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Sandia National Laboratories

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Recent research on stishovite: Hugoniot and partial release Z experiments and DFT EOS calculations

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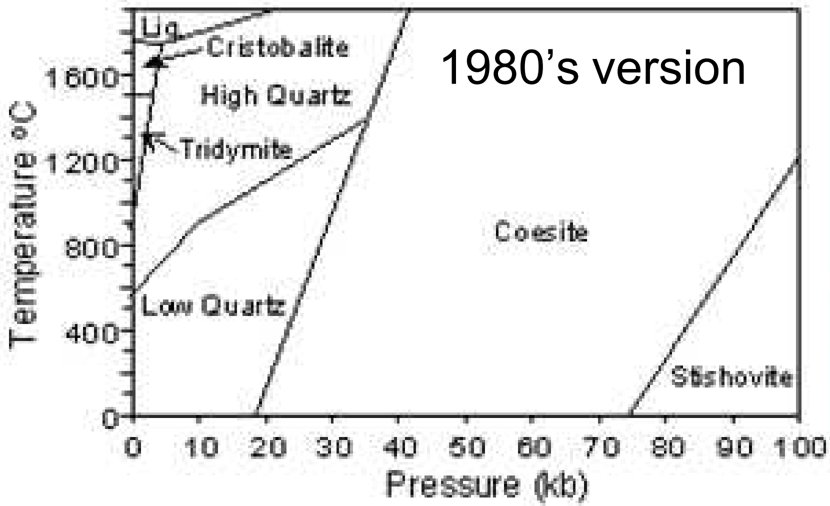
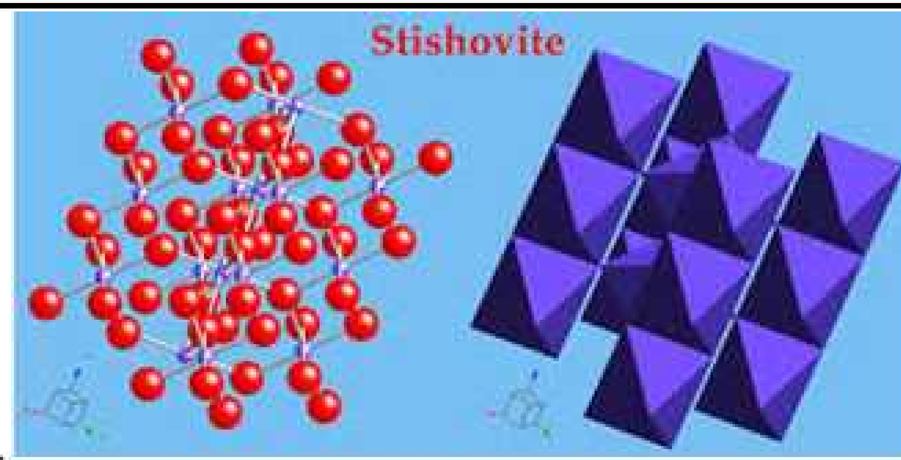
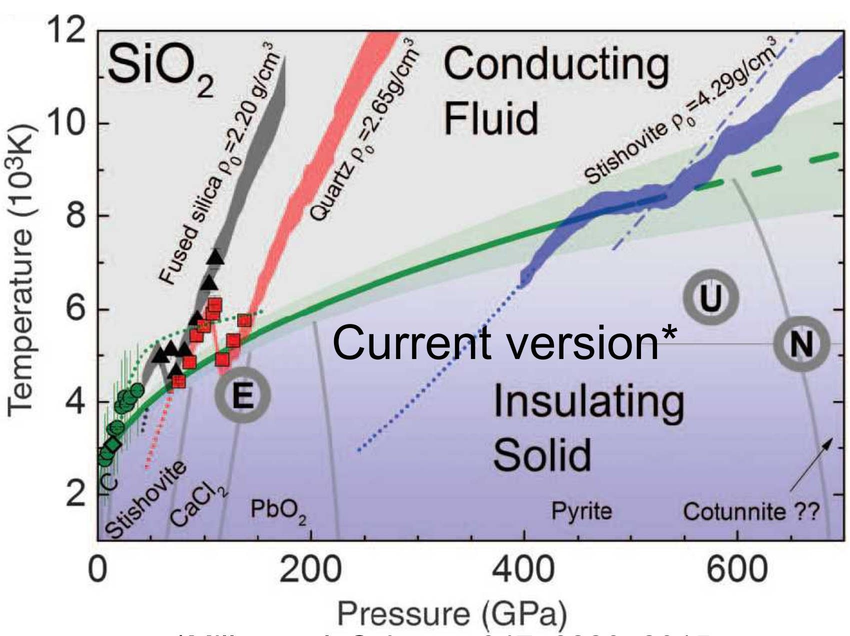
Stishovite is a high-pressure polymorph of SiO_2





Si atoms are 6-coordinated



*Millot et al, Science, 347, 6220, 2015

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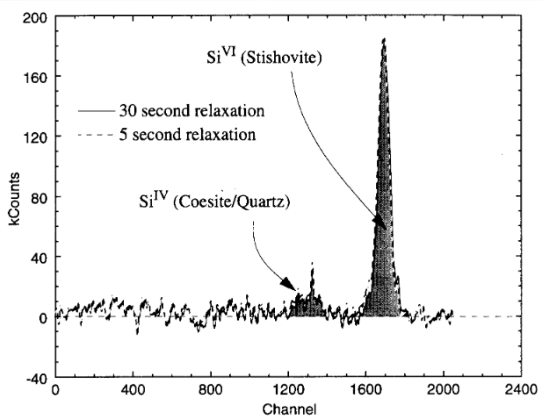
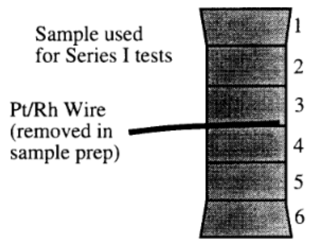
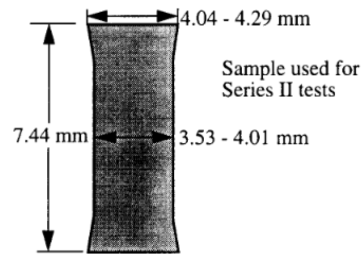
Early experimentation on gas guns was imprecise due to limitations of instruments and methods circa 1990.







