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Using THOR to manipulate the homogeneous phase transition and nucleation rates in freezing water

Erin J. Nissen and Daniel H. Dolan

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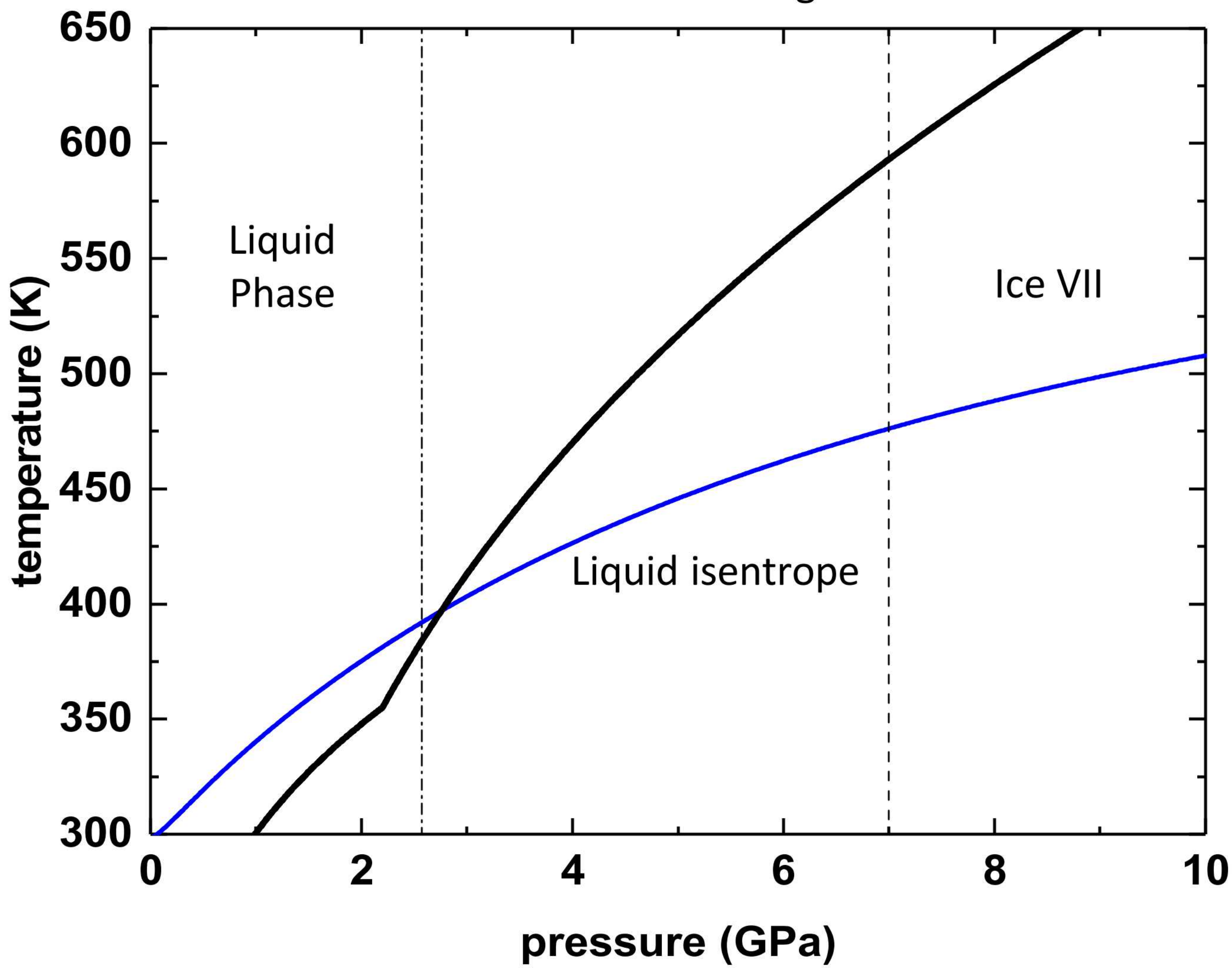
Previous Studies on Heterogeneous & Homogeneous Nucleation in Liquid Water

