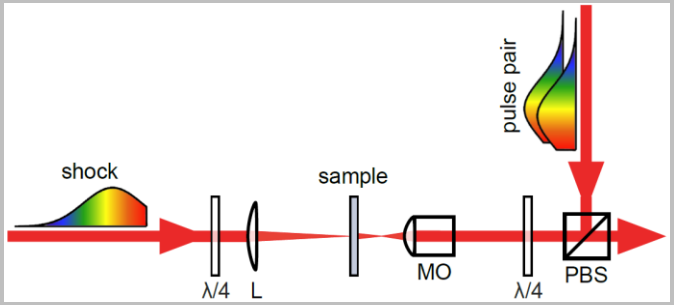
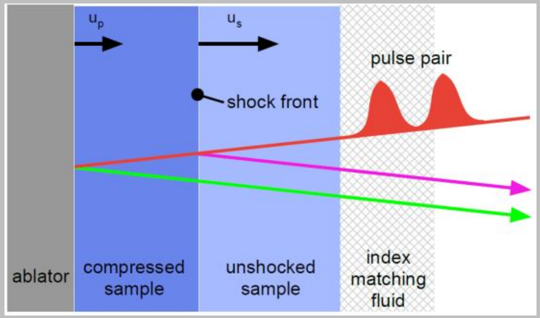
Exceptional service in the national interest

SAND2017-7026C

Sandia National Laboratories





Ultrafast Shock Interrogation of Polycrystalline Energetic Materials

Samuel D. Park*, Michael R. Armstrong‡, Ian Kohl*, Joseph M. Zaug‡, Robert Knepper*, Alexander S. Tappan*, Sorin Bastea‡, and Jeffrey J. Kay*

*Sandia National Laboratories, ‡Lawrence Livermore National Laboratory

APS SCCM 2017

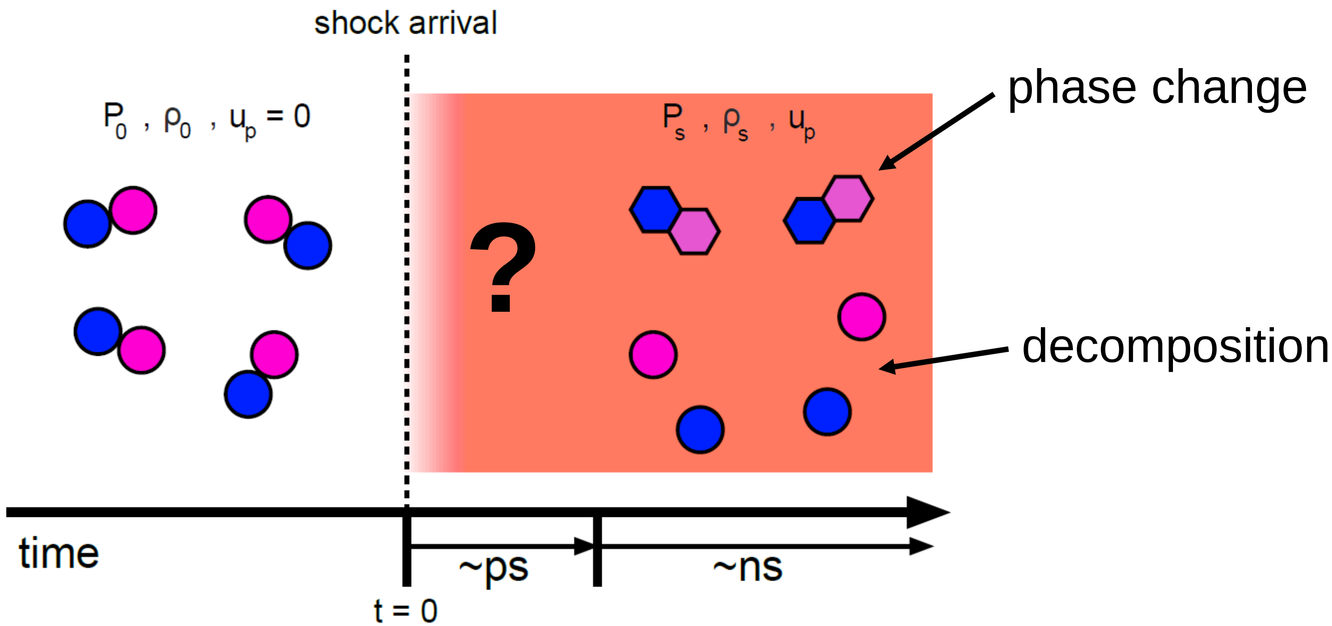
U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

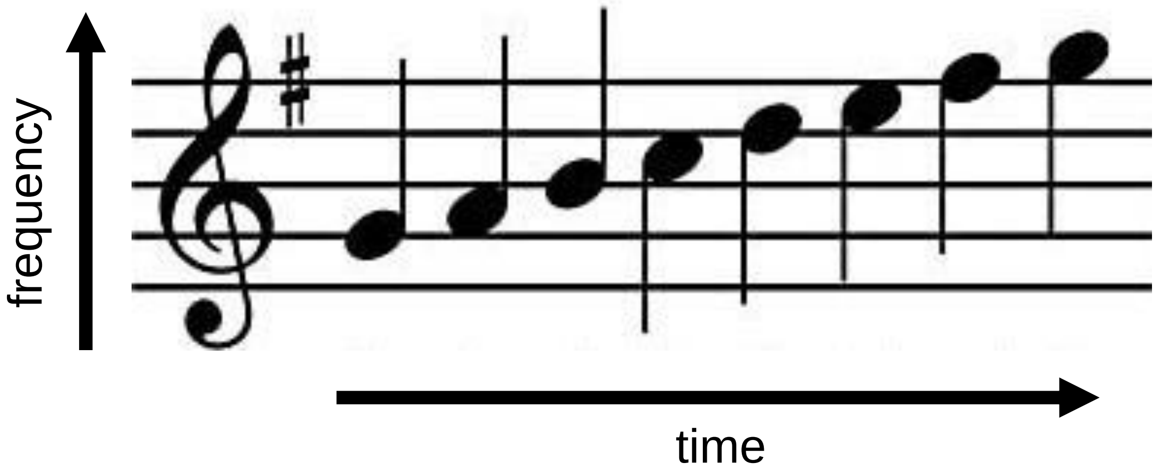
Introduction:



- Shock waves can change the thermodynamic state of a material over the picosecond time scale.
- Understanding shock initiation of energetic materials requires the ability to diagnose the state of materials on the picosecond time scale of shock compression.