SAND95-2342 Experimental measurements of the Hugoniot of Stishovite (M. D. Furnish and E. Ito)

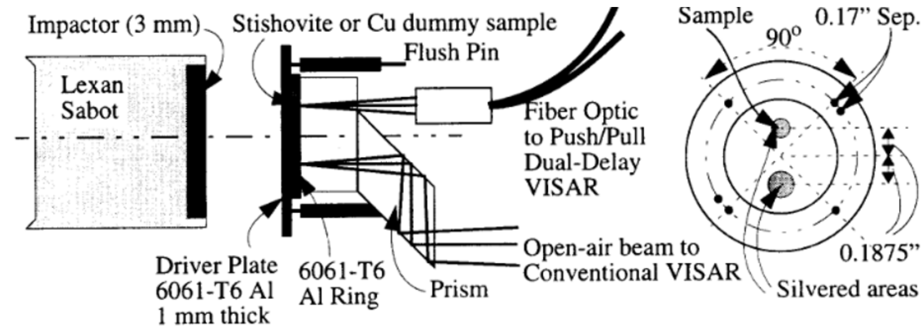
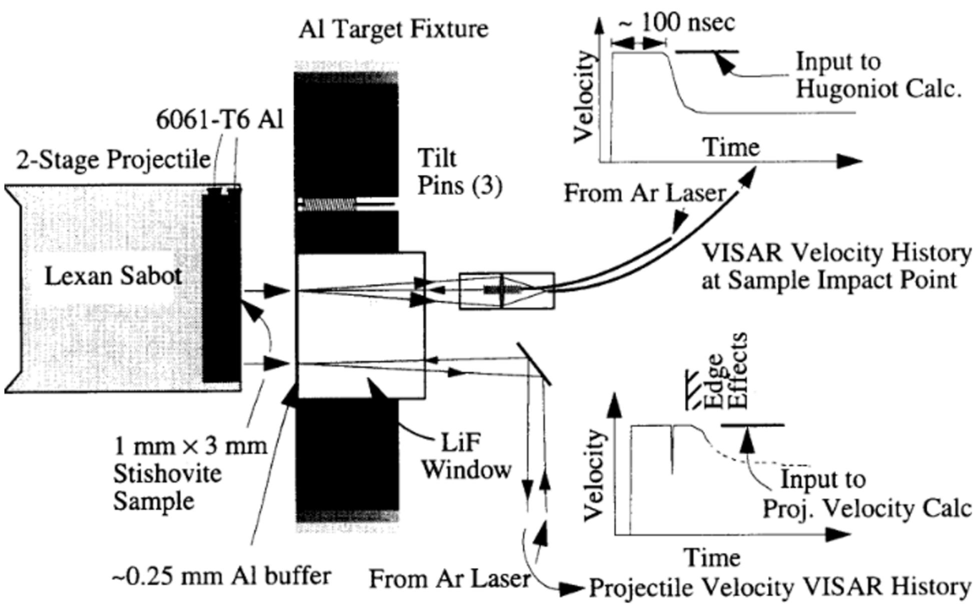


Figure 3.3. Configuration for forward-ballistic (Series II) stishovite tests



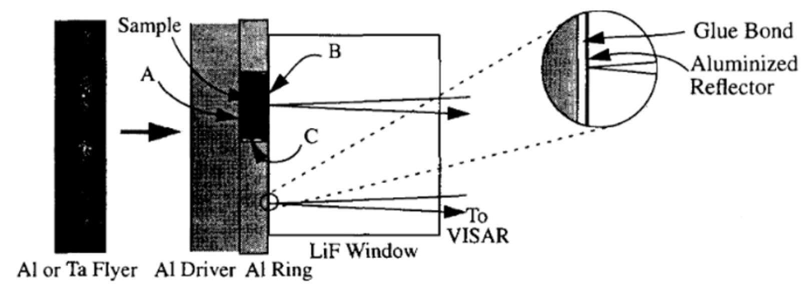
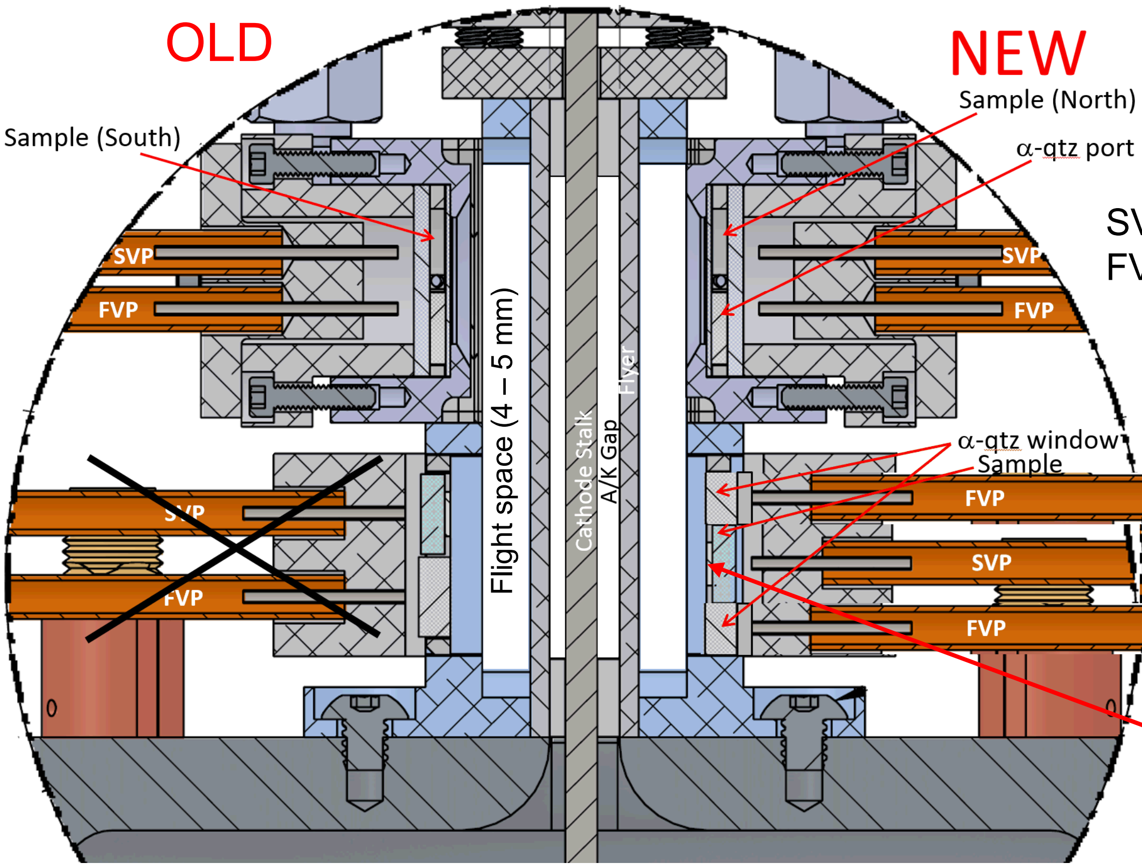