2.5 GPa ≤ Heterogeneous Nucleation

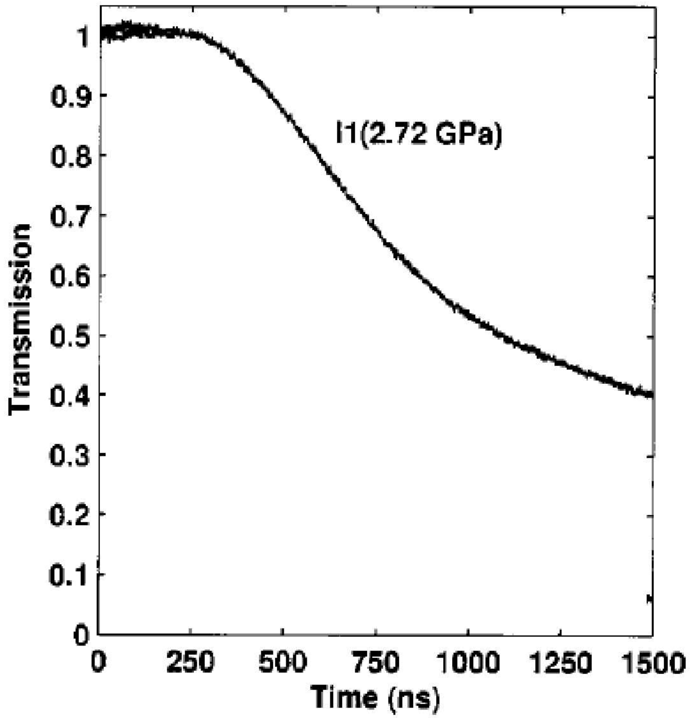
6.5 – 7 GPa = Homogeneous Nucleation



D. H. Dolan, et al. The Journal of Chemical Physics **121** (18), 9050 (2004); D. H. Dolan, et al. Nature Physics **3**, 339 (2007); S. J. P. Stafford, et al. AIP Conference Proceedings **1793** (1), 130005 (2017).

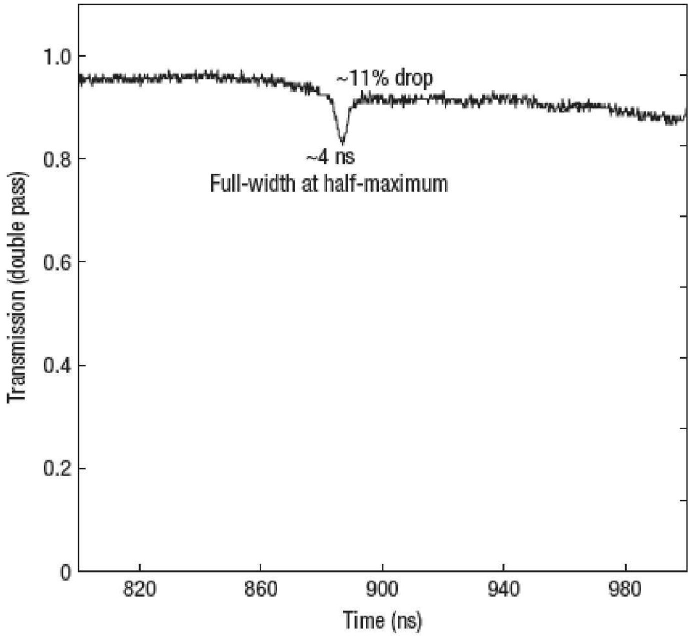
Transmission Loss of Water during Homogeneous & Heterogeneous Nucleation