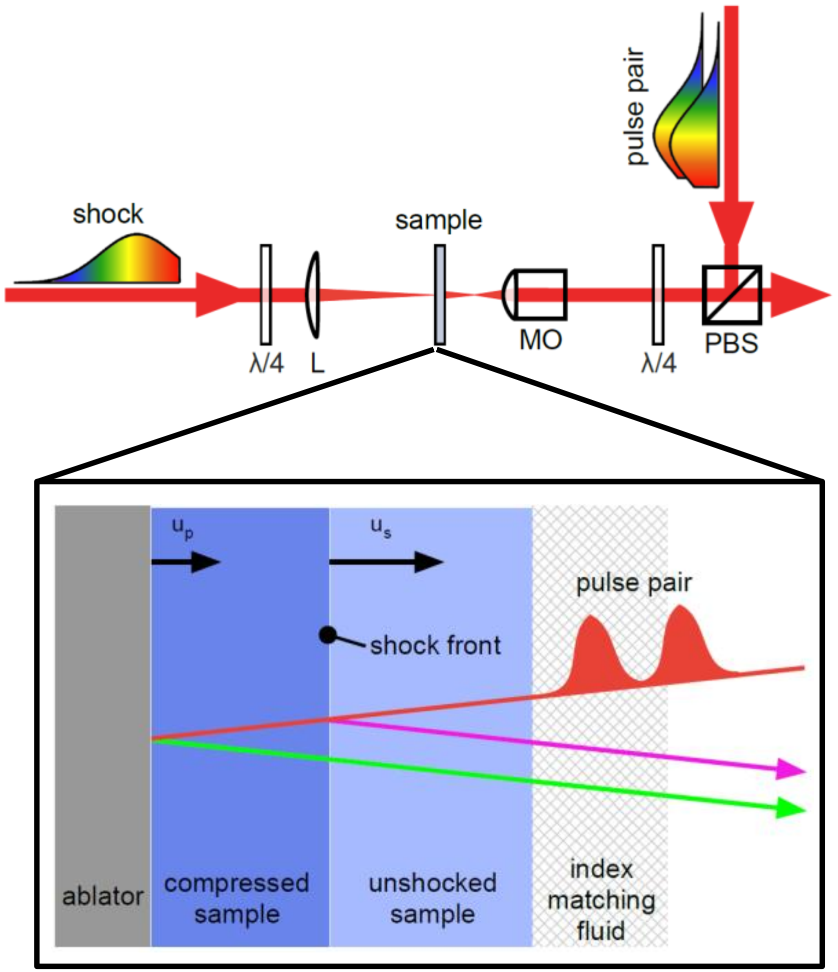
Nellis, *Rep. Prog. Phys.* (2006)
Zeldovich, *Theory of Detonation* (1960)

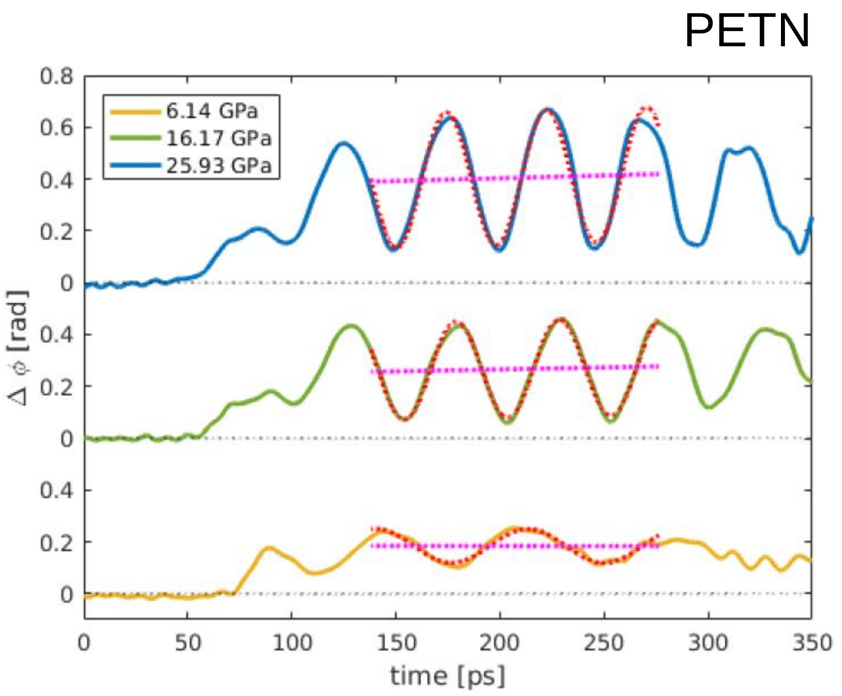
How do we achieve picosecond time resolution?



- Measure in time-frequency domain to probe the material during the initial stages of shock compression with fast time resolution.
- Ultrafast pulses are linearly chirped to ~350 ps, which governs the temporal range and resolution of our measurements.

Experimental USI Methods:



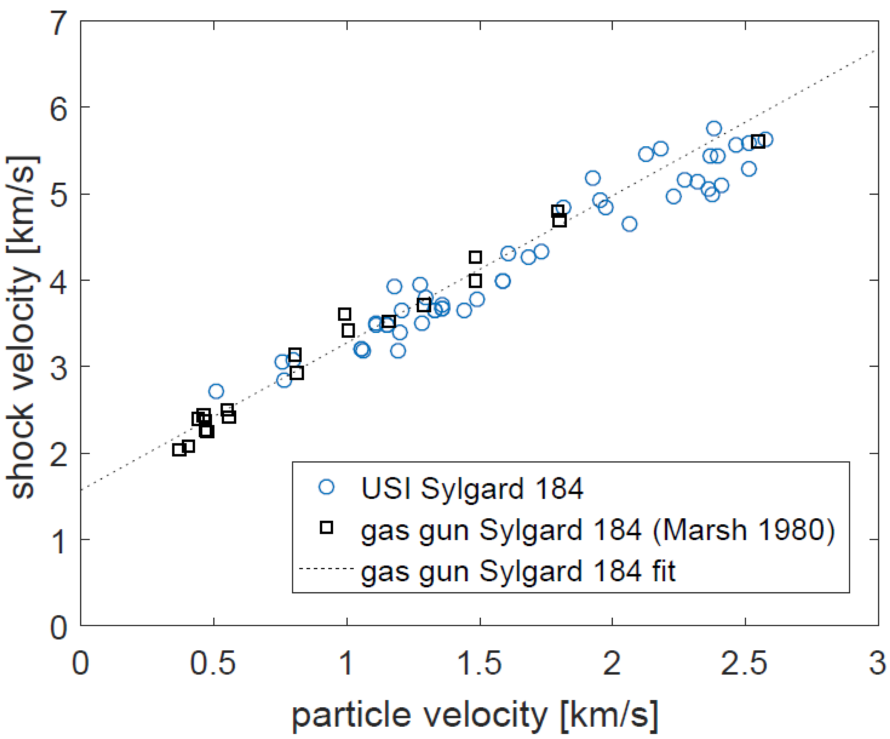


Armstrong et al., *J. Appl. Phys.* (2010)
Bolme et al., *J. Appl. Phys.* (2007)
Dlott et al., *J. Phys. Chem. B* (1998)

- The shock front and metallic ablator surface (typically Aluminum) act as a scanning optical etalon, with a total reflectance varying as the thickness of the shocked region.

Concept Validation:

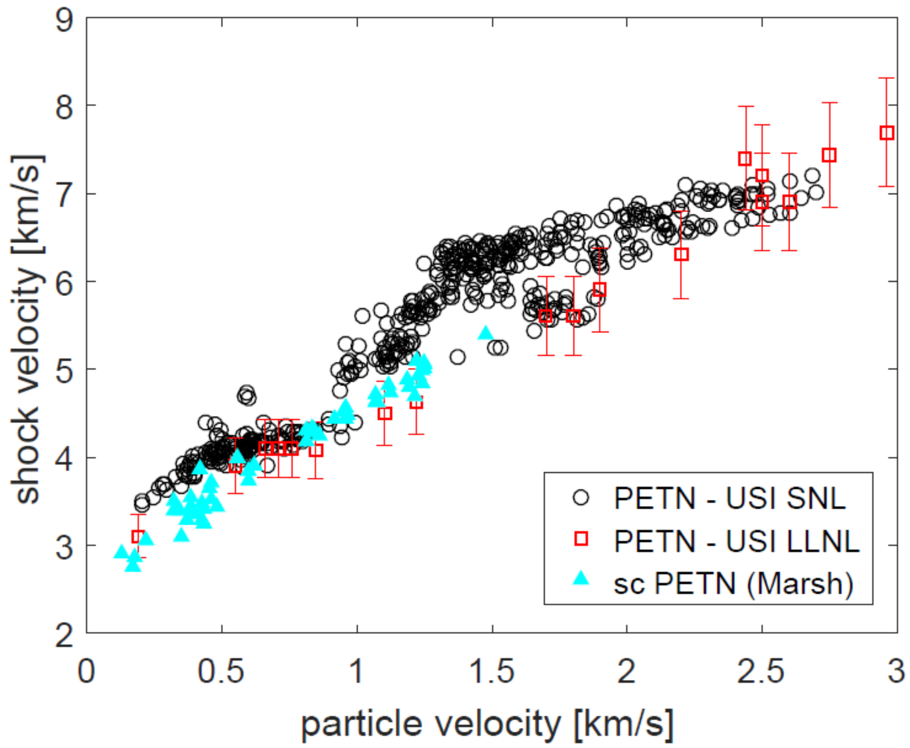
- Good agreement with previously reported gas gun results on polymer, Sylgard 184.
- USI results are expected to lie on gas gun results because there are no expected chemical or physical changes in the material under shock compression.