Figure 3.4. Important interfaces for forward ballistic configuration. (A) Sample-driver interface; gap delays shock; (B) Sample-window interface; gap delays shock; (C) Lateral interface; gap slightly accents edge effects.

Reverse-ballistic configuration

Forward-ballistic configuration

With the advent of better data acquisition and loading methods (Z, NiF, etc.), it has become worthwhile renewing these efforts.



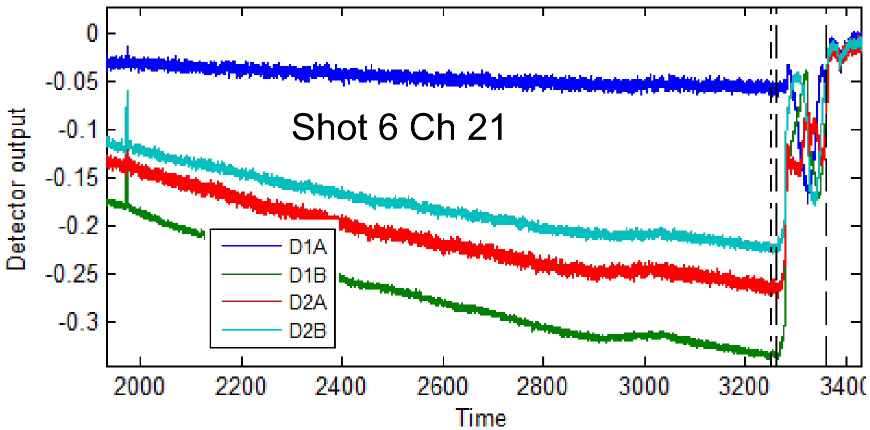
SVP = sample-viewing probe
FVP = flyer-viewing probe

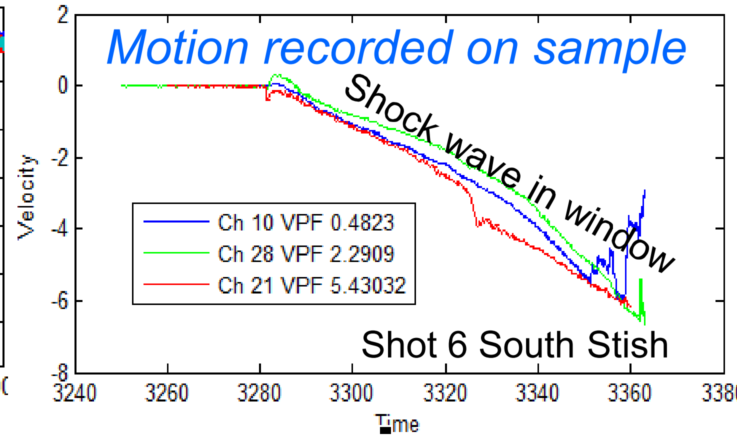
New configuration use flyer-viewing probes on both sides of sample

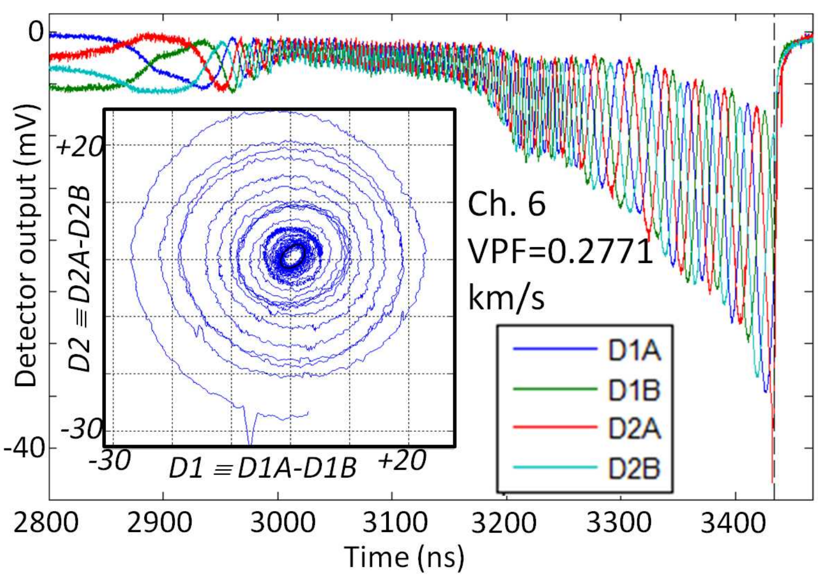
Stishovite samples 0.3 – 0.7 mm thick, 2 -2.5 mm dia.