2.5 GPa ≤ Heterogeneous Nucleation



z-cut quartz & fused silica

6.5 – 7 GPa = Homogeneous Nucleation



cubic zirconia & sapphire

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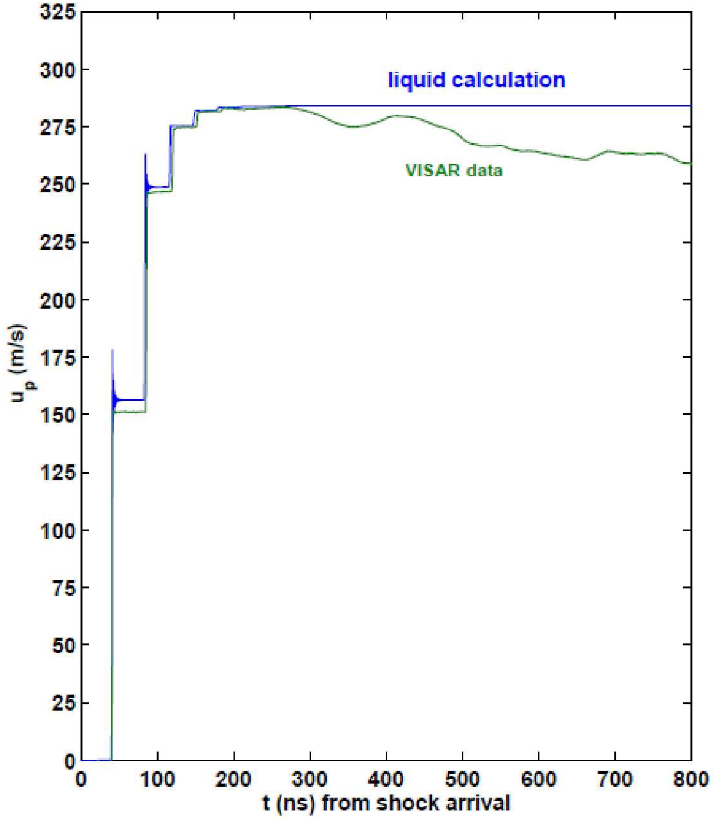

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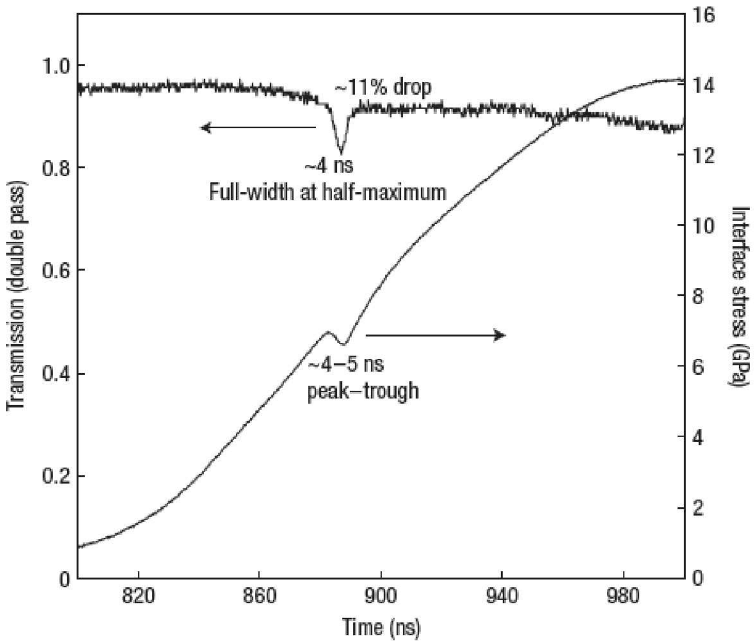