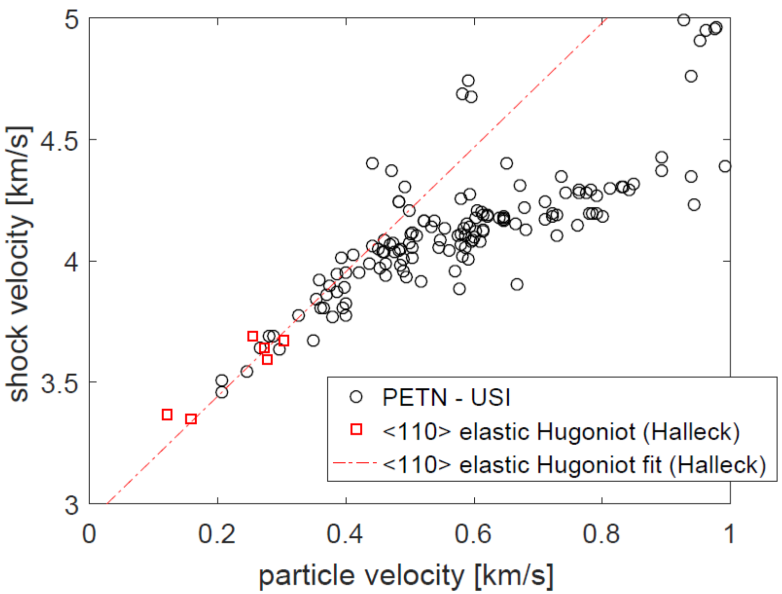


Marsh, *LASL SHOCK HUGONIOT DATA* (1980)

Polycrystalline PETN Films:

- Vapor deposited PETN – strongly preferred <110> orientation
- USI results *should* match/agree with unreacted equation of state (Marsh – quartz impact, wedge, and impedance matching)

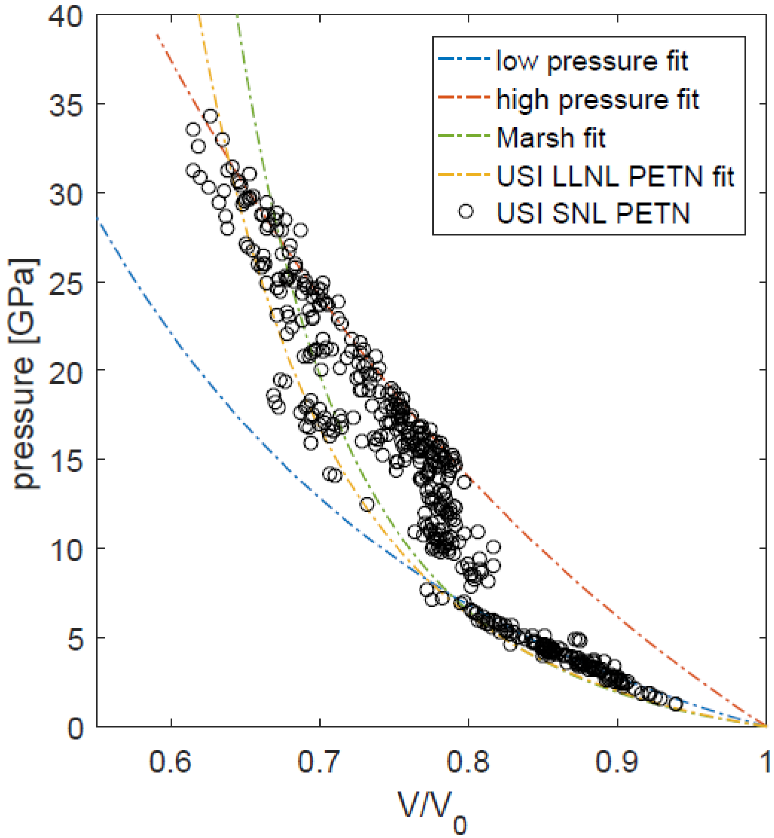




Marsh, *LASL SHOCK HUGONIOT DATA* (1980)

Halleck et al., *J. Appl. Phys.* (1976)

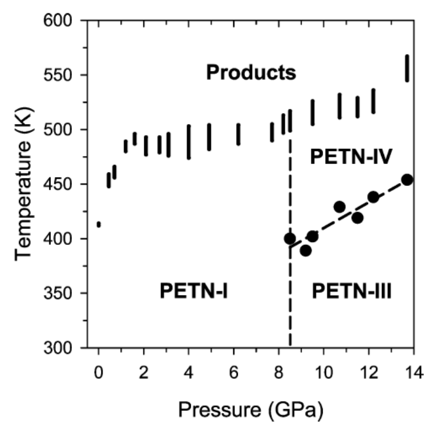
Polycrystalline PETN Films:



- Observation of volume expansion around ~7-12 GPa
- <110> sensitive from 8.5 – 12.5 GPa (most sensitive orientation)
- Exothermic Chemistry?

Assumptions:

- Sample does not absorb at the wavelengths of the pulse pair spectrum (does not change under shock compression)[1]
- Refractive index behind shock follows Gladstone-Dale relation

