X International Voevodsky Conference "Physics and Chemistry of Elementary Chemical Processes" (VVV-2022)

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Study of Shock Compressibility and Shock-Induced Temperature of Oxides by Mach Cumulative Explosive Generators

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Magnesium oxide (Periclase), Titanium oxide (Rutile) and Aluminium oxide (Sapphire) – a part of a set of oxides, composing a Earth and planetary core and mantle, Lunar regolith, asteroids, comets, etc. (MgO, SiO_2, Al_2O_3, CaO, FeO, TiO_2)

The modeling of space impact phenomena requires an equations of state of complex rocks, mix of oxides or oxides + silicates

Shock wave properties of oxides is required to develop such a equation of state (EOS)

Also, EOS of oxides is required to calculate an interior of Earth, rocky planets and rocky cores of giant gas planets, including newly discovered extra-solar system planets

A scope of this work to obtain new experimental data on shock compressibility and shock temperature of oxides in wide range of pressure

Study of the properties of matter at high pressures

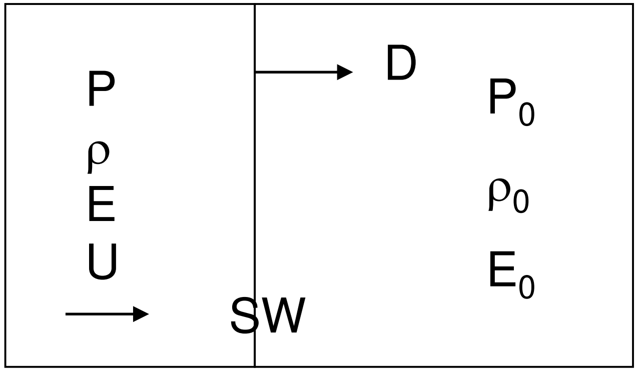
Static: Bridgman press or diamond anvil cell
Dynamic isentropic: electromagnet technique, Z-machine
Dynamic adiabatic with irreversible rise of entropy – **shock compression**

Rankine-Hugoniot relations at shock wave front directly derived from **conservation laws** (mass, momentum, energy):

$$\rho/\rho_0 = V_0/V = D/(D-U)$$

$$P = \rho_0 D U$$

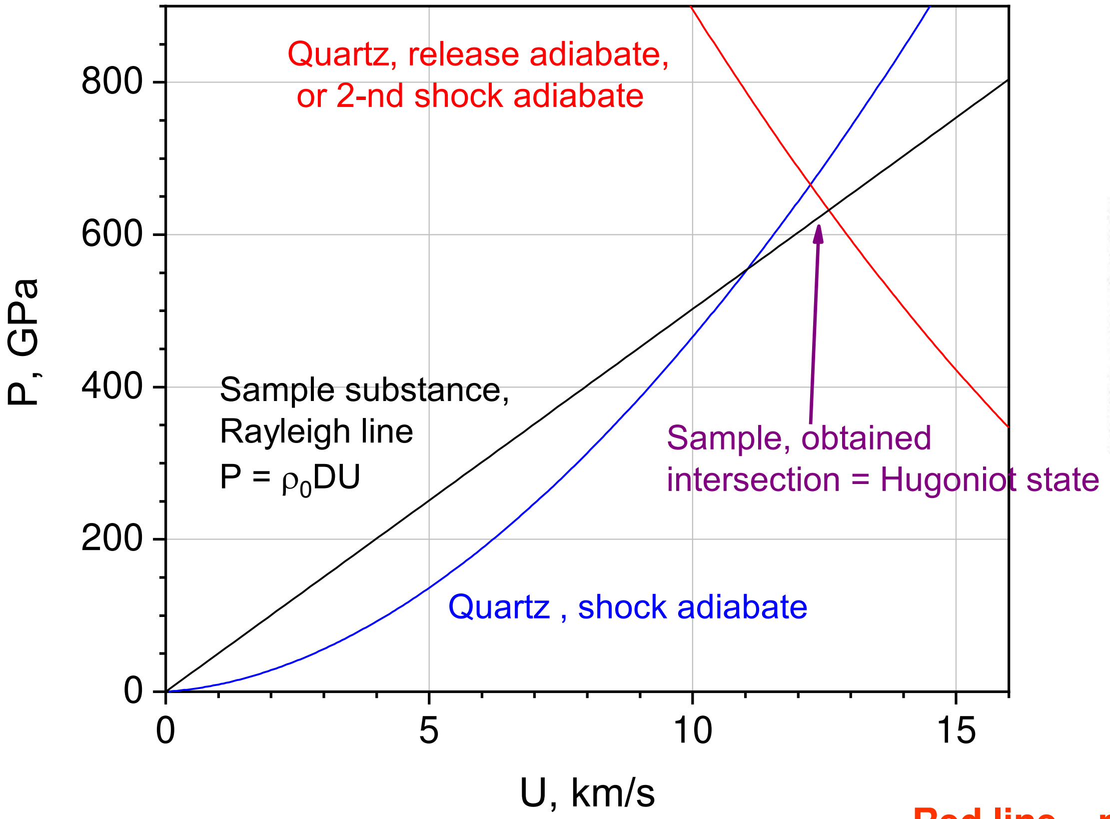
$$E = E_0 + P(V_0 - V)/2$$

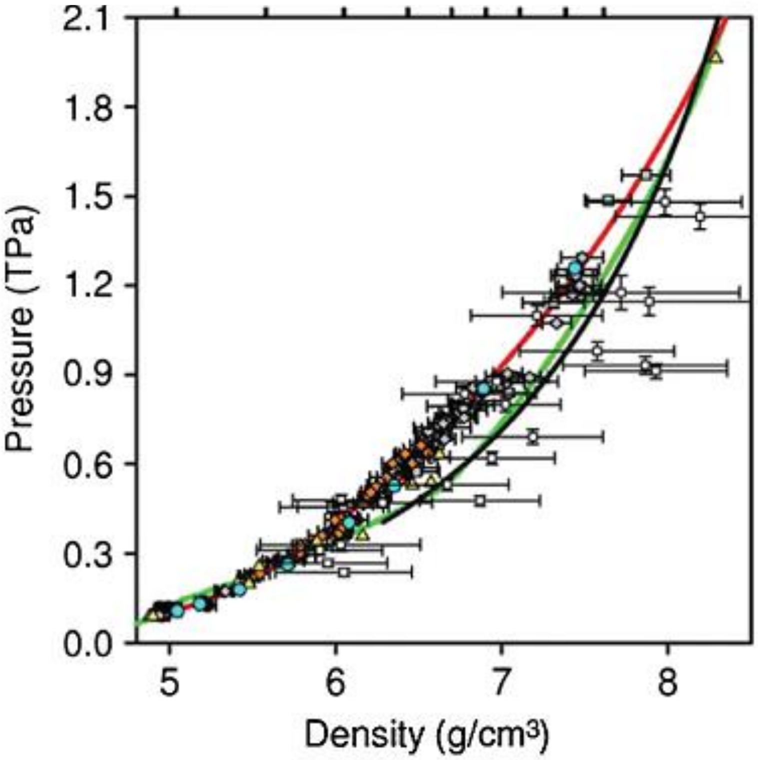


If one measure any two parameters, other can be calculated from conservation laws,
Not making any assumptions about EOS
For example – D and P is measured, U and ρ - calculated
Or D and U is measured, P and ρ - calculated

Temperature is not included in Hugoniot relations and depends on EOS
It must be measured separately

Determination of Shock adiabat: Impedance matching (Метод отражения)