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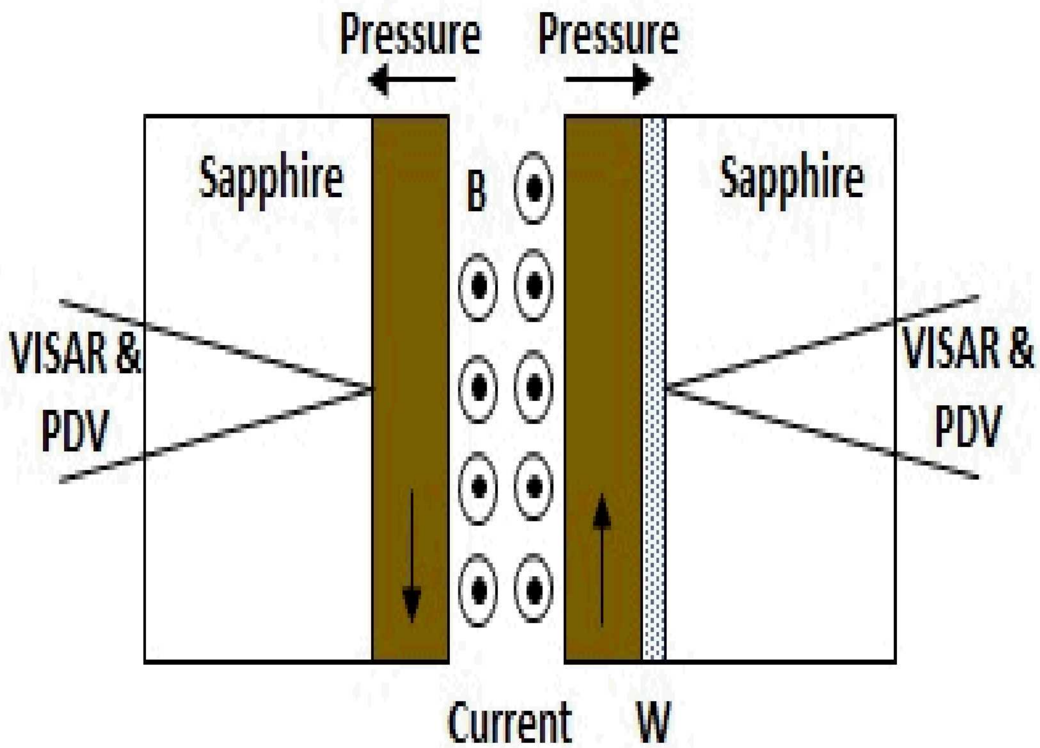
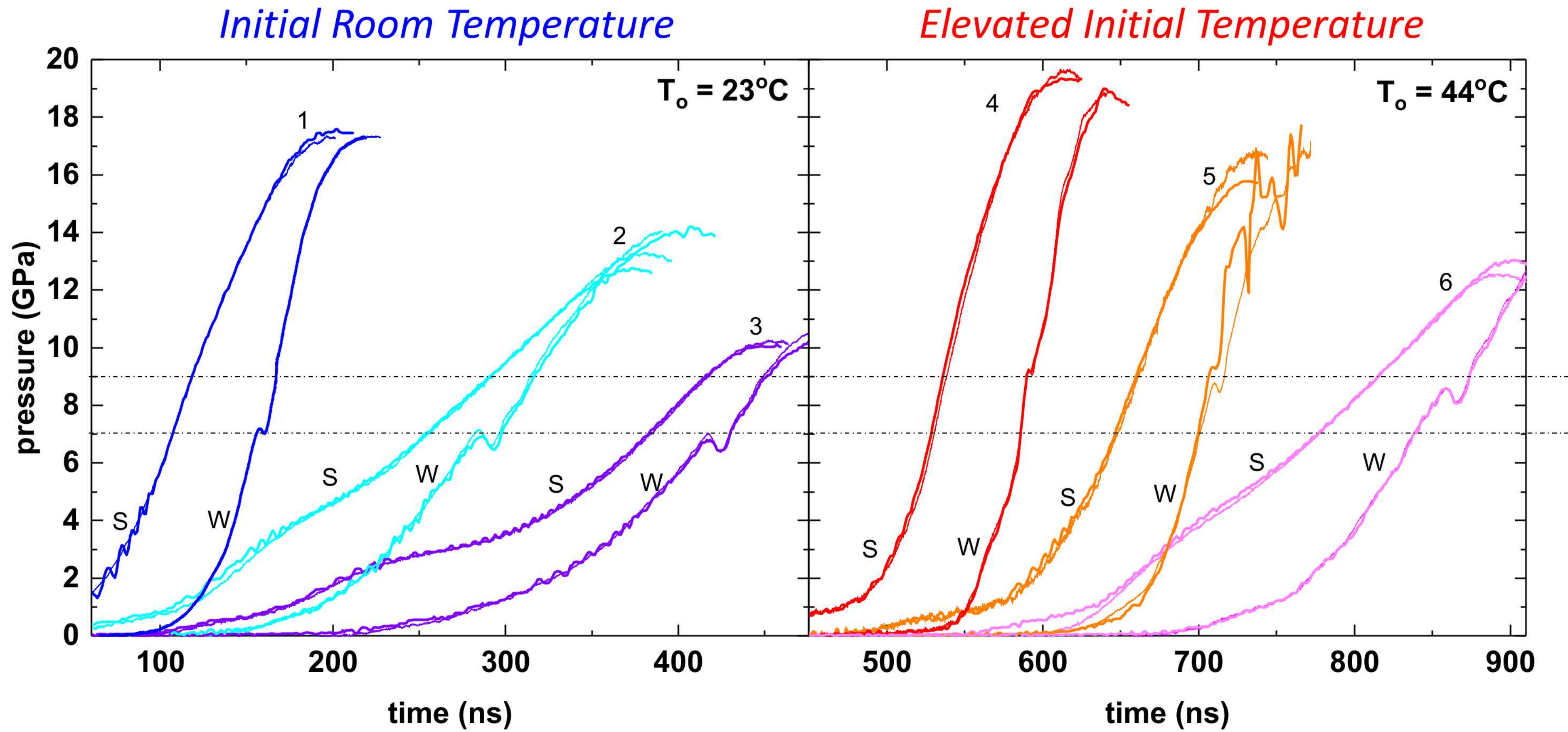
Sandia's THOR-64