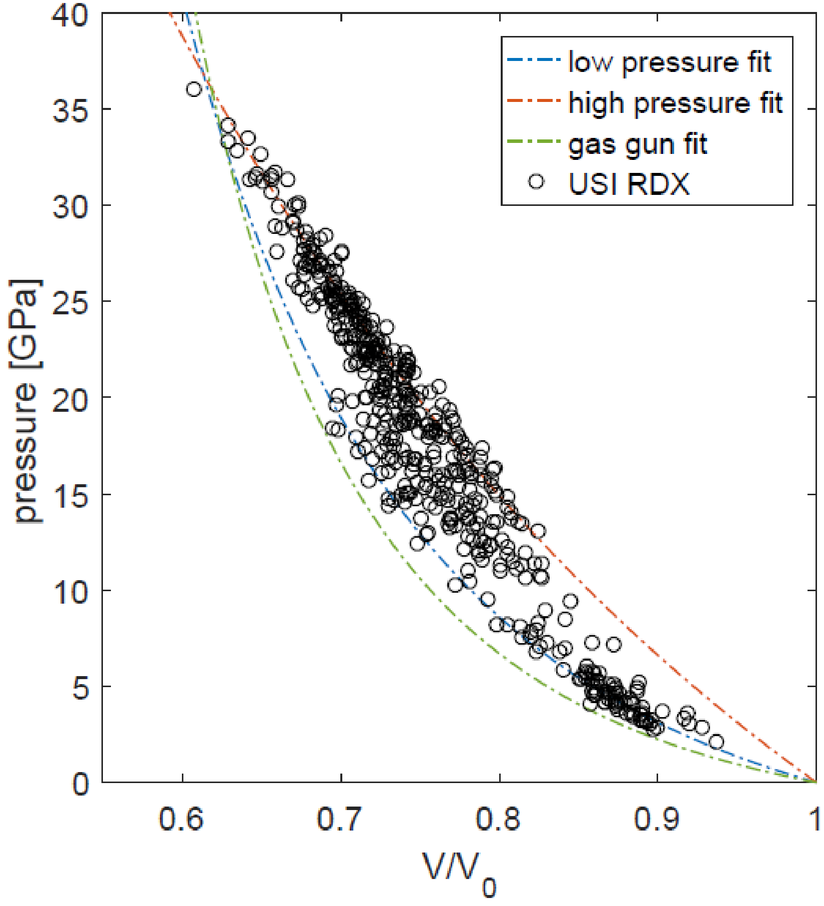


J. J. Dick et al., *J. Appl. Phys.* (1991)

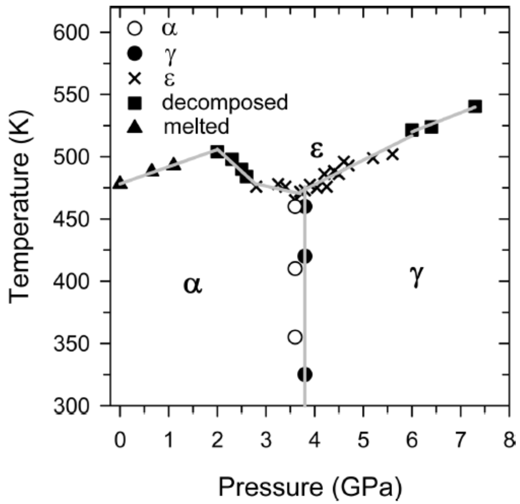
Dreger et al., *J. Phys. Chem. A* (2013)

[1] J. J. Kay, SCCM 2017 Session T2

Polycrystalline RDX (α) Films:

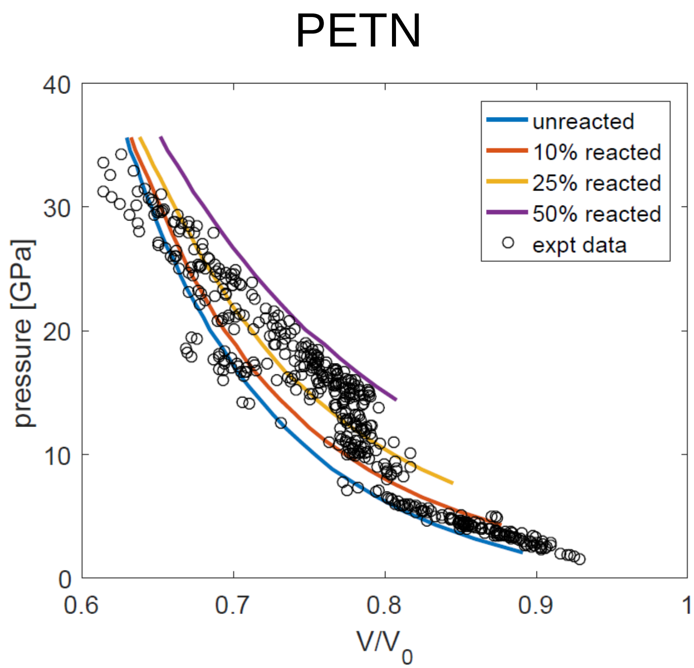


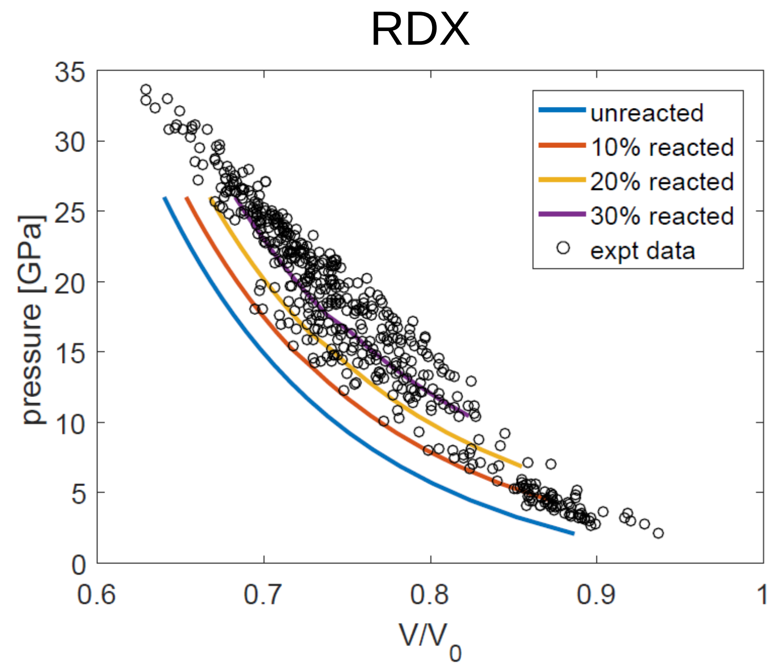
- Vapor deposited RDX – no strongly preferred orientation
- Observe a similar effect as polycrystalline PETN films but not as pronounced – possibly due to microstructure and orientation effects



Dreger et al., *J. Phys. Chem. A* (2010)
Ilhyukin et al., *Soviet Phys. Doklady* (1960)

Preliminary Simulations: Reaction?





- Shock initiation sensitivity for PETN: <110> sensitive from 8.5 – 12.5 GPa (most sensitive orientation)
- Extremely thin reaction zone for PETN (less than 1 ns)
- MD shock simulations – threshold shock velocity of 5 km/s to initiate chemical reactions for <110>

Sheffield et al., *9th Det. Symp.* (1989)
J. J. Dick et al., *J. Appl. Phys.* (1991)
Yoo et al., *J. Appl. Phys.* (2000)
T. Shan et al., *J. Phys. Chem. B* (2012)

Conclusions:

- USI has the temporal and spatial capabilities relevant for measuring shock initiation
- Measure particle and shock velocities right behind the shock front (< 350 ps)
- Anomalies in shock Hugoniot locus for energetic materials
- Assuming samples do not absorb at wavelengths used in the experiment (~800 nm), we observe a volumetric expansion
- Exothermic chemistry?

Acknowledgments:

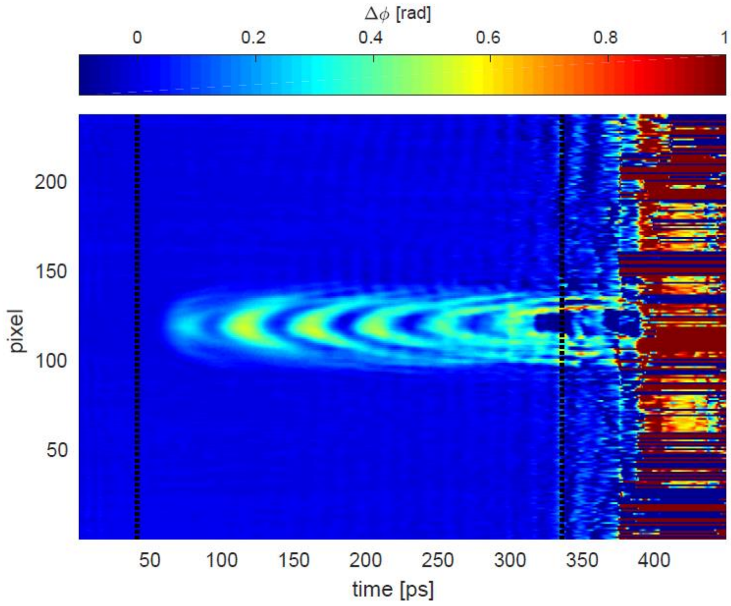
SNL:
- Jeff Kay
- Ian Kohl
- Rob Knepper
- Alex Tappan
- Yuki Horie
- Leanna Minier