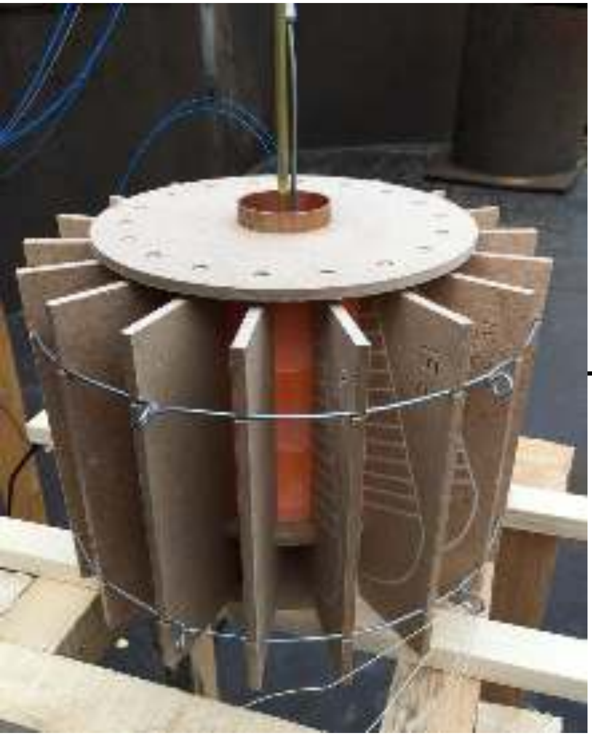


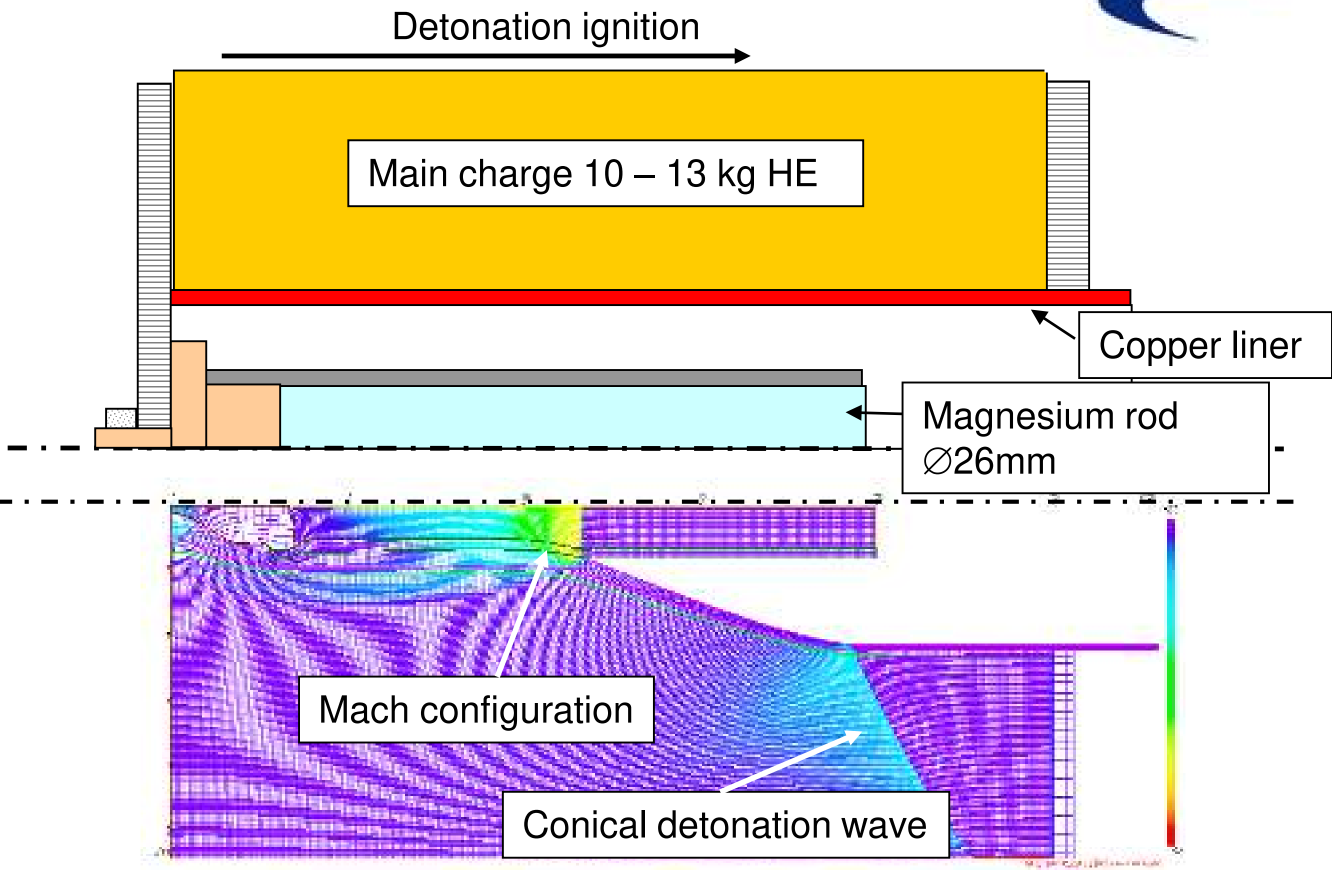
Red line – new Quartz shock adiabate [2,3]. 206 points

Shock state, double shock and release of Quartz is calculated according to new EOS [1], including data [2,3]

1. *I.V. Lomonosov, A.V. Bushman, V.E. Fortov, K.V. Khishenko.* Caloric equations of state of structural materials. In: High Pressure Science and Technology – 1993. Eds. *S.C.Schmidt, et al.* AIP Press, N.Y., 1994, Part 1. p.117 – 120.
2. *D. Knudson and M. P. Desjarlais.* Shock Compression of Quartz to 1.6 TPa: Redefining a Pressure Standard. Phys. Rev. Lett. 103, 225501 (2009);
3. *M. D. Knudson, M. P. Desjarlais.* Adiabatic release measurements in α-quartz between 300 and 1200 GPa: Characterization of α-quartz as a shock standard in the multimegabar regime. Phys Rev B 88, 184107 (2013).

Mach-type shock wave generator



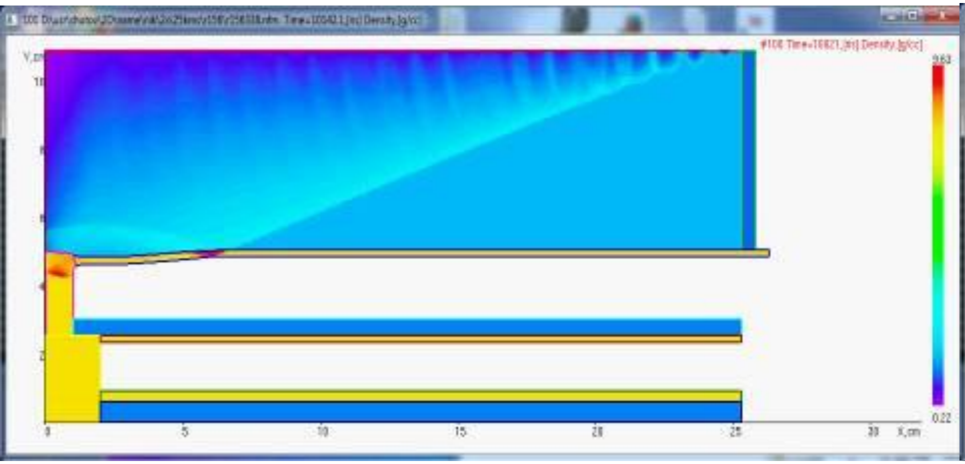


1-stage generator (2012-2014). Mass of explosive: 3.9 kg и 12.5 кг. Up to 500 GPa
2- stage generator (2015). Mass of explosive: 12.5 kg. Up to 2000 ГПа

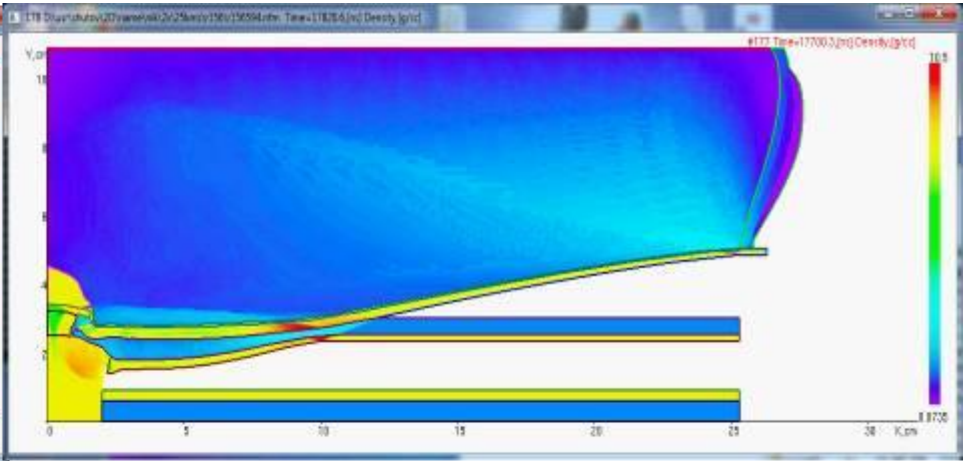
Nikolaev D., Ternovoi V., Kim V., Shutov A. Plane shock compression generators, utilizing convergence of conical shock waves // Journal of Physics: Conference Series. 2014. V. 500. № 14. P. 1-5.

Axisymmetric 2D - simulation of **2 - stage device**

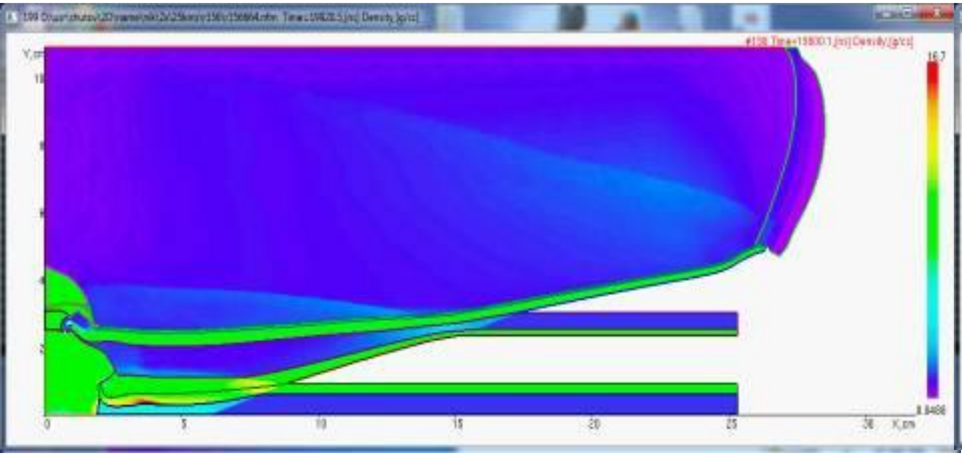
Velocity of detonation initiation point up to 25 km/s. 2th stage liner velocity is increased from 4.2 to 6 km/s. Color = density



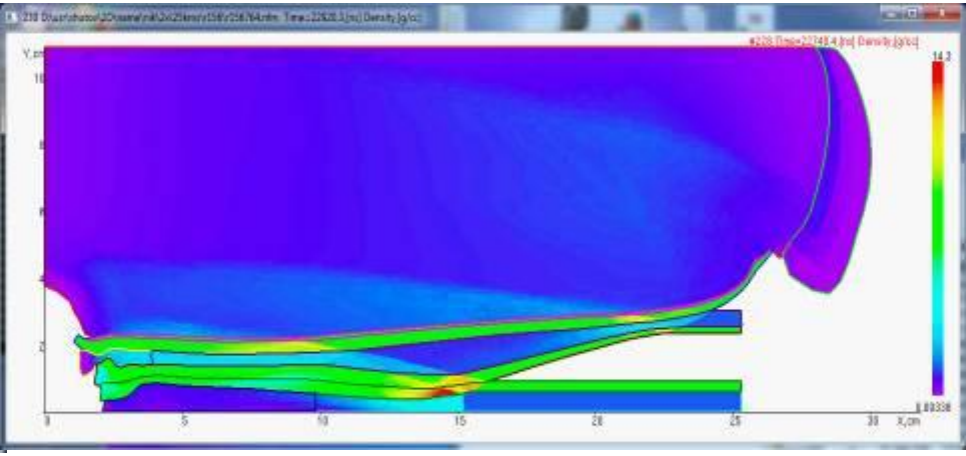
10020 ns. Launching of 1-st stage liner. Cone formation