Can change ramp rate by changing the timing at which each marx bank fires

The entire sample holder can be heated/cooled to maintain a temperature other than room temperature

PDV & VISAR Profiles for 6 Shots on THOR

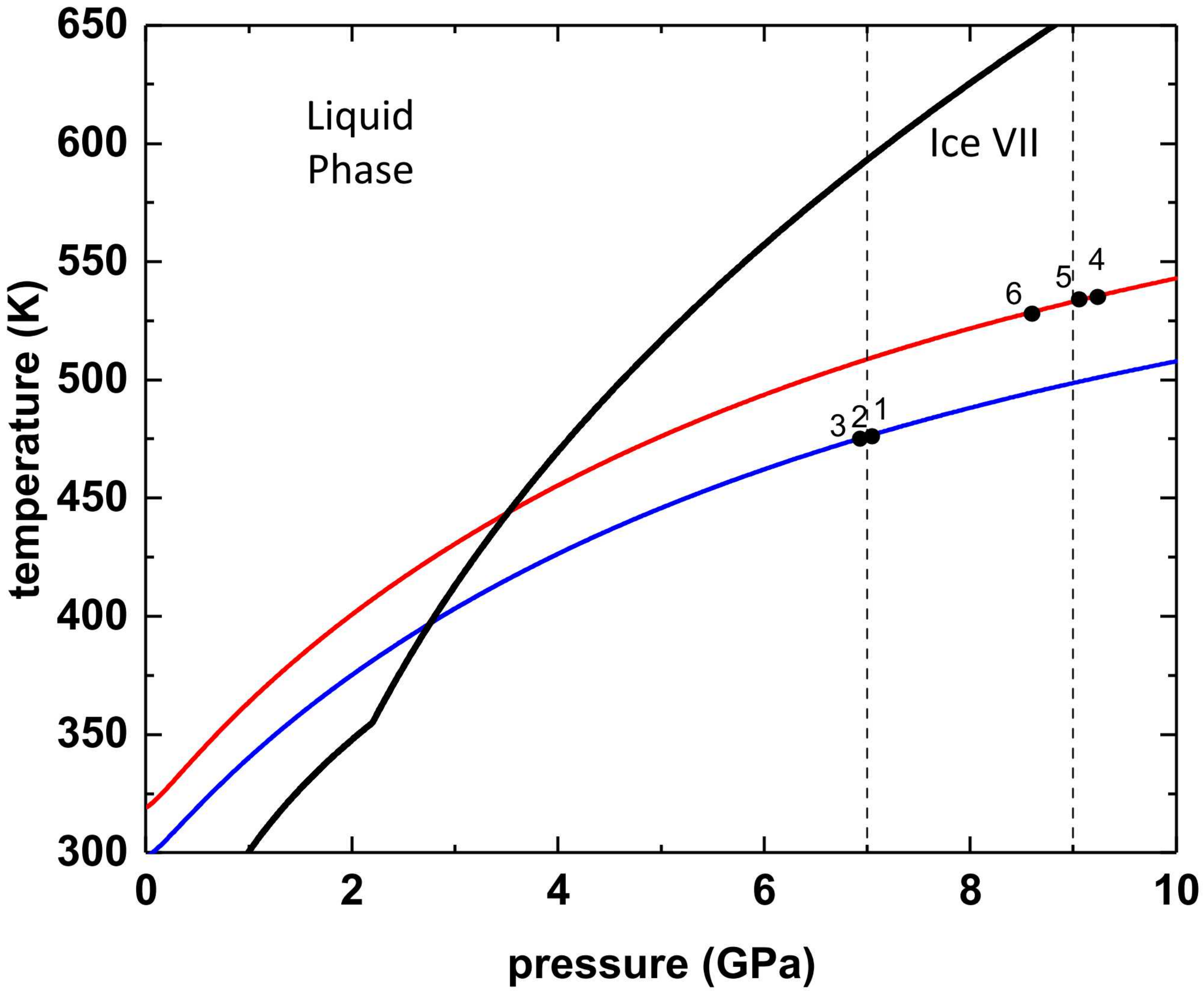


S – Sapphire (control)