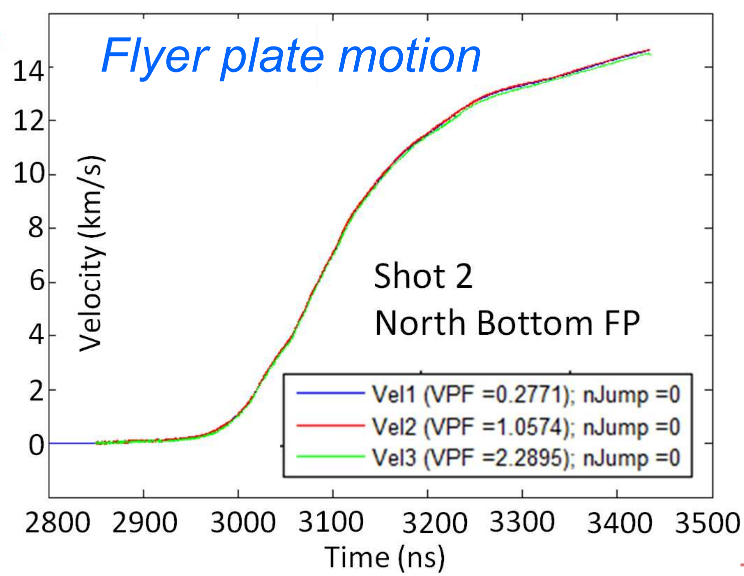
The upper sample was attenuating, required a supported shock. Thus, the option of using a layered impactor to measure sound speeds at the Hugoniot was not available

The VISAR equipment used includes a wide range of sensitivities, 38 spots, and timing giving ~300 ps transit time uncertainty (1σ)









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A set of 5 experiments was conducted, each with two stishovite samples impacted by an aluminum flyer at 12.25 – 25.39 km/s

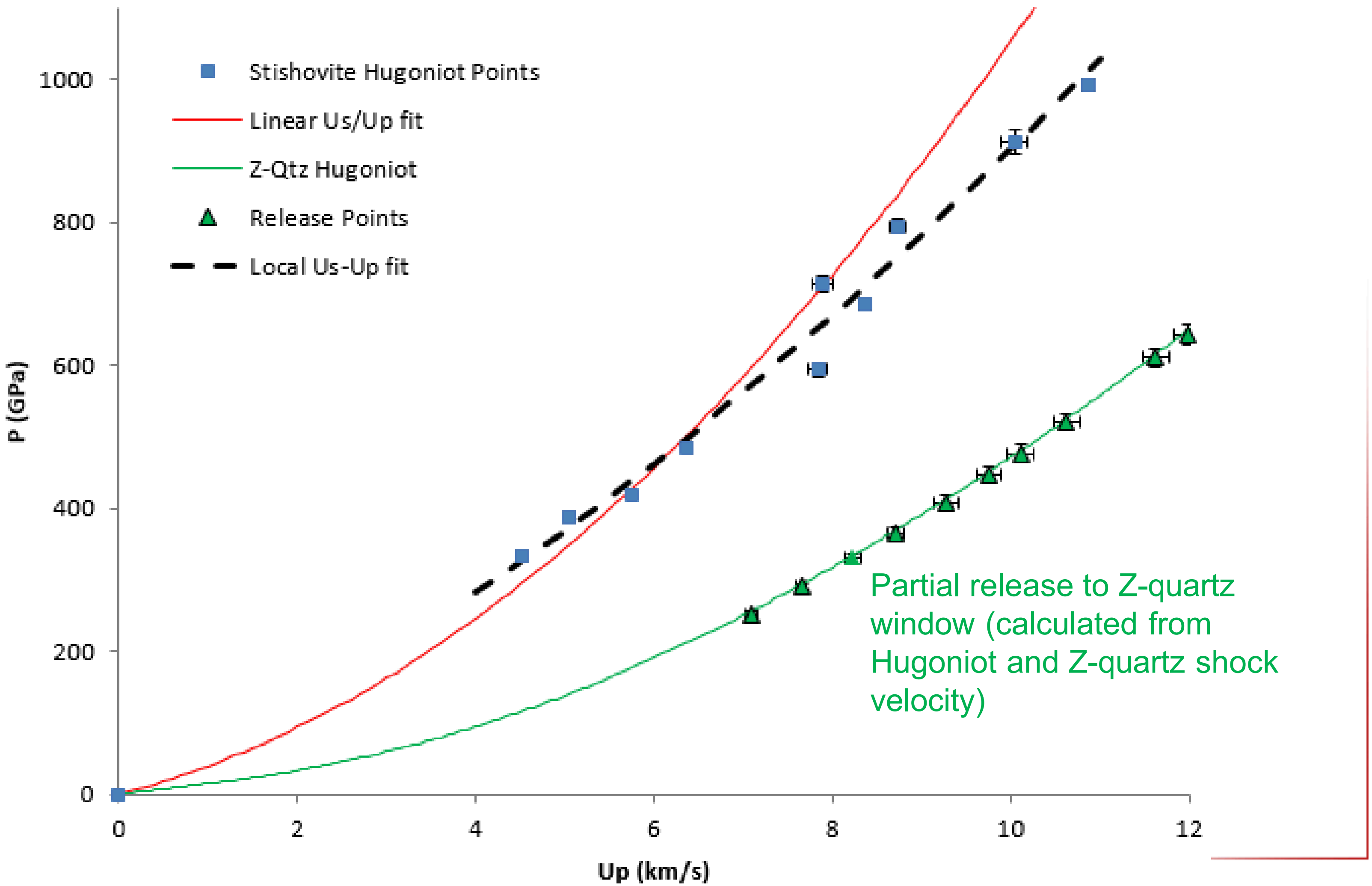
Test	Thickness	Rho0	Ufp	Impact	TOA	U(Rel)	dRho0	dUfp	dImpact	dTOA	dU(Rel)
31	0.363	4.31	12.25	2.8086	2.82988	20.8	0.02	0.05	0.0005	0.0004	0.15
32	0.418	4.34	13.5	2.80926	2.83299	22.1	0.02	0.05	0.0005	0.0003	0.15
21	0.62	4.26	14.62	3.36789	3.4041	23.4	0.02	0.05	0.0005	0.0003	0.2
22	0.656	4.28	16	3.38114	3.41819	24.5	0.02	0.05	0.0005	0.0003	0.2
41	0.6792	4.3	20.15	2.67994	2.7156	27.5	0.02	0.05	0.0005	0.00035	0.3
42	0.6159	4.27	21.55	2.68188	2.71078	28.6	0.02	0.05	0.0005	0.00035	0.3
51	0.3693	4.29	18.7	3.17893	3.19981	25.7	0.02	0.05	0.0005	0.00035	0.3
52	0.452	4.29	19.965	3.1633	3.184674	26.75	0.02	0.05	0.0005	0.00035	0.3
61	0.3187	4.29	23.91	3.07457	3.08962	30.64	0.02	0.05	0.0004	0.0003	0.3
62	0.7954	4.29	25.39	3.0737	3.111078	31.35	0.02	0.05	0.00035	0.00022	0.3