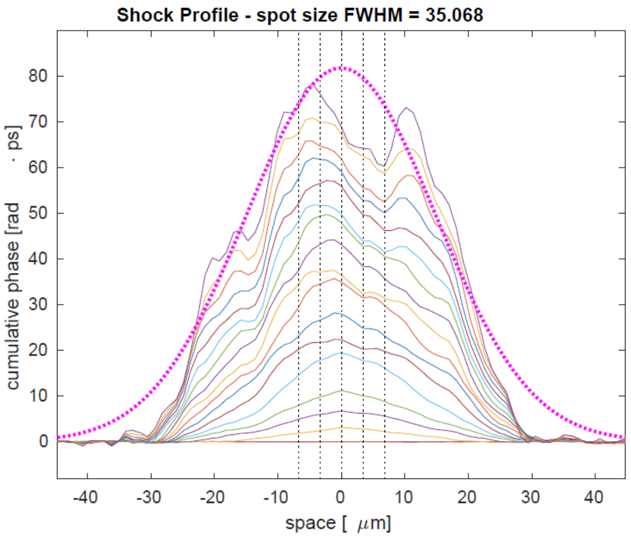
LLNL:
- Mike Armstrong
- Joe Zaug
- Sorin Bastea
- Paulius Grivickas

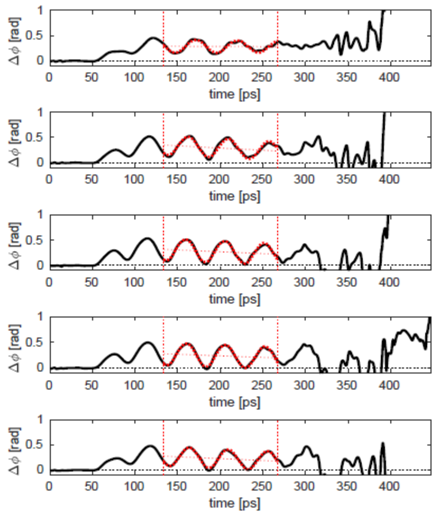
Funding is gratefully acknowledged from:

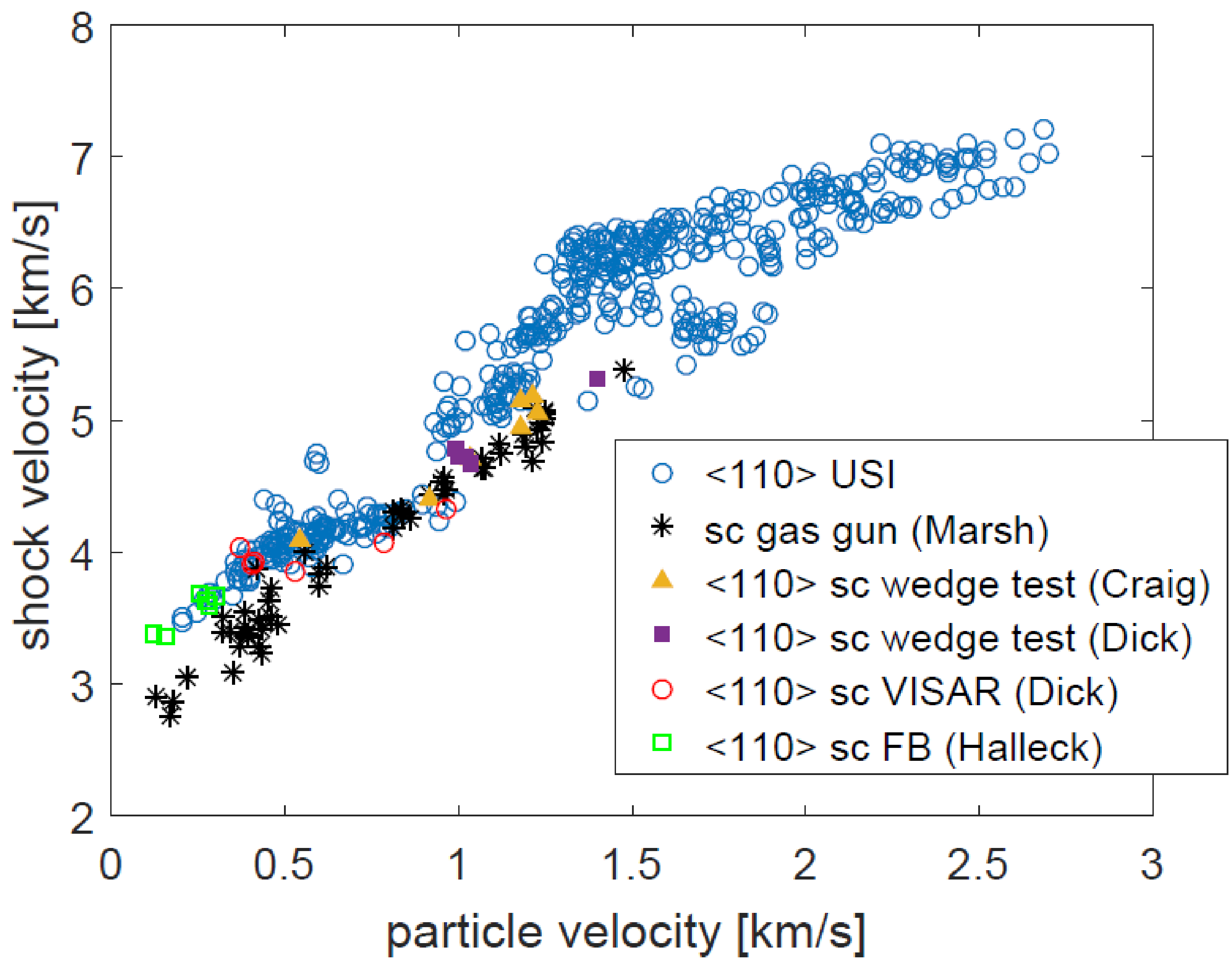
Sandia Laboratory-Directed Research and Development (LDRD) Program

begin extra slides

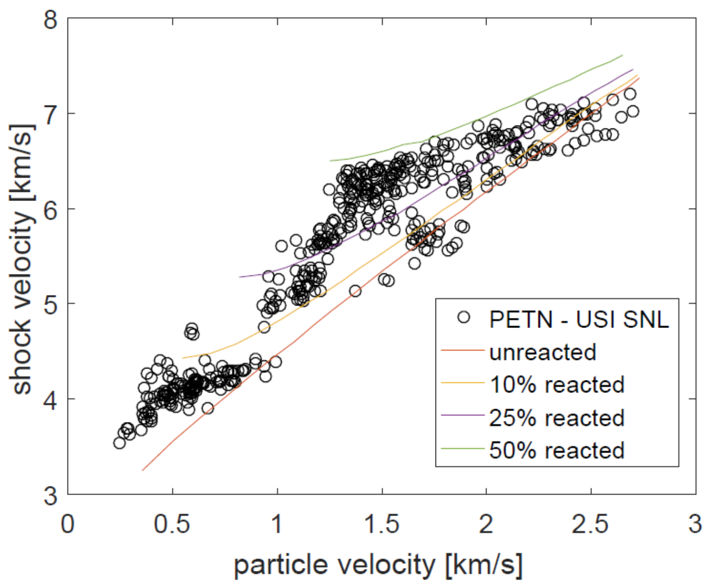

Δϕ [rad]
0
0.2
0.4
0.6
0.8
1
pixel
200
150
100
50
50
100
150
200
250
300
350
400
time [ps]