17700 ns. Launching of 2^{nd} stage liner. Cone formation

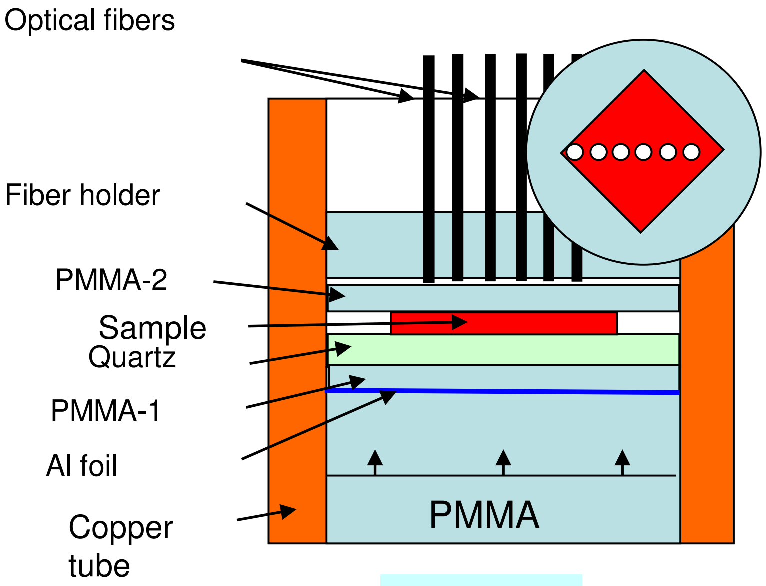


19800 ns. Conical shock wave convergence in central body

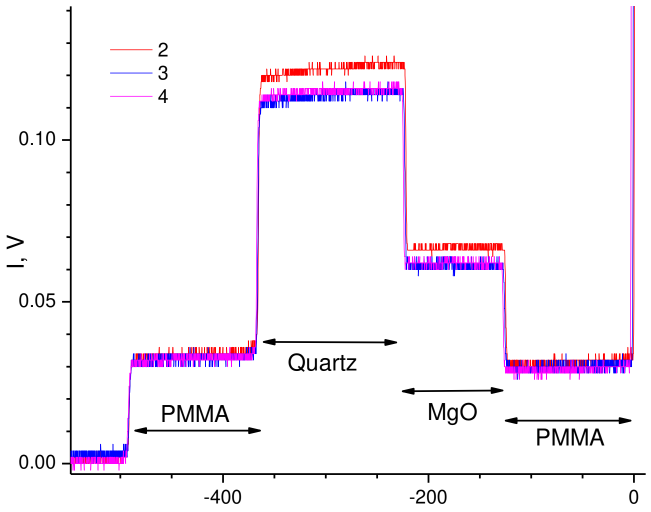


22740 ns. Mach disk formation in central body

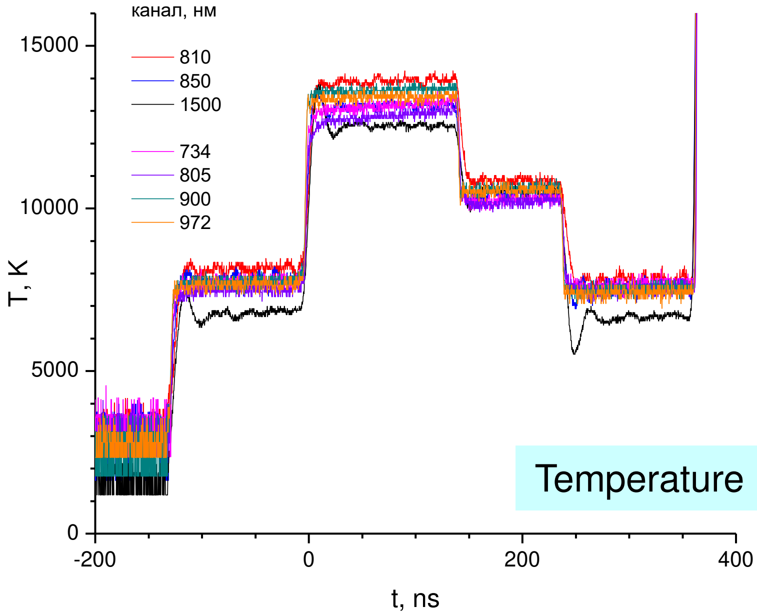
Shock adiabate of transparent samples (MgO and Al2O3) + temperature of shock compression.



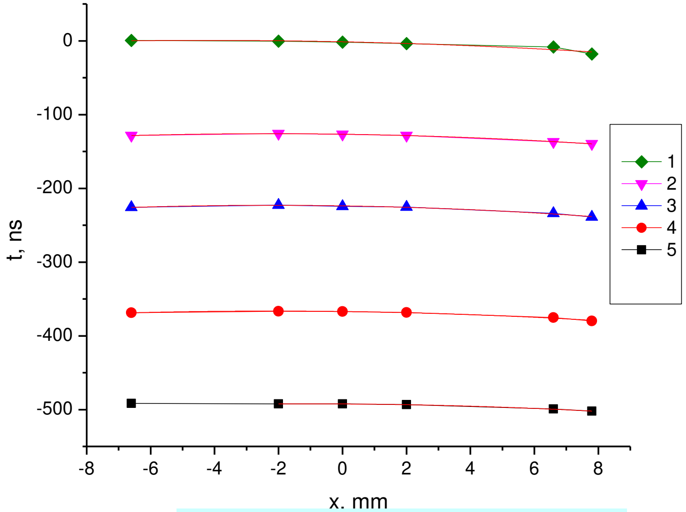
Assembly



Fast detectors record



Temperature

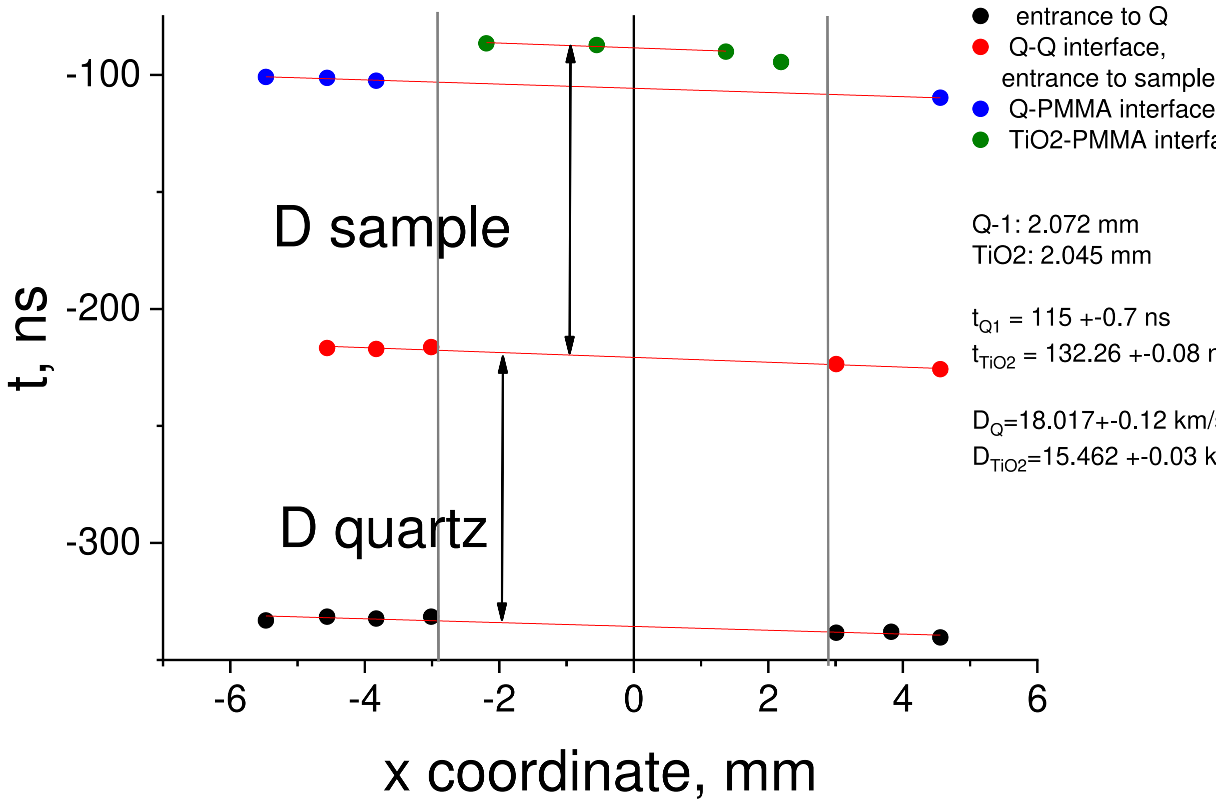


Processinf of experimets

Shock compression of opaque substance (porous TiO_2)

12 fast optical gauges

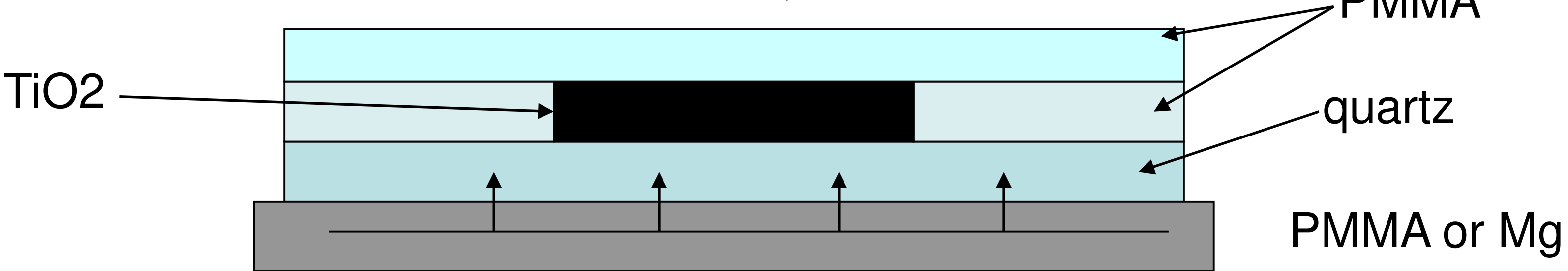
Wave velocities, precision from 0.1% to 0.6%. Density – 3%. Slightly tilted shock wave