Impact time was determined from 4 records for each of 6 – 10 VISAR spots, correlated via a common timemark and fiber measurements calibrated on each shot

Breakout time was determined from 4 records for each of 3 VISAR spots, correlated via a common timemark and fiber measurements calibrated on each shot

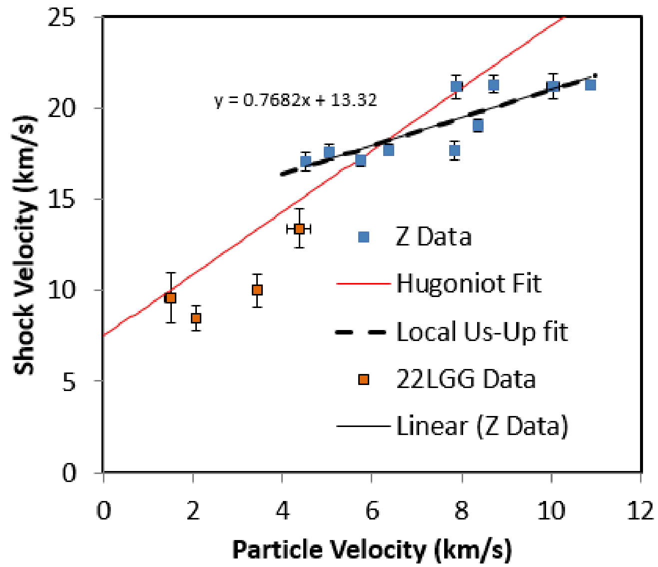
Samples were synthesized in a large-volume multi-anvil press at 15 GPa and 1773 K, with an initial density of 4.29 gm/cc.

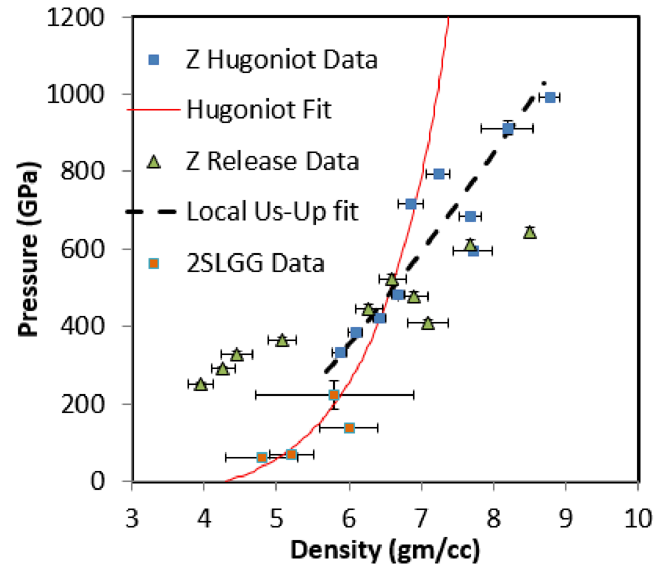
The Hugoniot family thus gathered spans the range 0.33 – 1.0 TPa