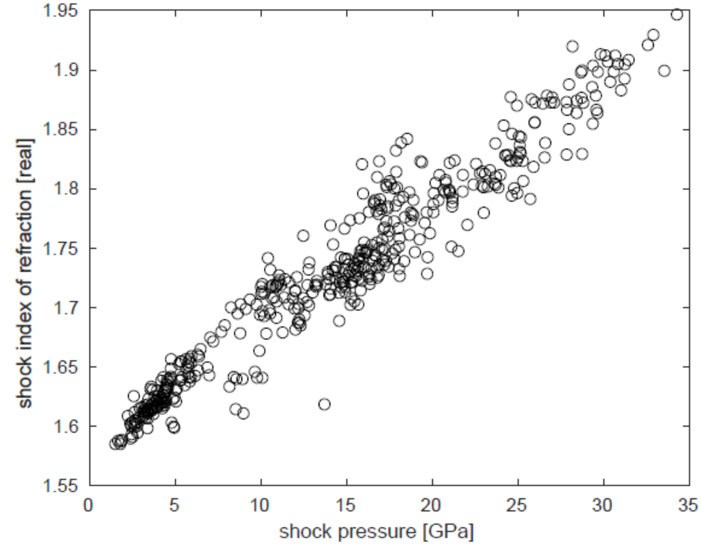

Shock Profile - spot size FWHM = 35.068
cumulative phase [rad · ps]
80
70
60
50
40
30
20
10
0
-40
-30
-20
-10
0
10
20
30
40
space [μm]

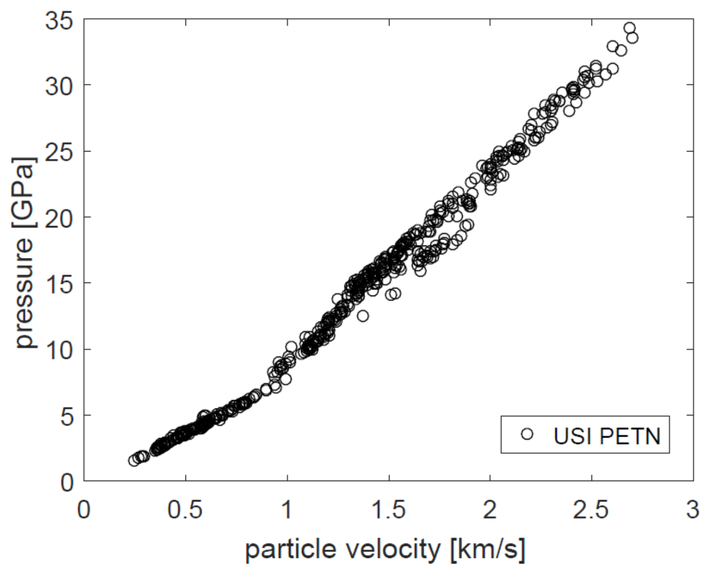

Δϕ [rad]
1
0.5
0
0
50
100
150
200
250
300
350
400
time [ps]



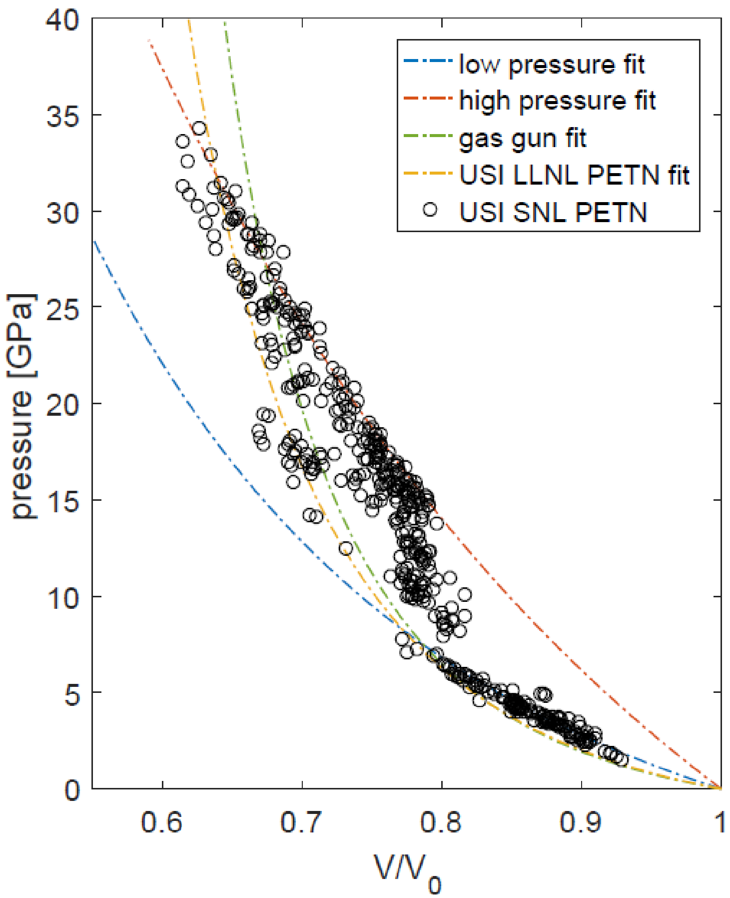
shock velocity [km/s]
particle velocity [km/s]
8
7
6
5
4
3
2
0
0.5
1
1.5
2
2.5
3
<110> USI
sc gas gun (Marsh)
<110> sc wedge test (Craig)
<110> sc wedge test (Dick)
<110> sc VISAR (Dick)
<110> sc FB (Halleck)


shock velocity [km/s]
particle velocity [km/s]
3
4
5
6
7
8
0
0.5
1
1.5
2
2.5
3
PETN - USI SNL
unreacted
10% reacted
25% reacted
50% reacted


shock index of refraction [real]
shock pressure [GPa]
1.55
1.6
1.65
1.7
1.75
1.8
1.85
1.9
1.95
0
5
10
15
20
25
30
35


pressure [GPa]
particle velocity [km/s]
0
5
10
15
20
25
30
35
0
0.5
1
1.5
2
2.5
3
USI PETN

Elastic stiffness modulus <110> Longitudinal ~ 15.235 GPa
Bulk Modulus ~ 9.58 GPa

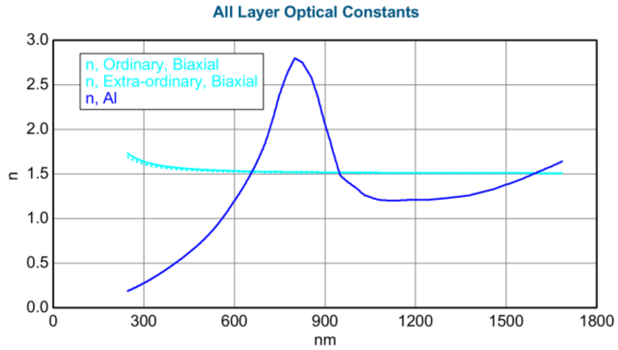


Morris, *6th Det. Symp.*

PETN:

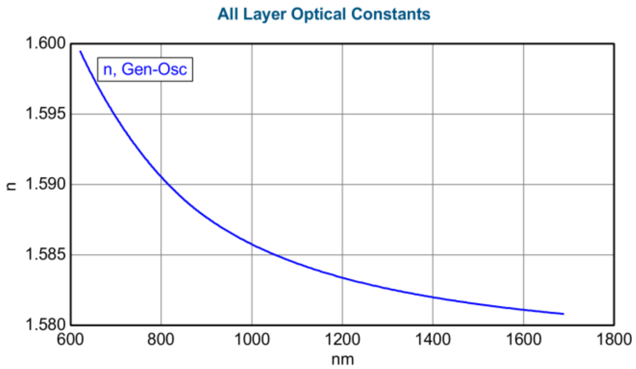
n = 1.552 @ 785 nm
density = 1.77 g/cc

RDX:



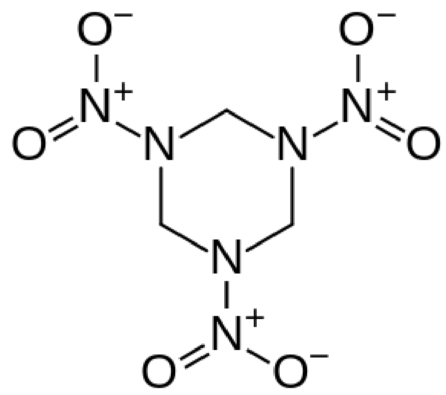
n = 1.52 @ 785 nm
density = 1.816 g/cc

CL-20:

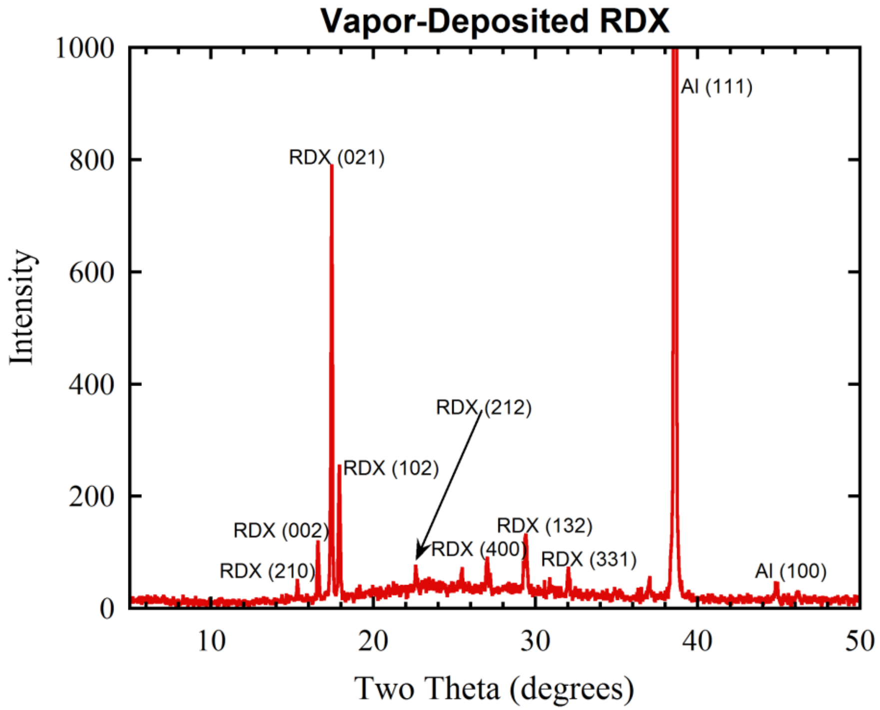


n = 1.592 @ 785 nm
density = 2.04 g/cc

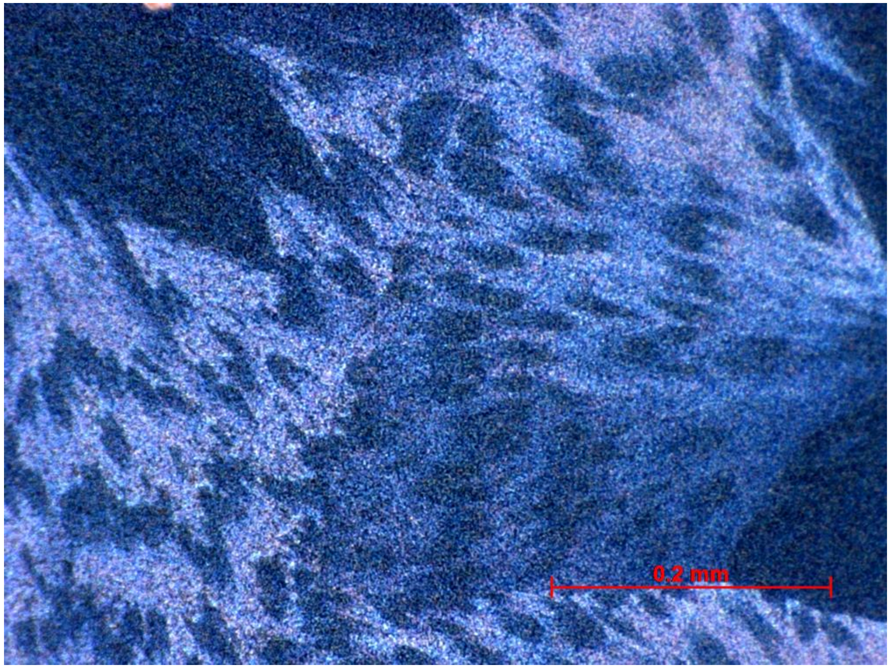
RDX



O⁻
N⁺
O
N
N
N
N⁺
O⁻
O
N⁺
O
O⁻



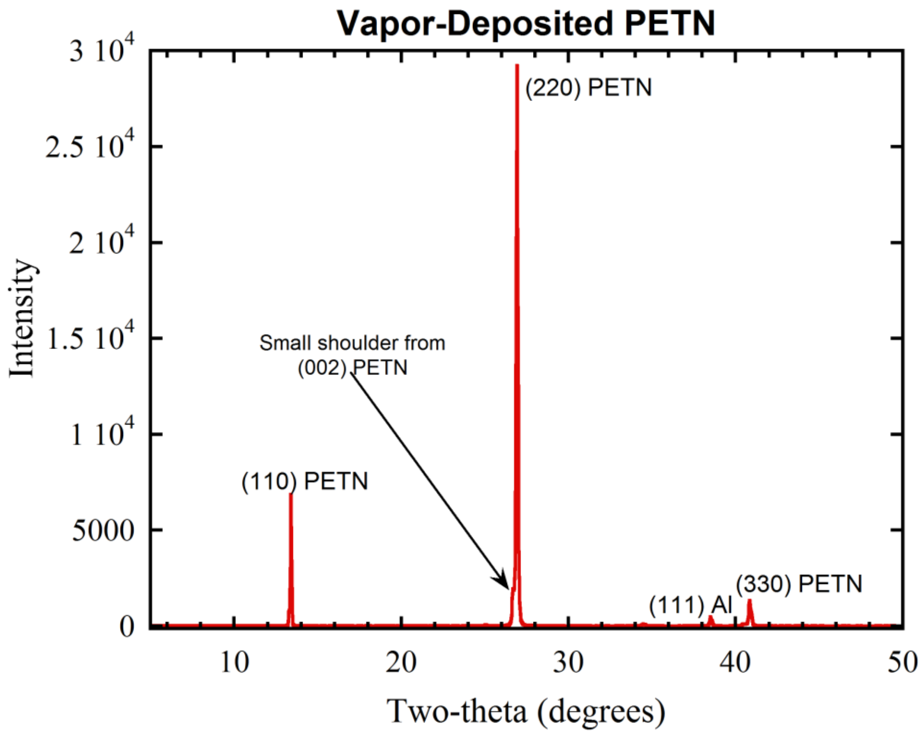
Vapor-Deposited RDX
Intensity
Two Theta (degrees)
0
200
400
600
800
1000
10
20
30
40
50
RDX (021)
Al (111)
RDX (212)
RDX (102)
RDX (002)
RDX (210)
RDX (400)
RDX (132)
RDX (331)
Al (100)

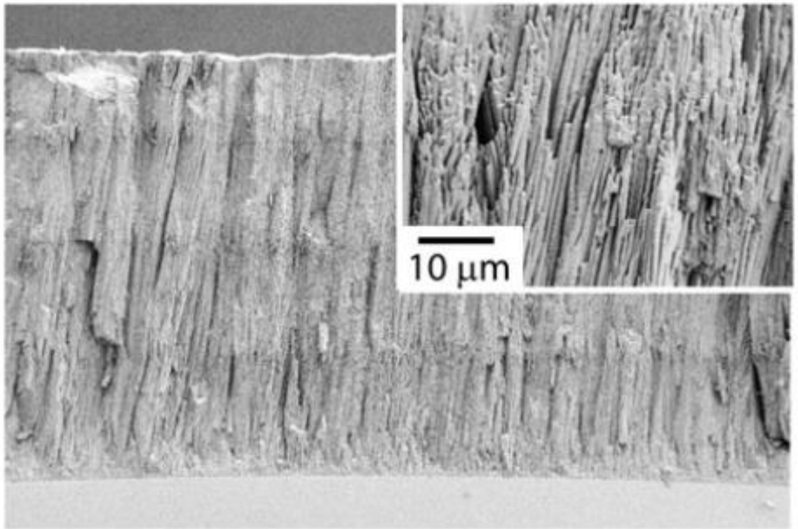


0.2 mm

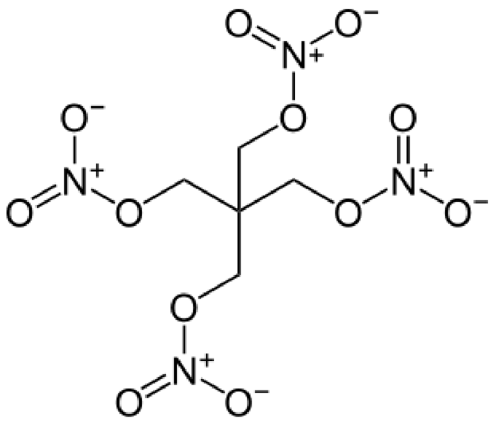
PETN

- Tetragonal crystal structure: 42m symmetry
- Elastic sound speed <110>: 2.9308 km/s
- Bulk modulus: 9.58 GPa