W – Water

E. J. Nissen and D. H. Dolan, The Journal of Applied Physics. Accepted.

Peak Phase Transition for Each Shot Shown on its Respective Isentrope



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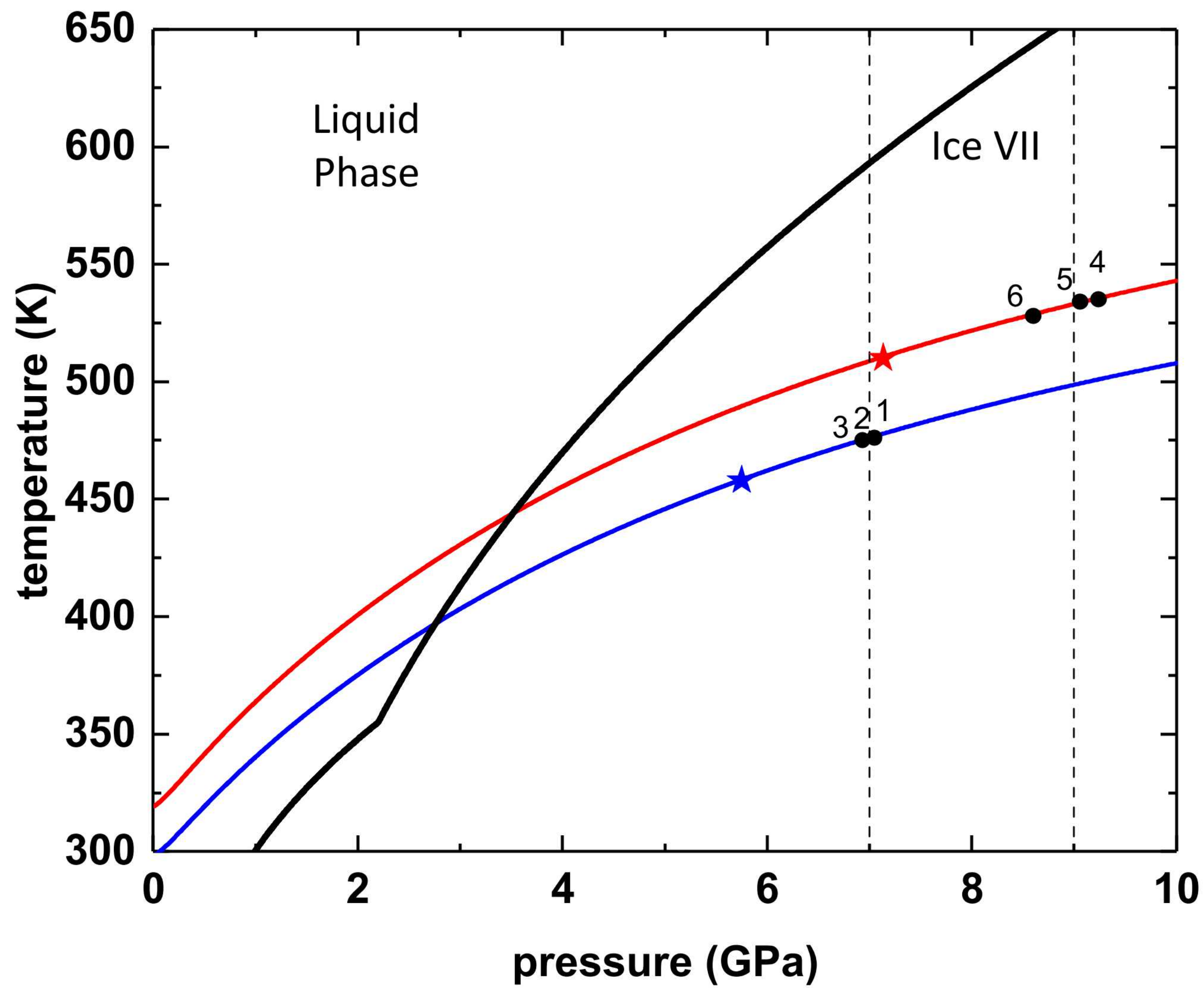

$$\Delta T_U = \Delta T_Q$$

E. J. Nissen and D. H. Dolan, The Journal of Applied Physics. Accepted.

Calculating the Freezing Duration & Nucleation Rate

Deconvolute Thickness of each Sample from the Observed Freezing Duration:

$$t_k = \frac{\tau_k W_F}{W_k}$$

Variables:
t_k – freezing duration
τ_k – observed freezing duration
W_F – thickness of the fastest sample
W_k – thickness of the sample
k – shot number
J – nucleation rate
γ – growth rate

Time-Independent form of the Kolmogorov-Johnson-Mehl- Avrami (KJMA) equation:

$$J_k = t_k^{-4} * \gamma^{-3}$$

If we assume γ is a constant,

$$\frac{J_k}{J_i} = \frac{t_i^4}{t_k^4}$$

Philip C. Myint and Jonathan L. Belof, Journal of Physics: Condensed Matter **30** (23), 233002 (2018).
E. J. Nissen and D. H. Dolan, The Journal of Applied Physics. Accepted.