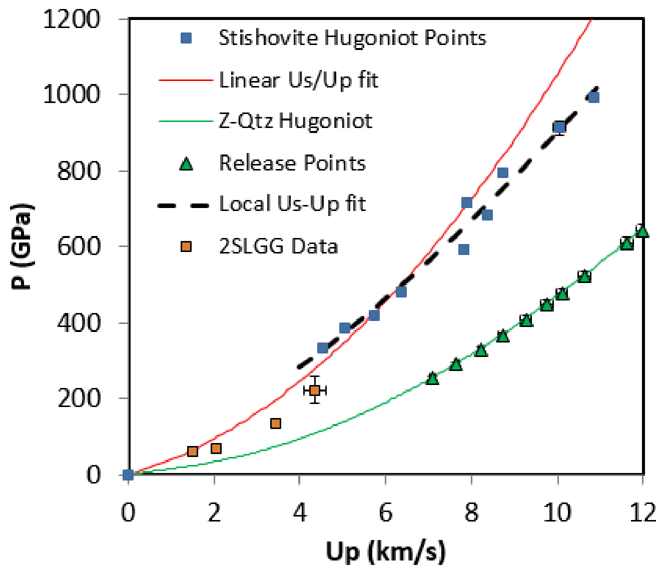


Uncertainties were calculated by 5000-element Monte Carlo methods

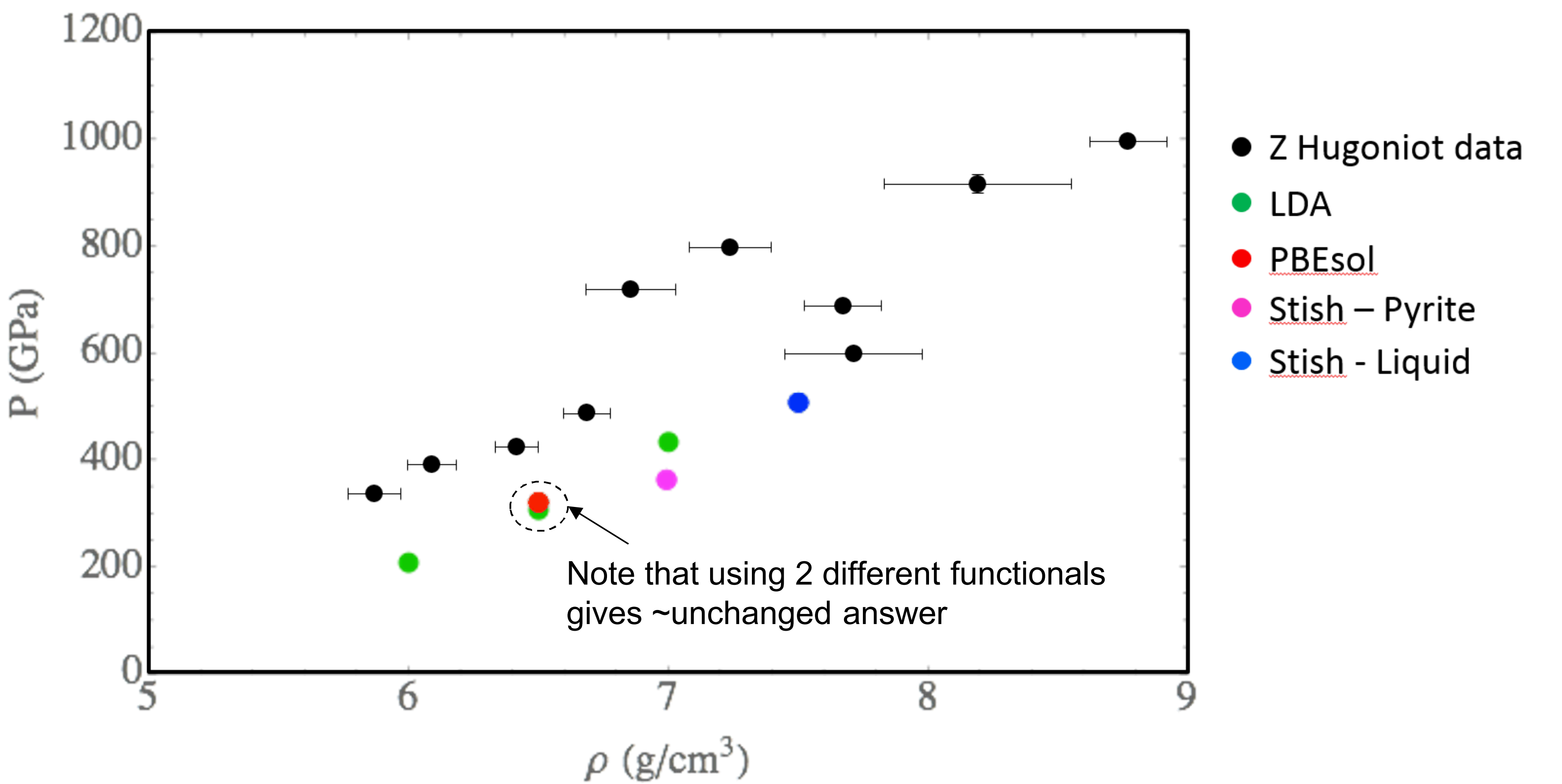
The data may be plotted to include the older STAR data as well







The experimental Hugoniot points show a much stiffer