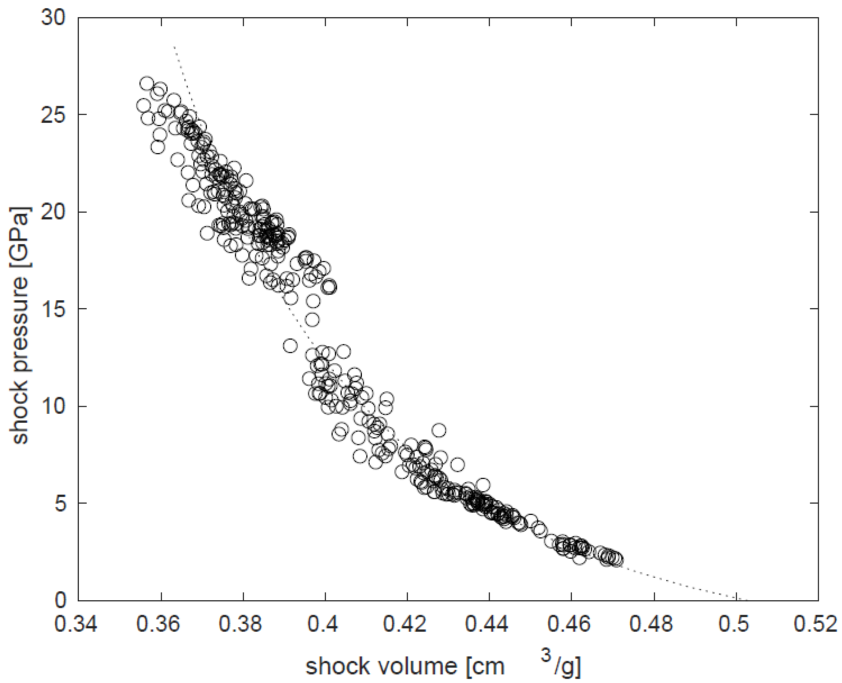


(a)

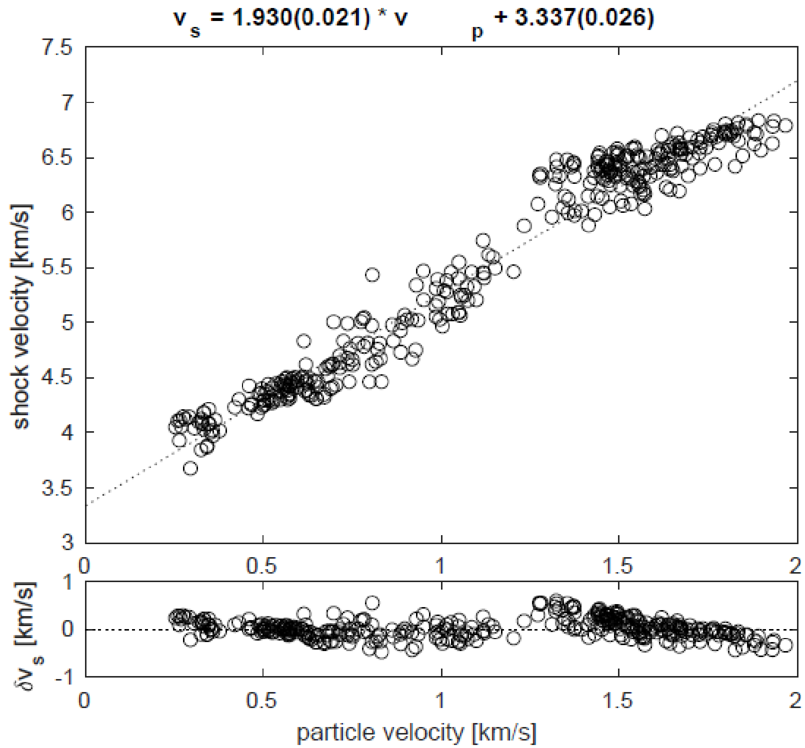


Knepper et al., *J. Mater. Res.* (2011)

CL-20 (beta)

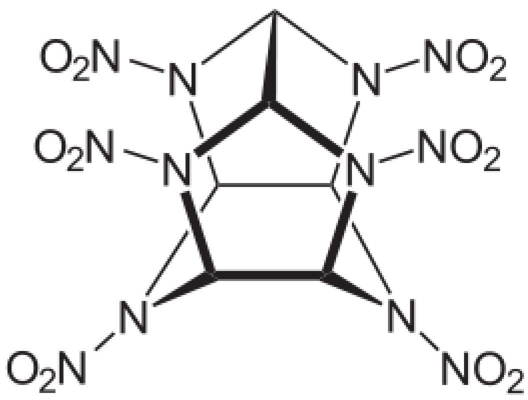


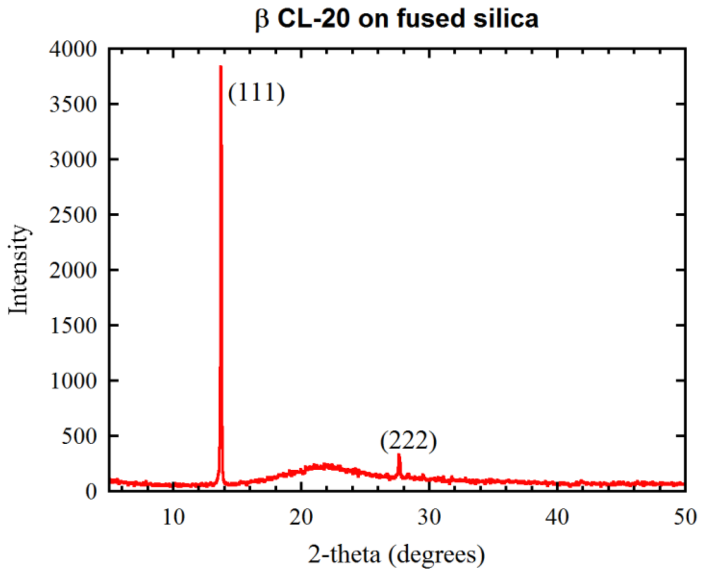
shock pressure [GPa]
shock volume [cm³/g]



v s = 1.930(0.021) * v p + 3.337(0.026)
shock velocity [km/s]
δv s [km/s]
particle velocity [km/s]

CL-20


O2N
NO2
O2N
NO2
O2N
NO2
N
N
N
N
N
N


β CL-20 on fused silica
Intensity
2-theta (degrees)
(111)
(222)
0
500
1000
1500
2000
2500
3000
3500
4000
10
20
30
40
50

Notes:

Sandia National Laboratories

$$U^2 = \frac{v_0^2 \cdot P}{v_0 - v}$$

$$\frac{\delta U}{U} = \frac{\delta v \cdot U}{2 v_0 u_p}$$