Q-1: 2.072 mm
TiO2: 2.045 mm

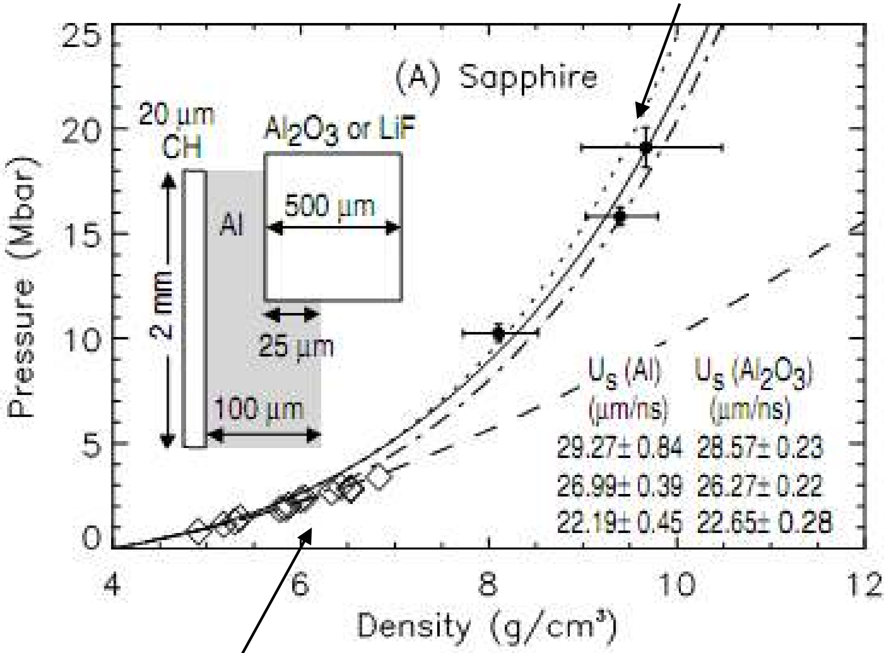
t_{Q1} = 115 +-0.7 ns
t_{TiO2} = 132.26 +-0.08 r

D_Q=18.017+-0.12 km/:
D_{TiO2}=15.462 +-0.03 k



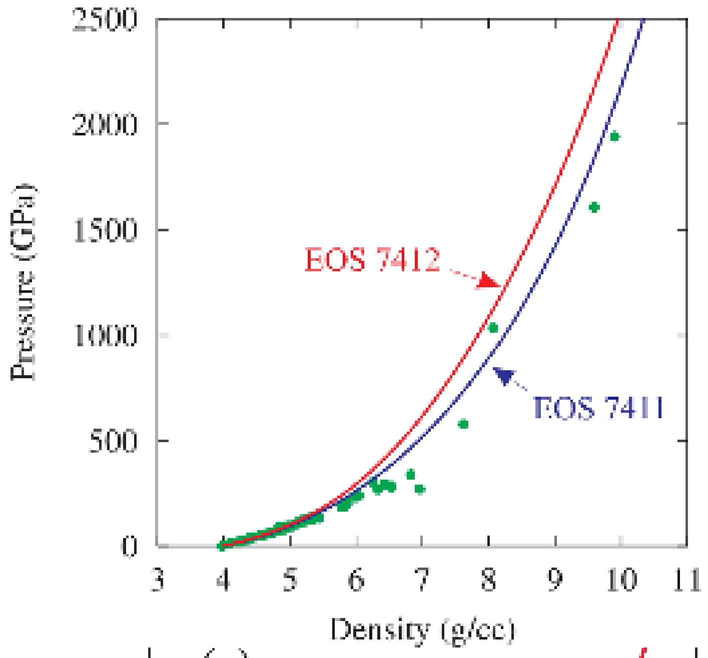
Shock adiabate of Sapphire

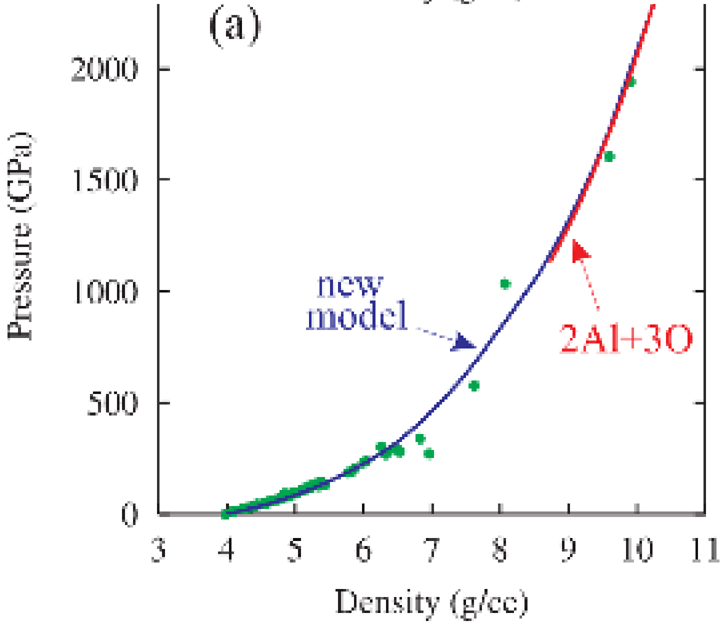
Hicks's new laser data



Erskine's old gas gun data

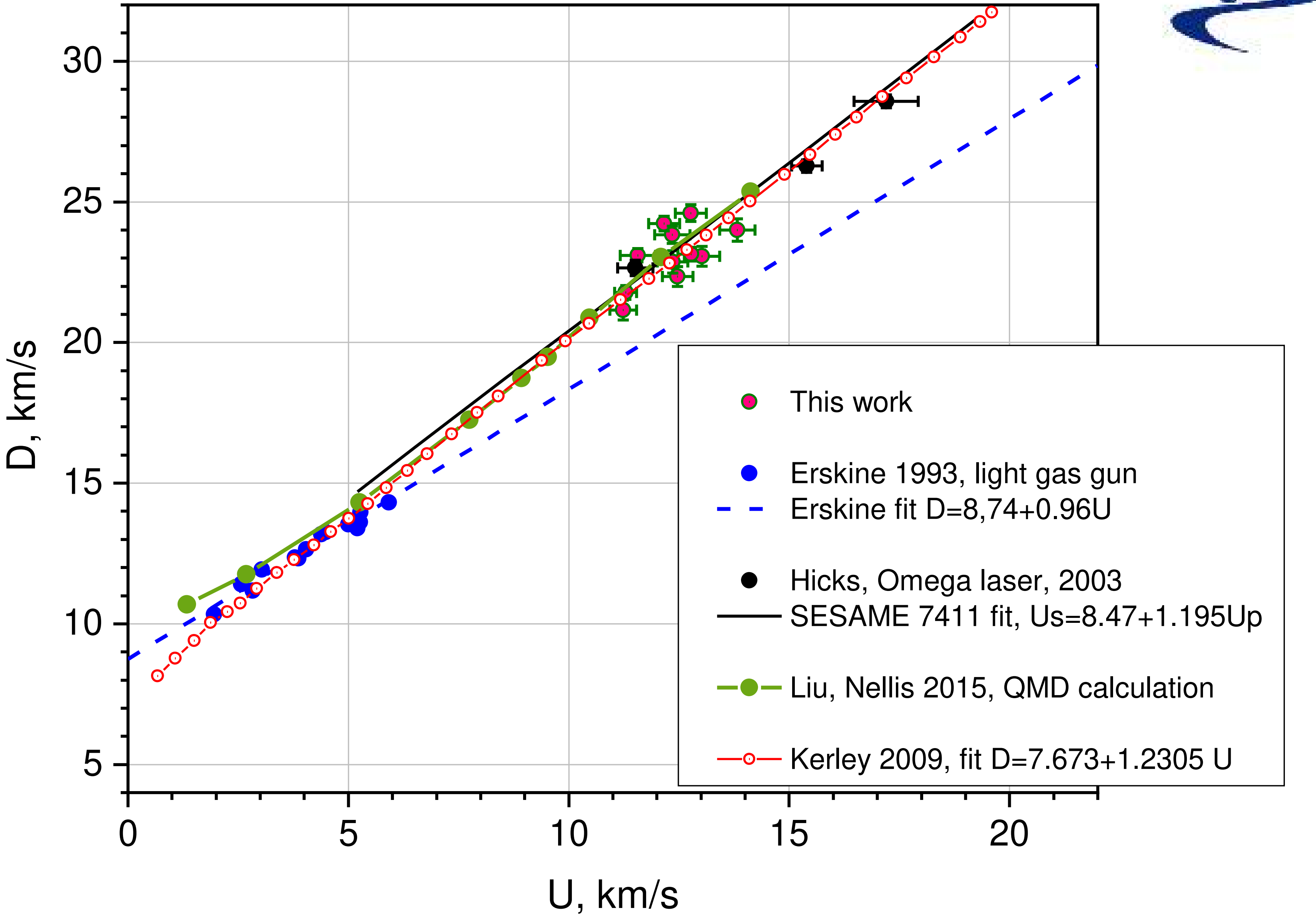
D.G. Hicks, P.M. Celliers, G.W. Collins, J. H. Eggert, and S. J. Moon
Shock-Induced Transformation of Al2O3 and LiF into Semiconducting Liquids. PRL VOL 91, 035502 2003





Gerald I. Kerley. Equation of State and Constitutive Models for Numerical Simulations of Dust Impacts on the Solar Probe Report on Contract #949182, 2009