Hugoniot than predicted by Density Functional Theory for the SiO_2 system in the 2 – 6 MBar area



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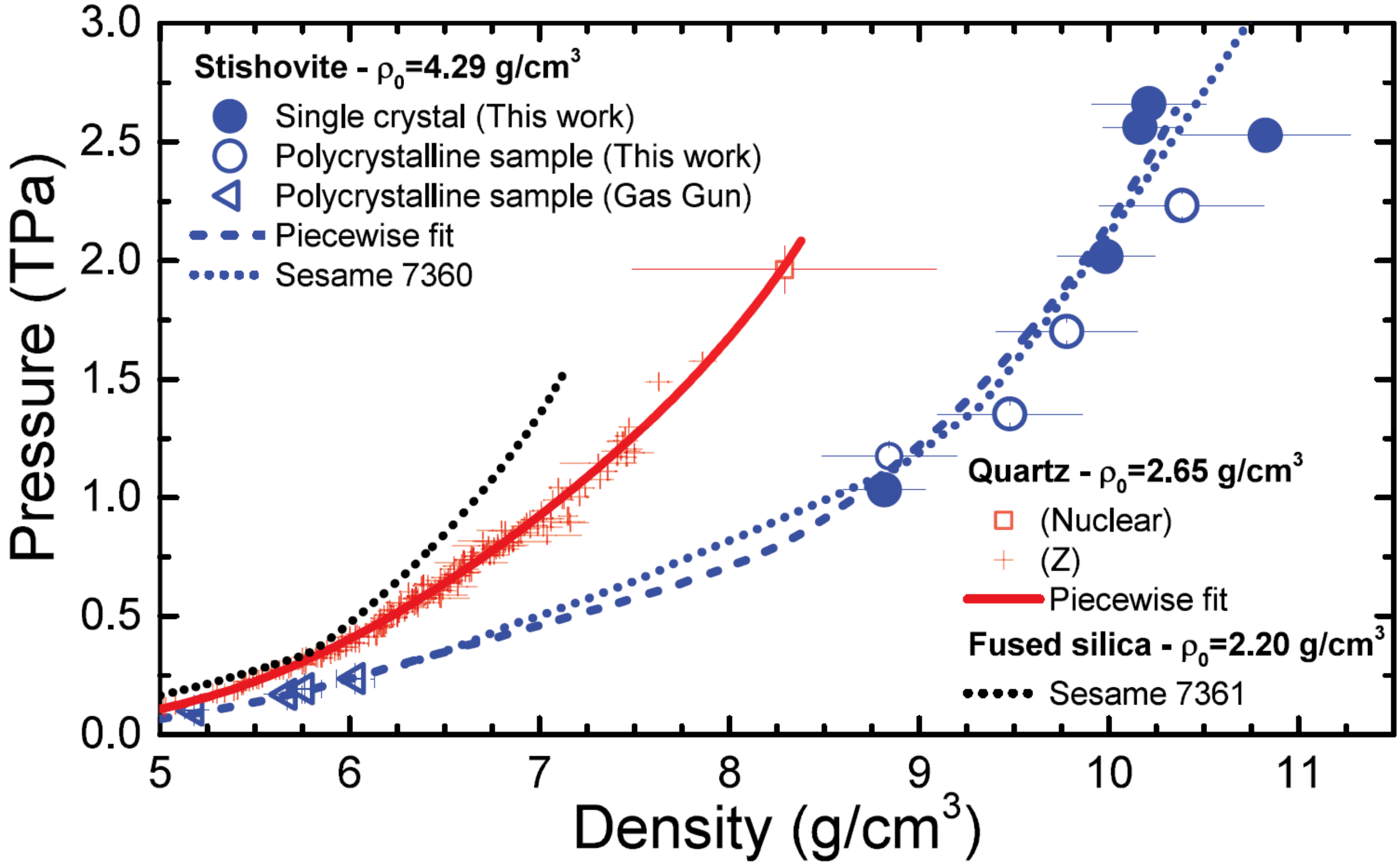
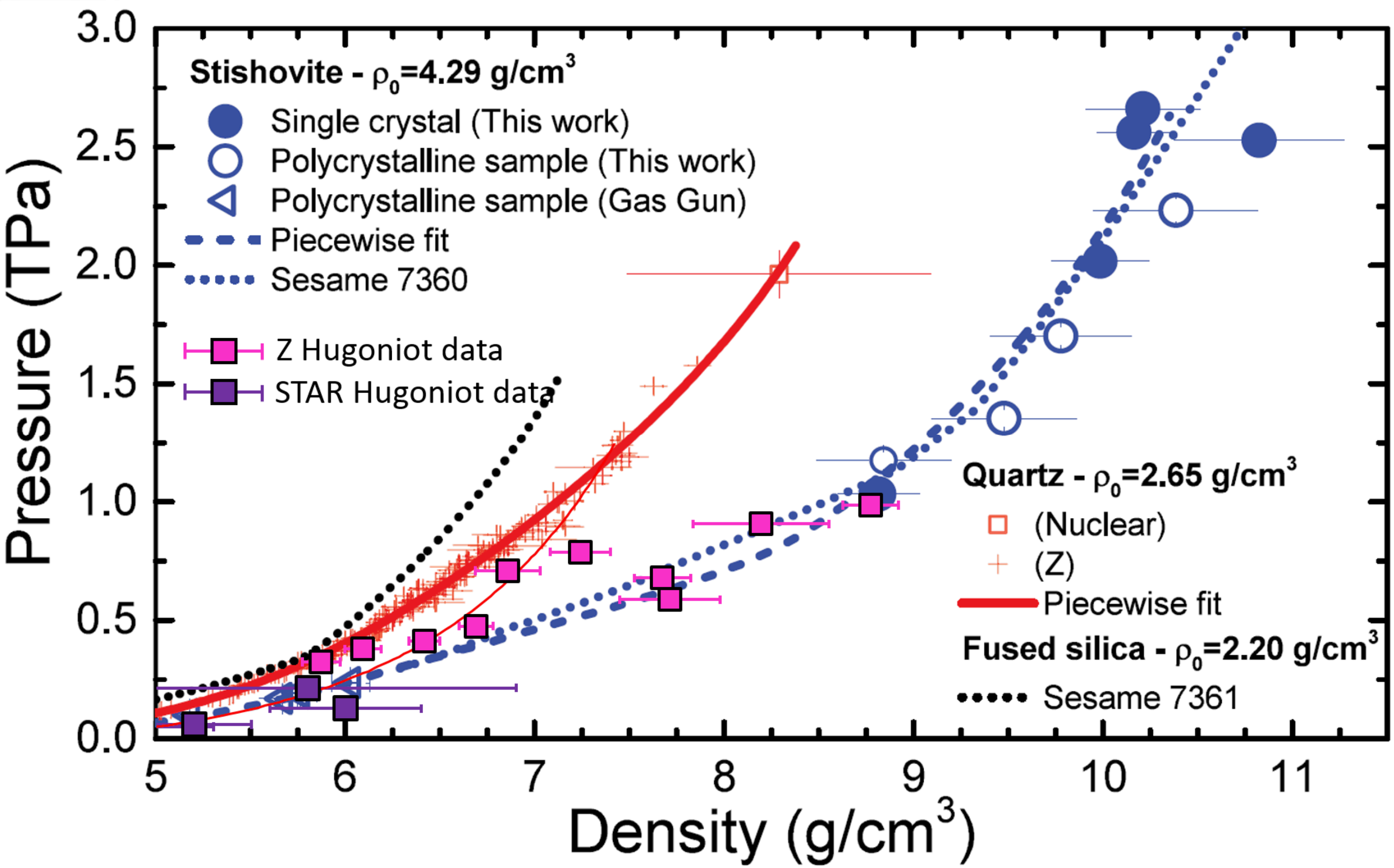
Recent OMEGA data picks up at ~1 TPa