NEJ1

Initial Sample Temperature & Compression Rate Effect on Dynamic Freezing in Water

Shot	Temperature (°C)	Thickness (μm)	Ramp (GPa/ns)	Transition Pressure (GPa)	Freezing Duration (ns)	Nucleation Rate Ratio ($J_4/J_{\text{shot}\,\#}$)
4	44	72	0.233	9.2	2.2	1
1	25	63	0.163	7.2	2.7	2.3
5	44	69	0.141	9.1	2.7	2.3
2	25	56	0.052	7.1	7.4	130
3	25	53	0.054	6.9	8.2	193
6	44	63	0.050	8.6	7.4	130

Ramp Rate

Freezing Duration

Nucleation Rate

Initial Temperature

Transition Pressure

Slide 10

NEJ1 Transition times decrease more slowly than (rate)-1, but more experiments at different ramp rates are needed to better constrain the trend.

Nissen, Erin J, 6/3/2019

Acknowledgements

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STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

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Randy Hickman
Josh User
Eric Breden
SCCM (Krell Institute)
Mom & Dad

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Sandia National Laboratories

Svjetlana Stekovic Monday, 12:15 PM
Computational studies of laser-driven flyer impact experiments to probe properties of inert and energetic materials.

Erin Nissen Monday, 2:15 PM
Using THOR to manipulate the homogeneous phase transition and nucleation rates in freezing water.

Sergey Matveev Tuesday, 2:15 PM
Shock initiation of reactive nanolaminates

Will Bassett Wednesday, 11:15 AM
Hot Spot Chemistry in Several Polymer-bound Explosives under Nanosecond Shock Conditions

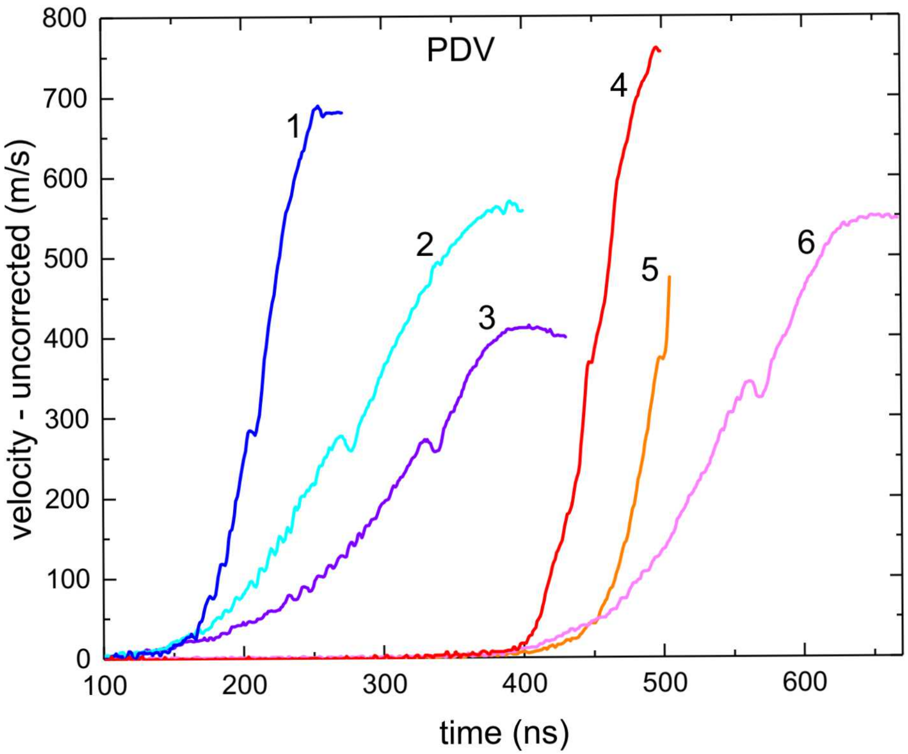
Erin Nissen Wednesday, 11:30 AM
Imaging the Reactive Flow Structure Evolution in Shocked Nitromethane and Nitromethane with Additives.