Shock adiabate of Sapphire

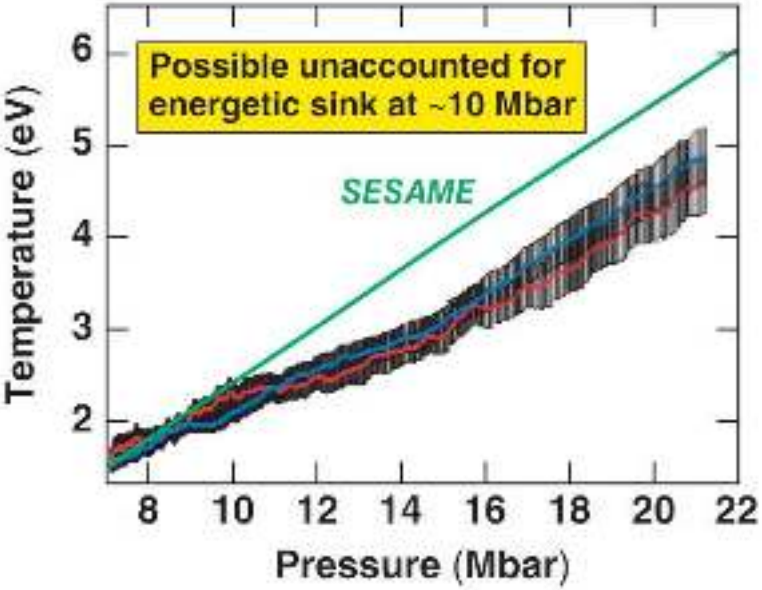


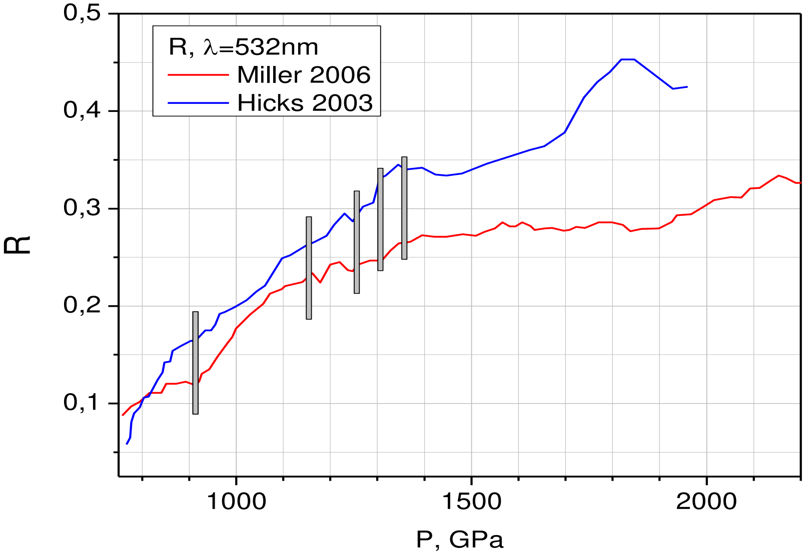
Our points indicates, that Hicks's "laser" "stiff" points is truth!

Later, Kerey's fit was used to calculate **P** and ρ from measured **D**

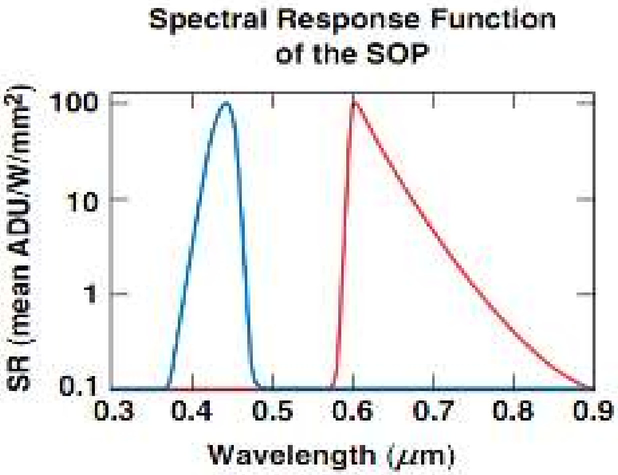
Temperature of shocked Sapphire. Pictures from: J. E. Miller, T. R. Boehly, D. D. Meyerhofer, P. Celliers, J. Eggert, D. G. Hicks, A. Melchior. University of Rochester. 48th Annual APS Meeting, Division of Plasma Physics, Philadelphia, PA. 2006.

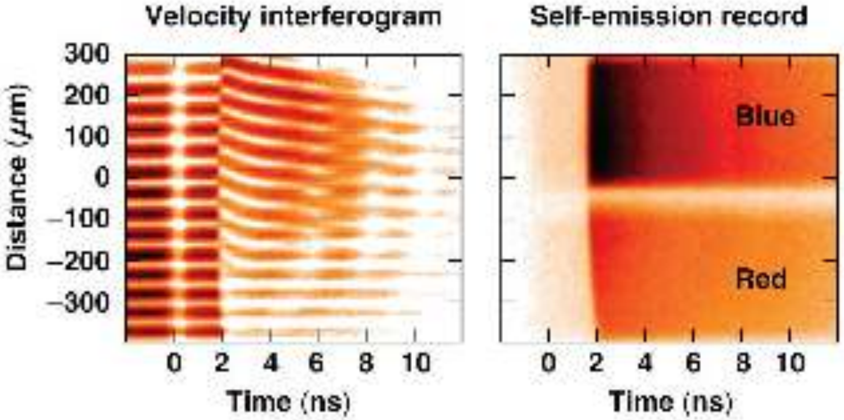
Not published, presentation located at University of Rochester web page



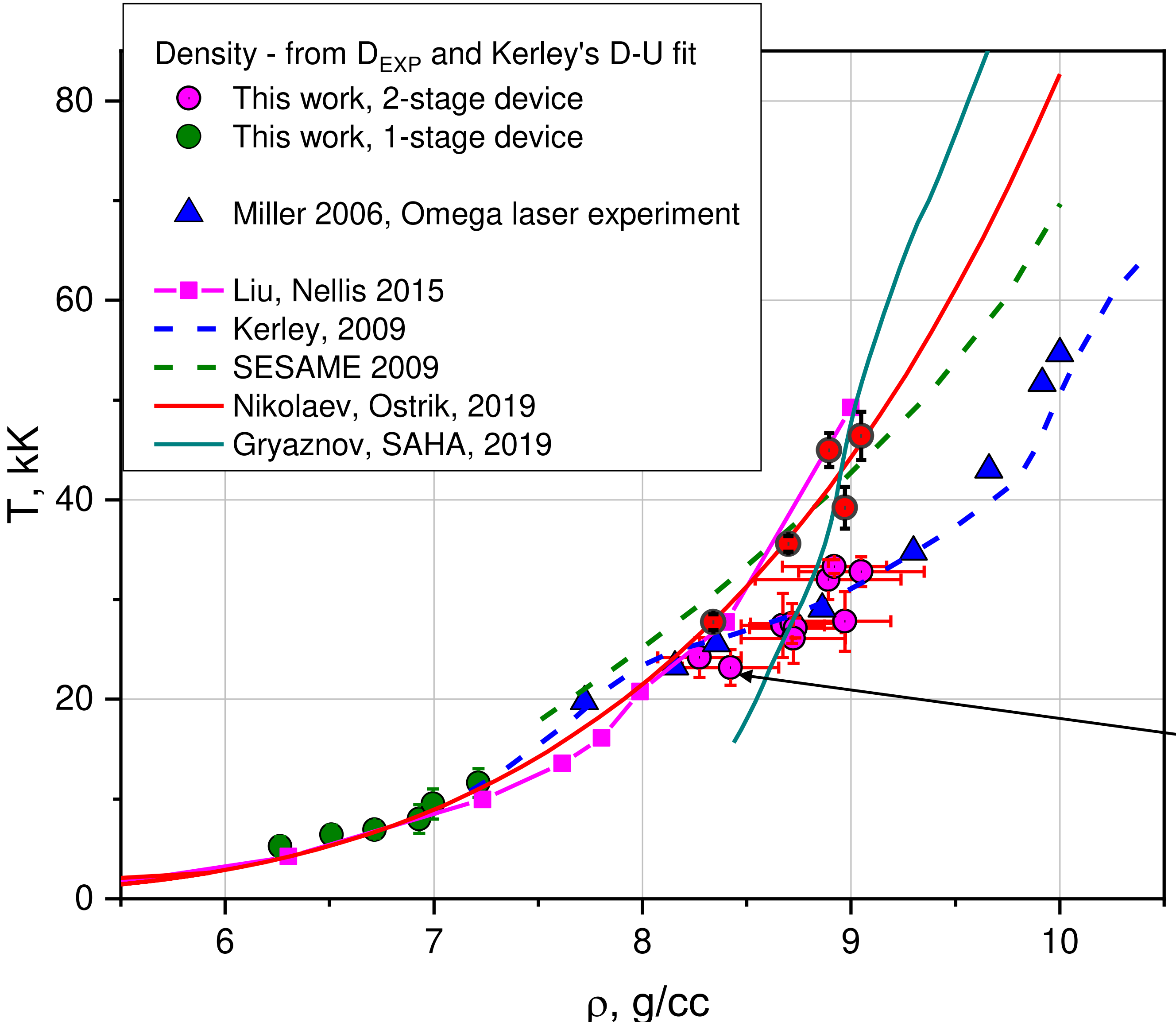


Emissivity $\varepsilon = 1 - R$





Taking in account the non black-body emissivity of shock front: our points is moving from Miller 2006 experiment and Kerley 2009 calculations directly to calculations of SESAME, Liu Nellis 2015, Ostrik 2019 and Gryaznov 2019