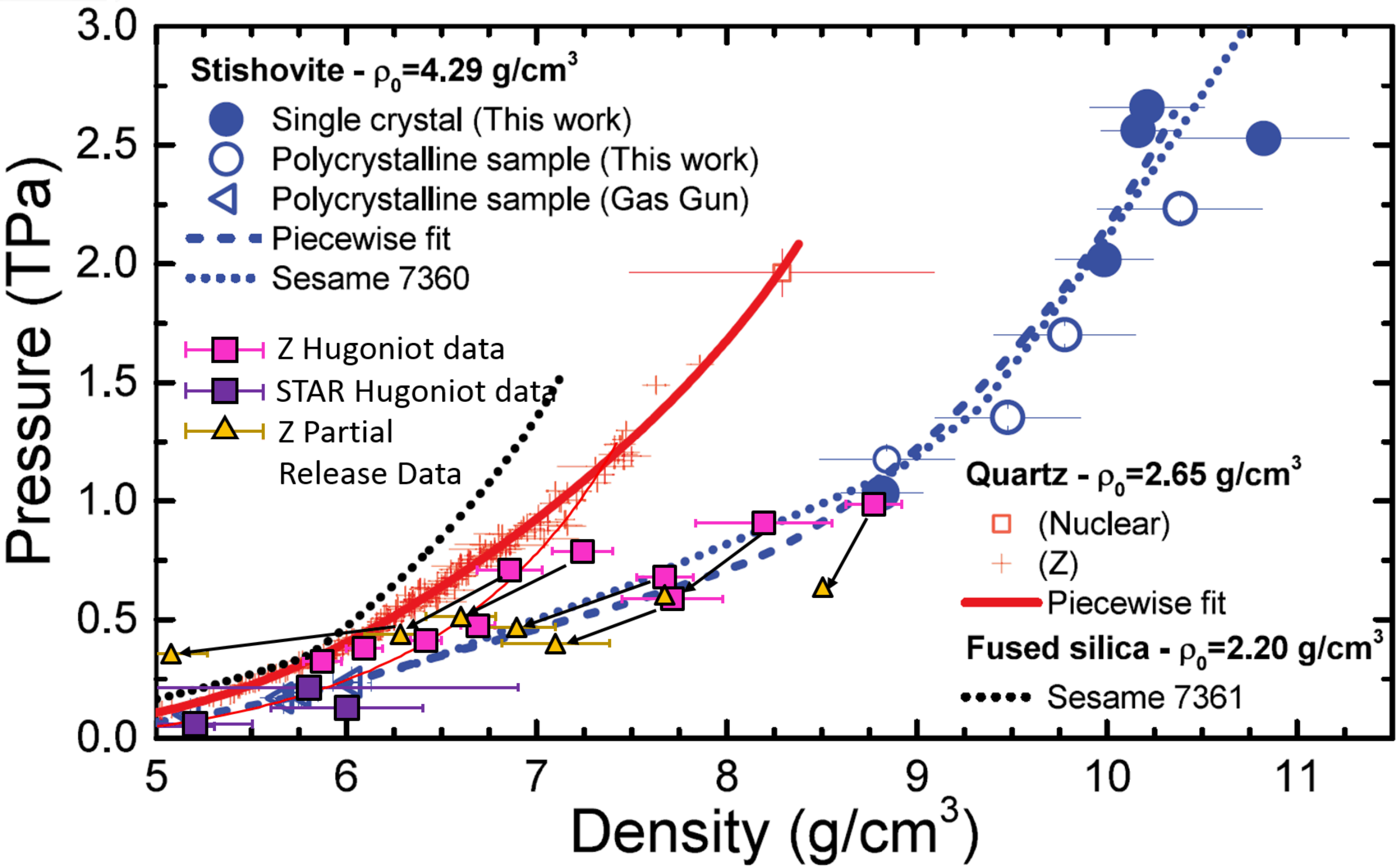
*Millot et al, Science, 347, 6220, 2015

The present dataset fills in the gap between this and gas gun data. But there are some surprises.



*Base figure from Millot et al, Science, 347, 6220, 2015

Adding the partial release data may aid in resolving the DFT questions as well.



*Base figure from Millot et al, Science, 347, 6220, 2015

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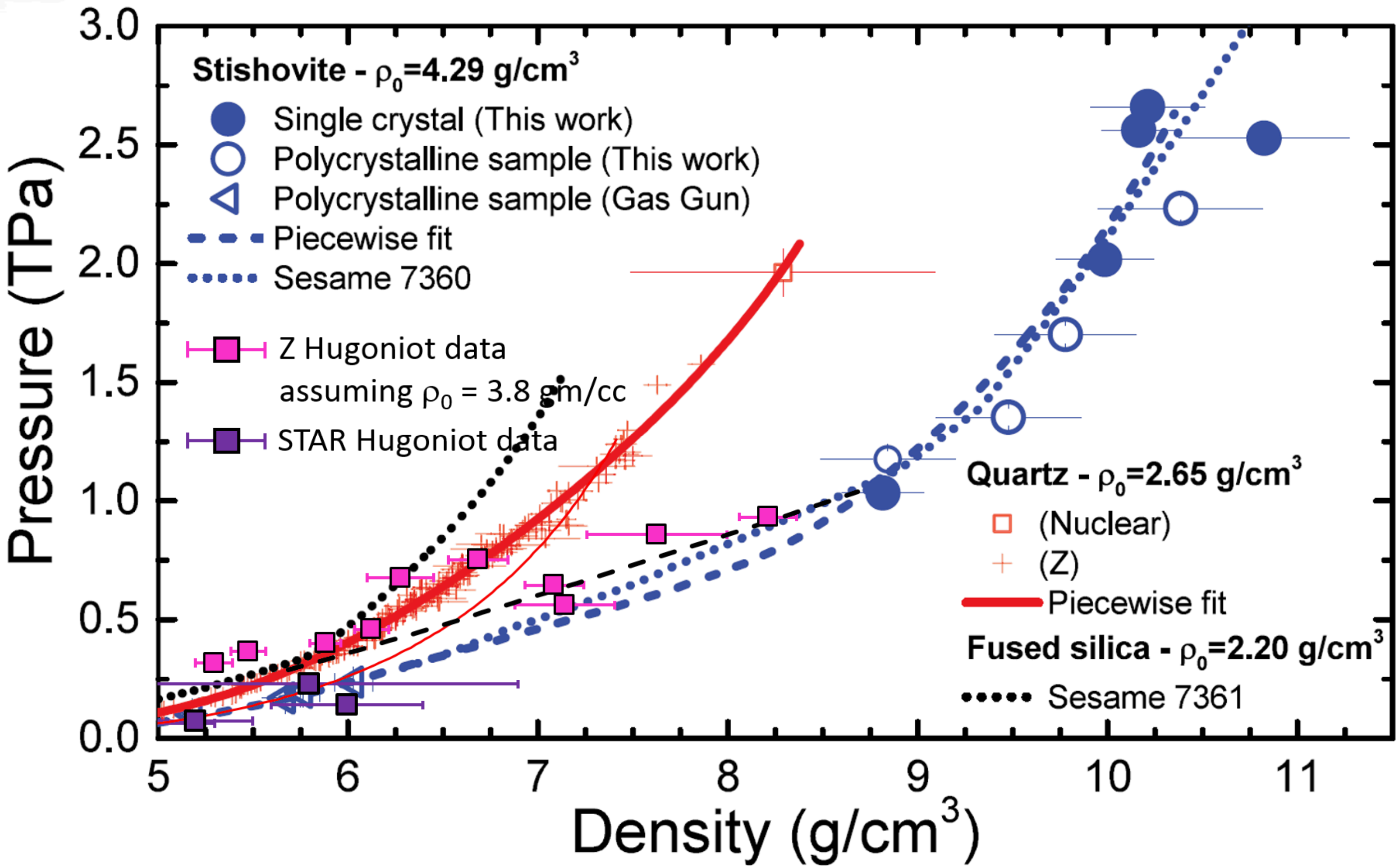
Conclusions

- Hugoniot and partial release measurements have been obtained for stishovite over the pressure range 0.33 – 1.0 TPa.
- The present data suite fills in a large gap of stishovite EOS data between gun gun measurements and NIF measurements.
- Sound speeds were not available from these measurements.
- The lower half of this suite is more stiff than gas gun data and current DFT calculations. The reason for this is unclear at present.
    - The DFT calculations appear to be solid
    - The experimental data are also carefully vetted, including sample characterization, diagnostics, and analysis.

Assuming the samples actually had a smaller initial density does NOT resolve the discrepancy.



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