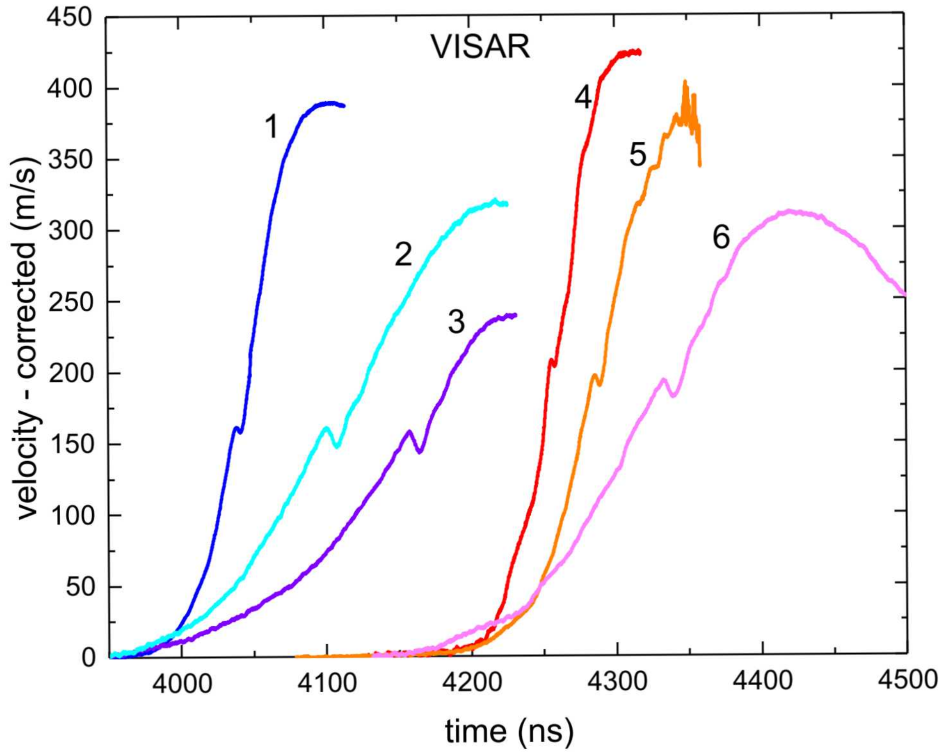
Belinda Johnson Thursday, 9:30 AM
Tracking Temperatures and Growth of Hot Spots in a Simplified Plastic-Bonded Explosive Under Shock Compression.

Wei Zhang Thursday, 3:30 PM
Shock Compression Dynamics of Double-layer Explosive Charges*

Lawrence Salvati Friday, 10:30 AM
Probing Shock-Initiation of Plastic-Bonded Explosives with a Tabletop Microscope

Raw PDV & VISAR Measurements





$$u_{True} = u_{Measured} * 1.783$$

$$P = \rho_o c u_p$$

Undercooling vs. Latent Heating by Solidification

$$\Delta T_U > \Delta T_Q$$

$$\Delta H = 6.36 \text{ kJ/mol}$$

$$\Delta T_Q = \frac{\Delta H}{C_P}$$

$$C_P \approx C_{v,VII} = \frac{c_{max} * 3}{\left(\frac{T_D}{T}\right)^3} \int_0^{T_D/T} \frac{x^4 (e^x) dx}{(e^x - 1)^2}$$

Sarah T. Stewart and Thomas J. Ahrens, Journal of Geophysical Research: Planets **110** (E3) (2005).
P. W. Bridgman, The Journal of Chemical Physics **5** (12), 964 (1937).

Table with Error Bars

Shot #	T_o (C)	Thickness (μm)	Ramp (GPa/ns)	Transition Pressure (GPa)	Observed Duration (ns)	Freezing Duration (ns)	Nucleation Rate Ratio $(J_4/J_{shot\ \#})$
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2	23	56	0.052	7.05 ± 0.18	6.6 ± 0.6	7.4	130
3	23	53	0.054	6.93 ± 0.16	6.9 ± 0.2	8.2	193
6	44	63	0.05	8.60 ± 0.04	6.5 ± 0.5	7.4	130