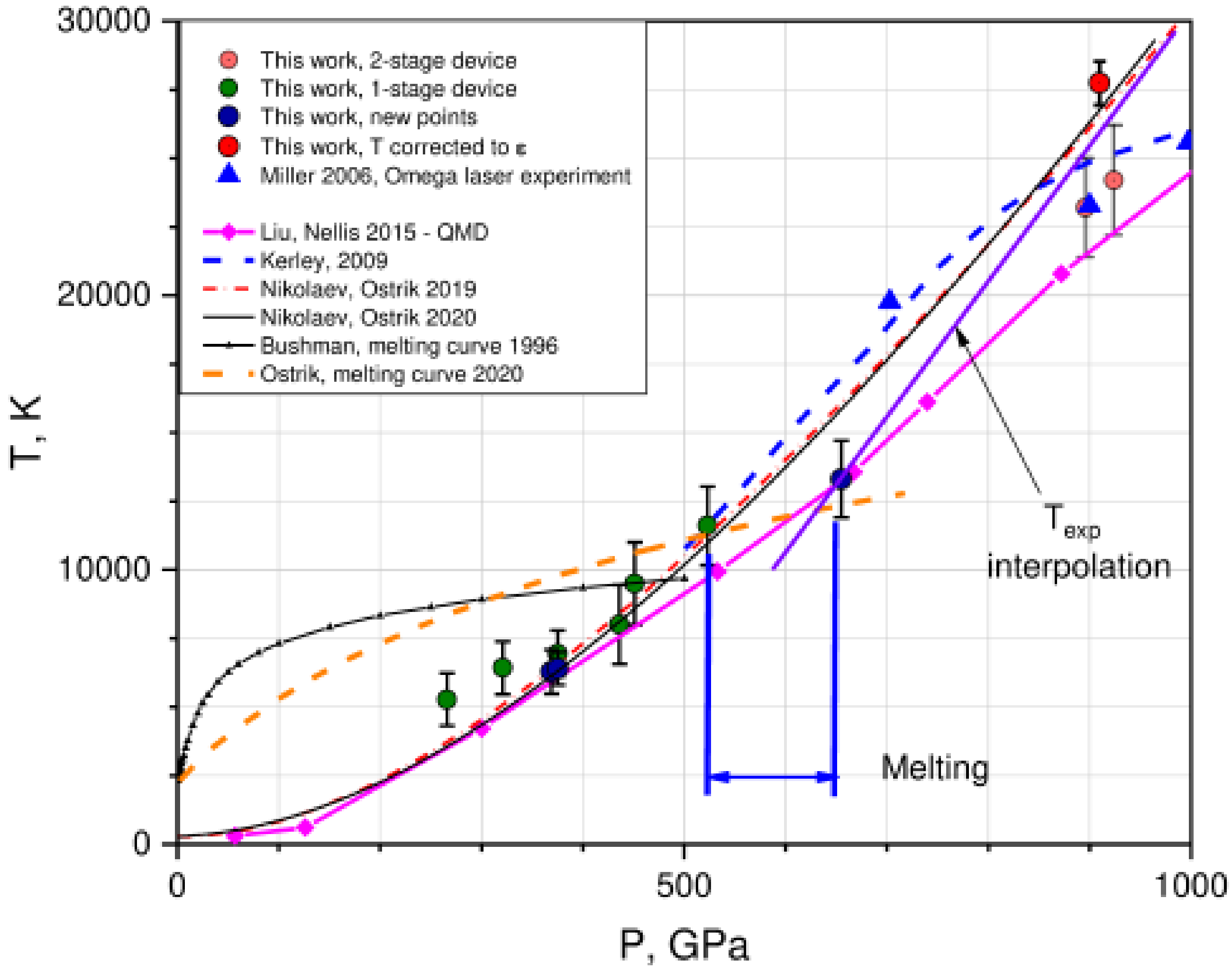


Possible start of decomposition: 900 GPa

Shock-induced melting of sapphire

Temperature EOS, Mi-Gruneisen type, accounting the Debye temperature model

Melting curve calculated according the Lindemann melting rule



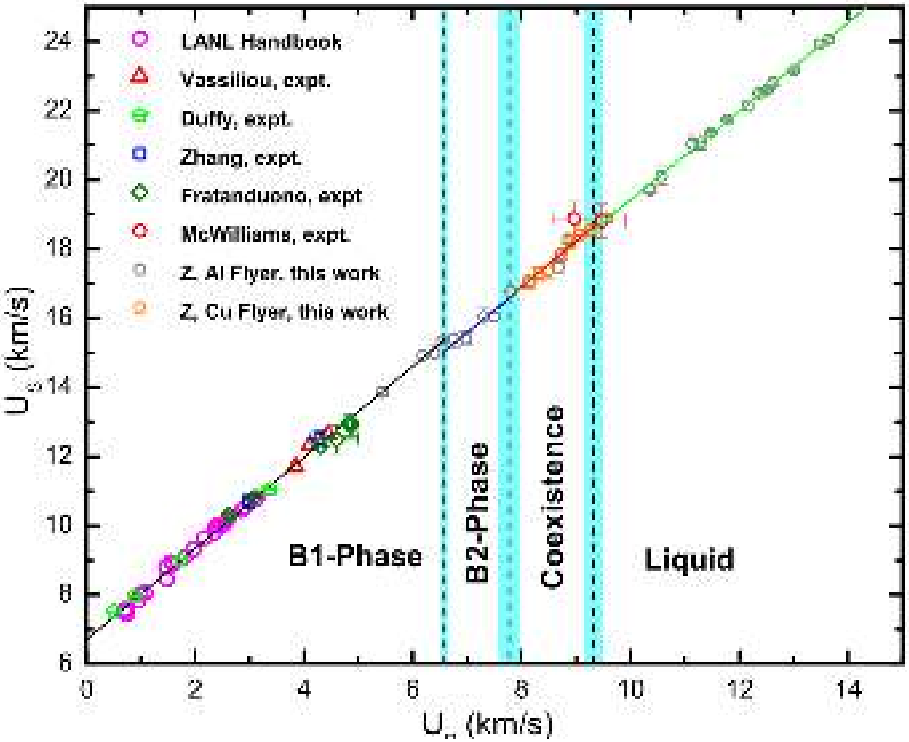
Al_2O_3 melting at shock compression:
500 – 650 GPa
11000 – 12500 K

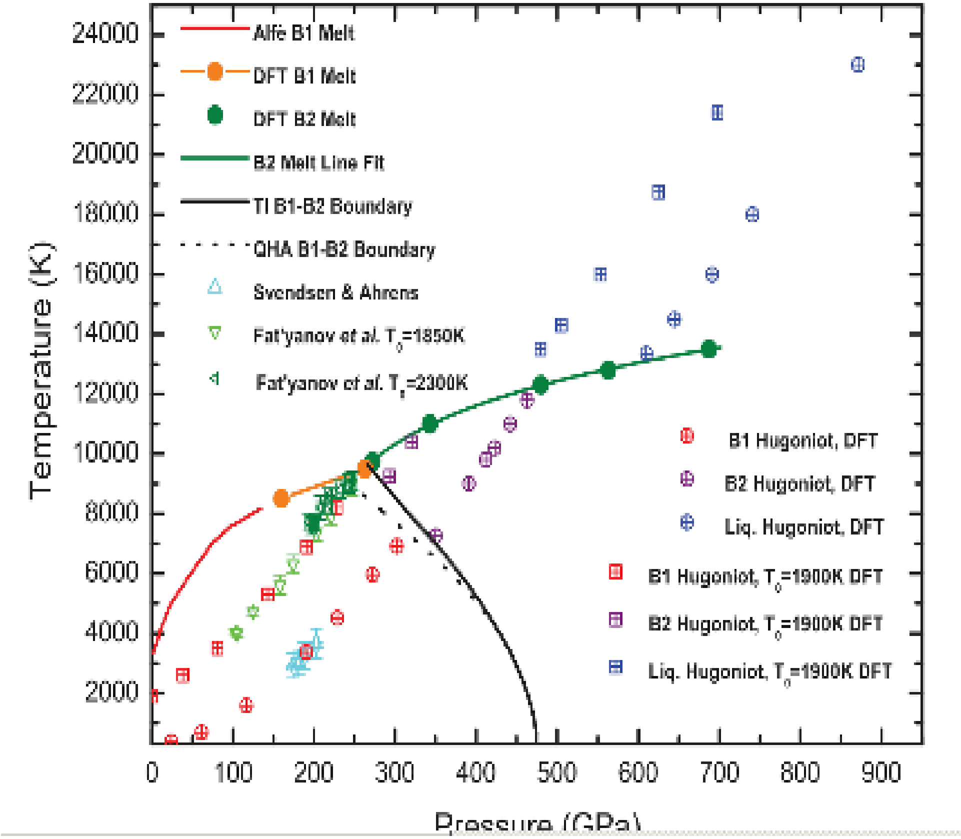
Shock adiabate of MgO (Periclase)

Explosive and gas gun points don't reach even B1-B2 transition

Big data set from Sandia Z-machine. Only compressibility was measured, no temperatures. Supported by DFT-calculation of temperatures.

Polymorph transition B1-B2 (fcc NaCl structure – bcc CsCl structure) is seen at the shock adiabate, also melting



