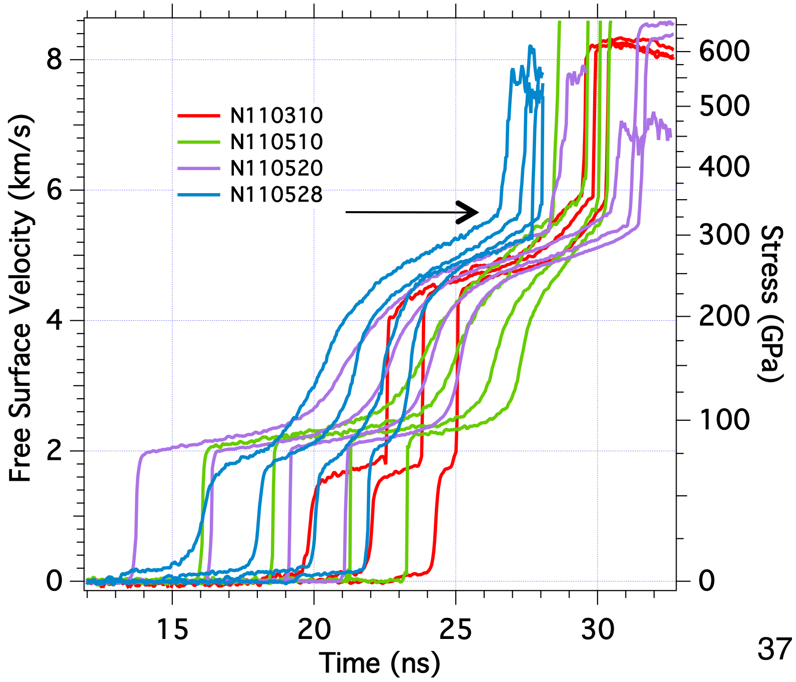
We need to continue to develop experimental techniques for this regime.

Supporting Slides

On the NIF Tantalum shocks up at the same velocity on each shot

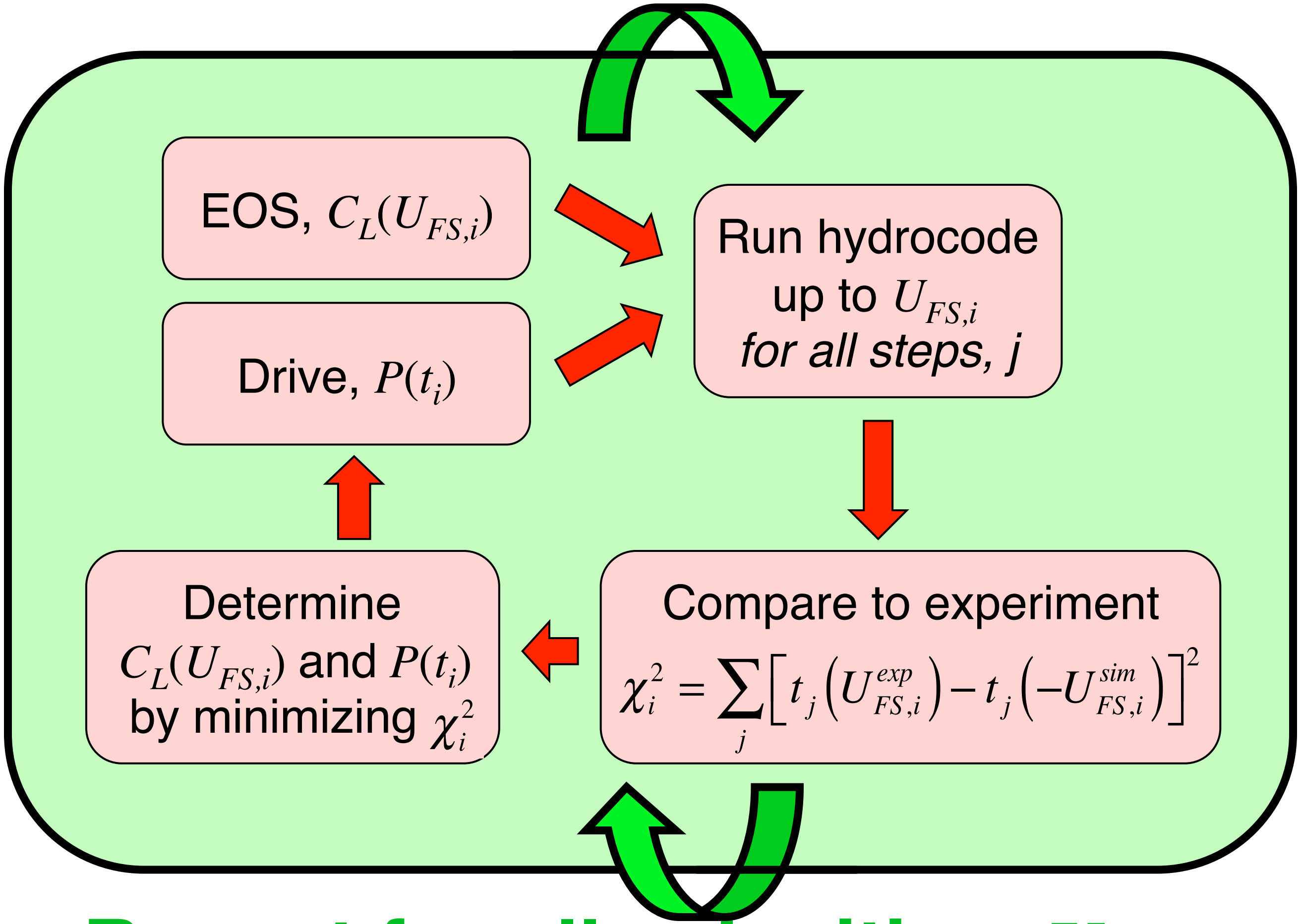


Shock initiation at ~ 3.4 Mbar repeatedly with minor dependence on sample thickness or drive profile.



We will use a Forward-Only Analysis Method to deal with time-dependent transitions and growing shocks.

The National Ignition Facility



EOS, $C_L(U_{FS,i})$

Drive, $P(t_i)$

Run hydrocode up to $U_{FS,i}$ *for all steps, j*

Compare to experiment

$$\chi_i^2 = \sum_j \left[t_j\left(U_{FS,i}^{exp}\right) - t_j\left(-U_{FS,i}^{sim}\right)\right]^2$$

Determine $C_L(U_{FS,i})$ and $P(t_i)$ by minimizing χ_i^2

Repeat for all velocities, $U_{FS,i}$

- **This method still requires a model for time-dependent phase transitions.**
- **Exact methods being developed by Evan Reed and by Bryan Reed potentially offer a very attractive alternative.**