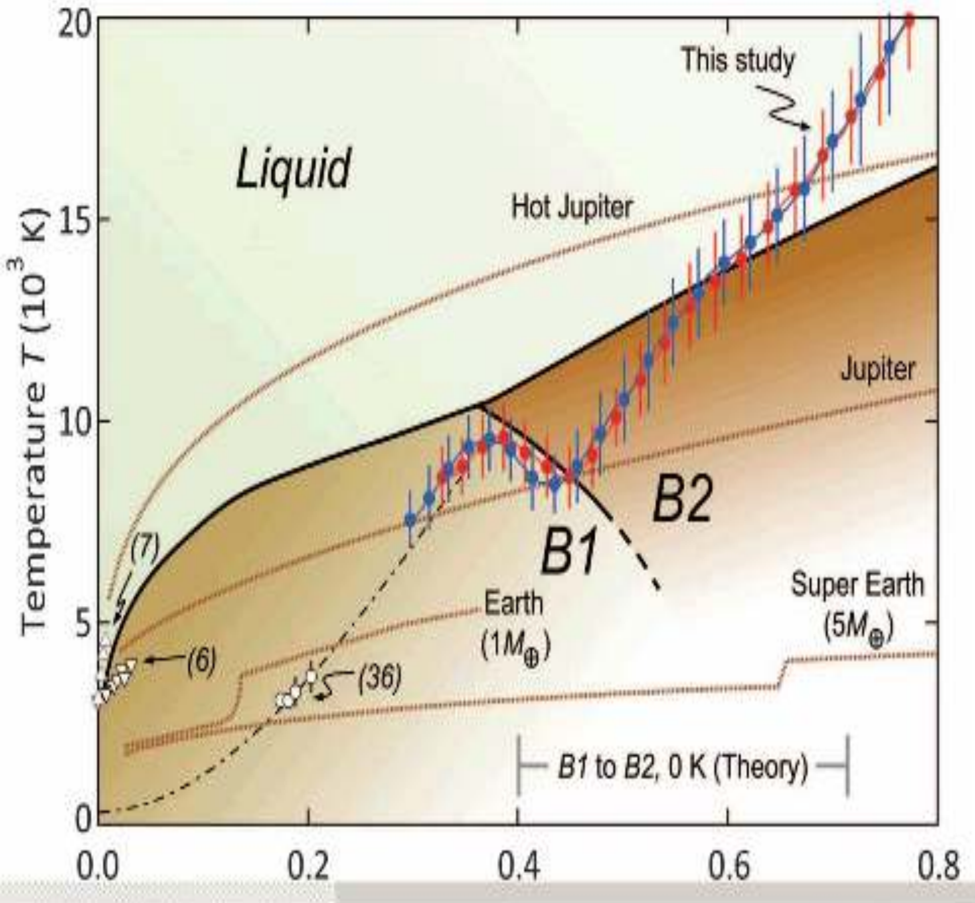


Root, Desjarlais 2015. Z-Machine

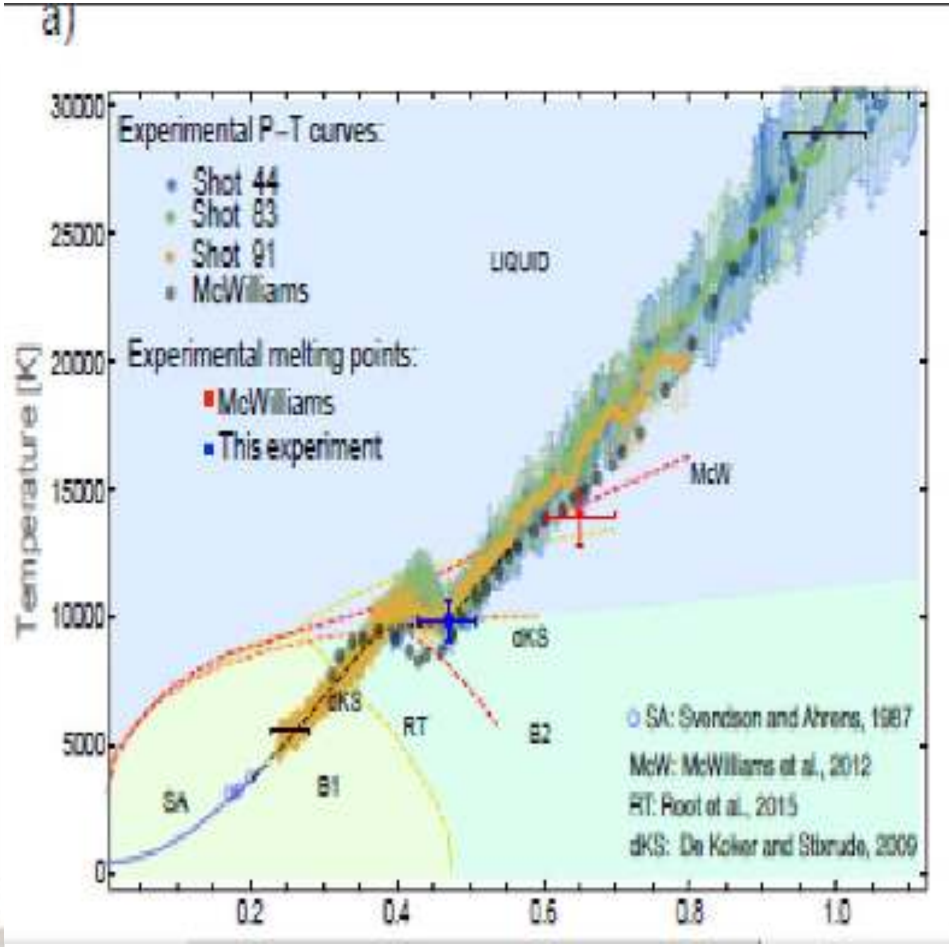
Laser shock waves experimental data Omega and LULI

Analogous to sapphire, decaying shock. 1 shot = temperature, shock velocity and reflection vs time curves.

Kink at temperature vs pressure identified as: B1-B2 transition (McWilliams) or melting (Boilis)

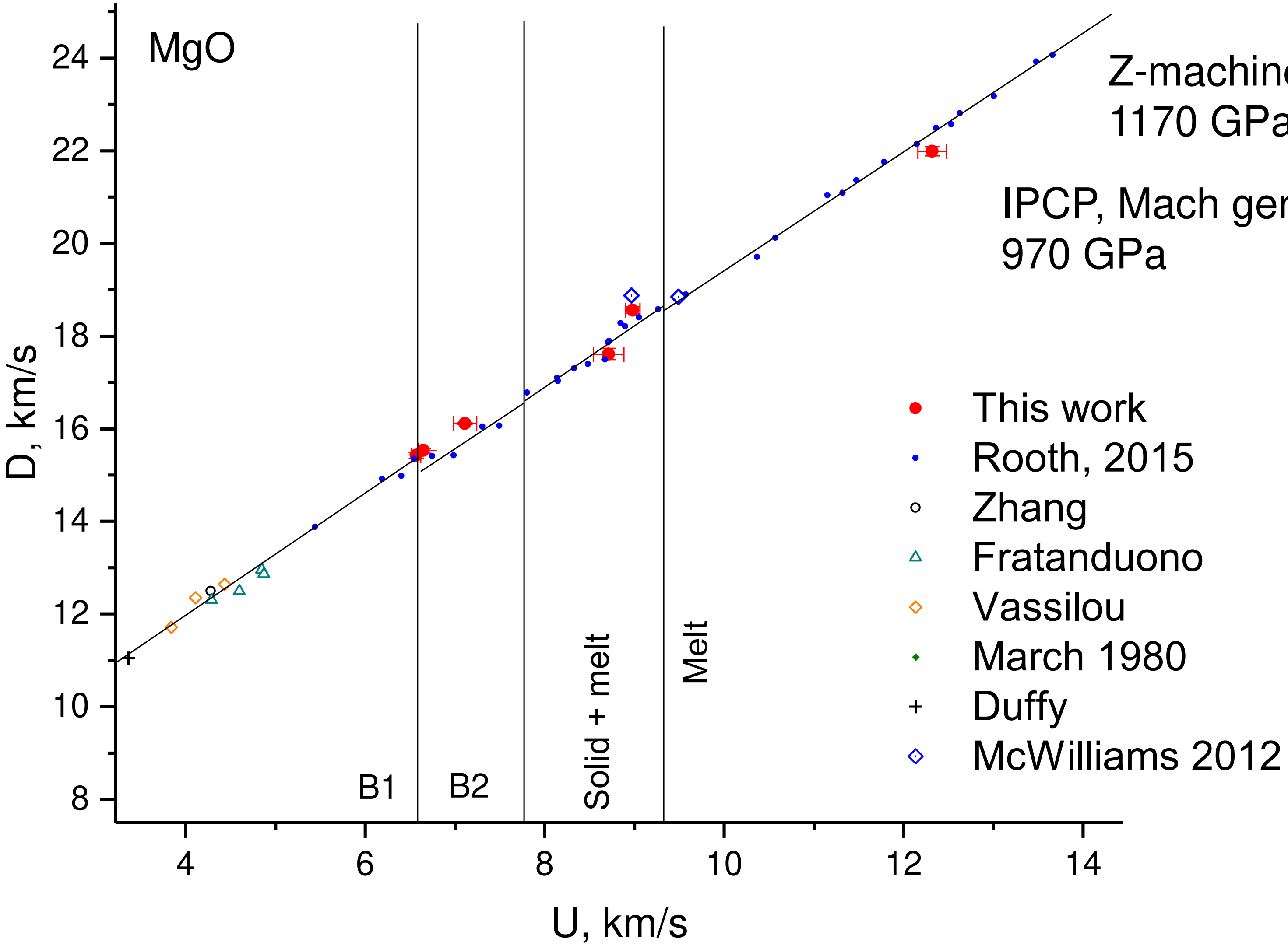


McWilliams 2012, OMEGA



Boilis, Brambrink 2016, LULI

Shock adiabate of MgO: this work

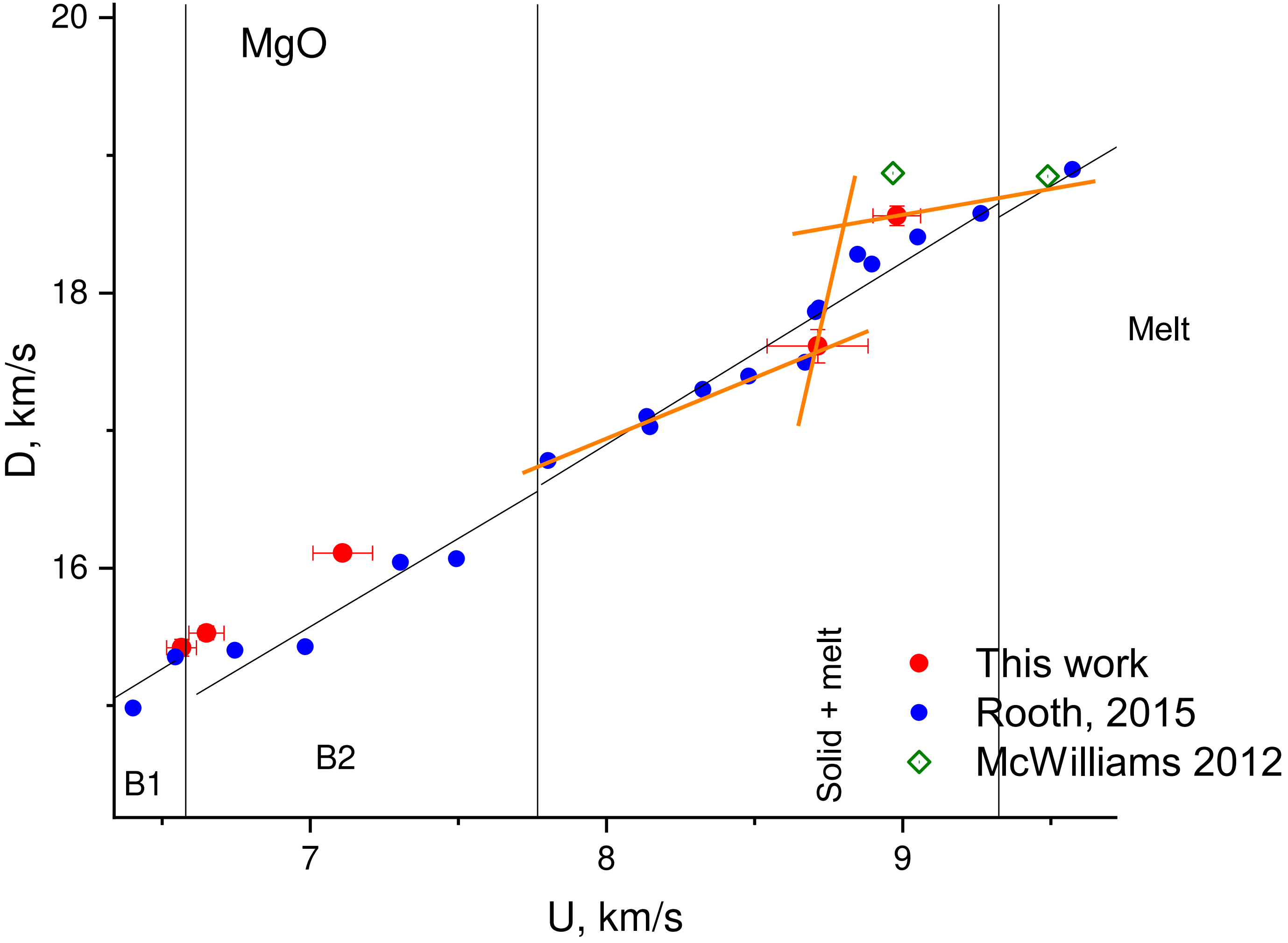


Z-machine:
1170 GPa

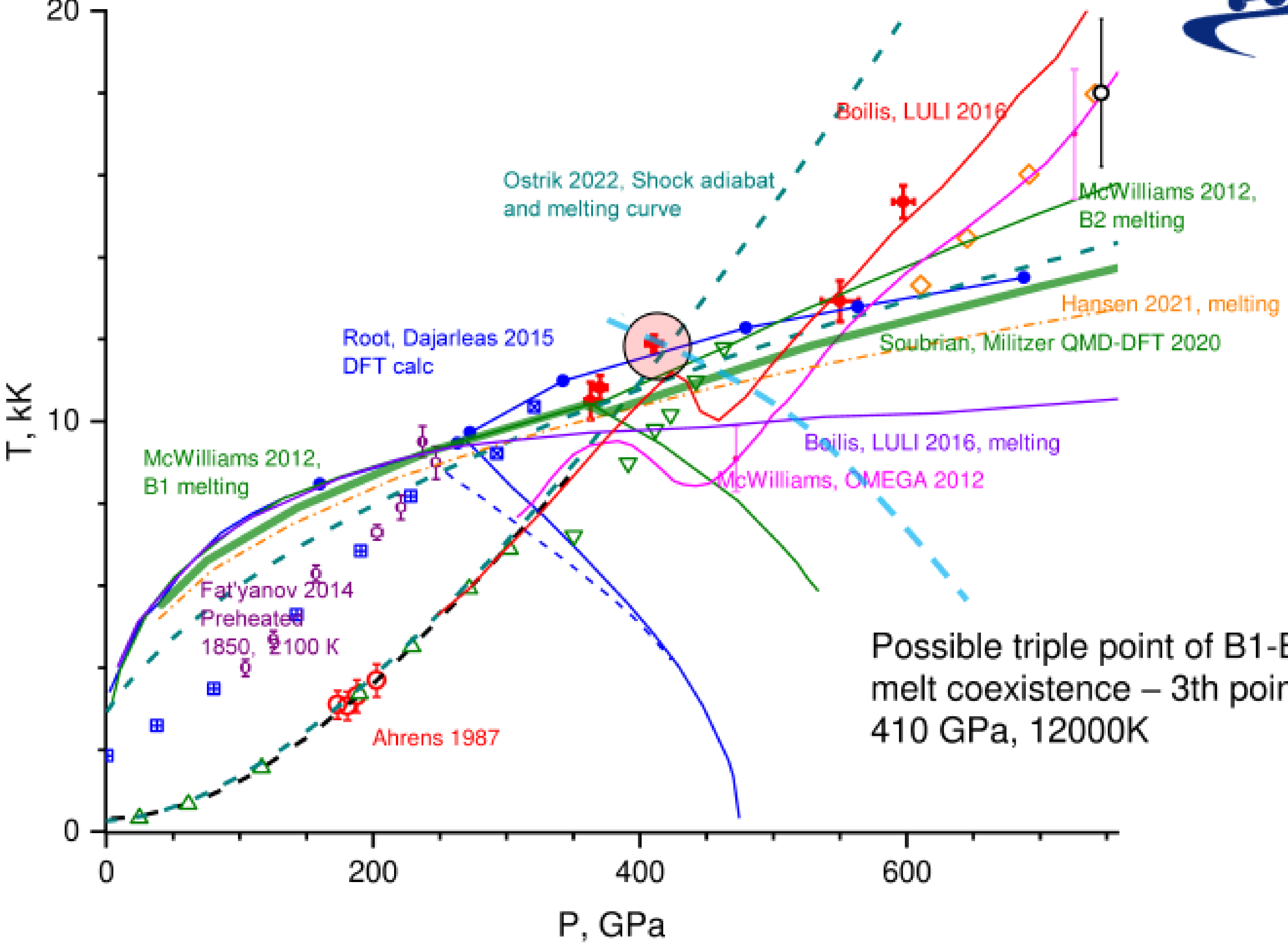
IPCP, Mach generator:
970 GPa

Shock adiabate of magnesium oxide

First 3 points clearly extrapolates shock adiabat of B1 phase
At particle velocity 8.7 – 9.1 км/с (550 – 600 GPa) - kink of the slope.
Possible end of melting. It is in agreement with Rooth data and McWilliams data. DFT calculations provide value 620 GPa

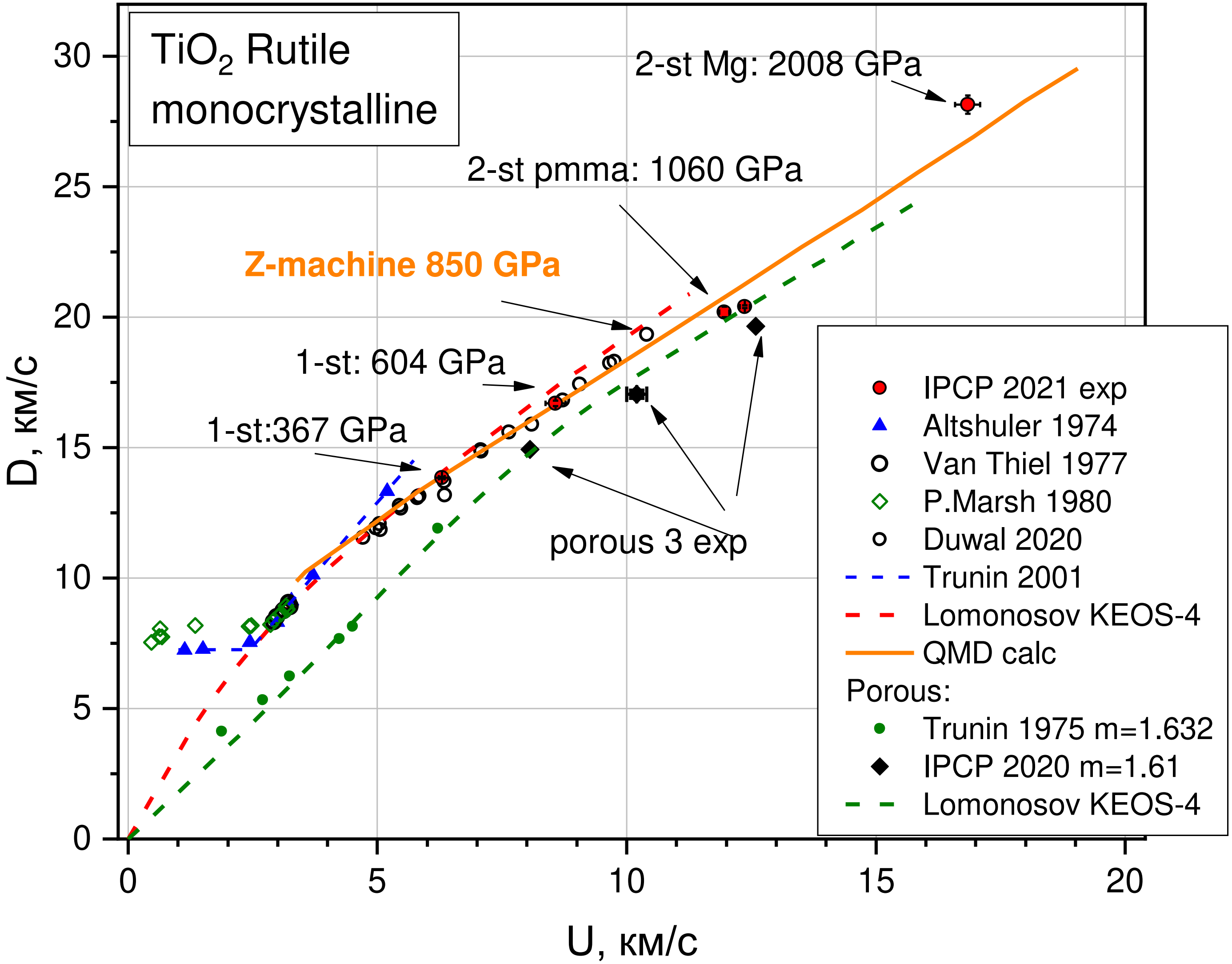


Shock wave temperatures

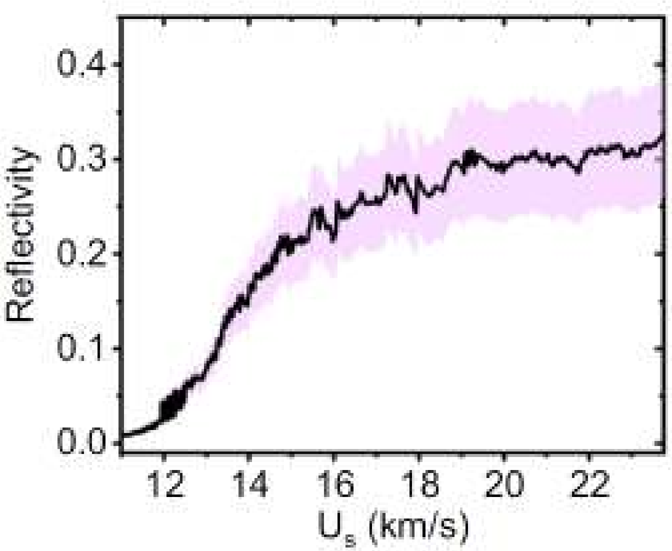


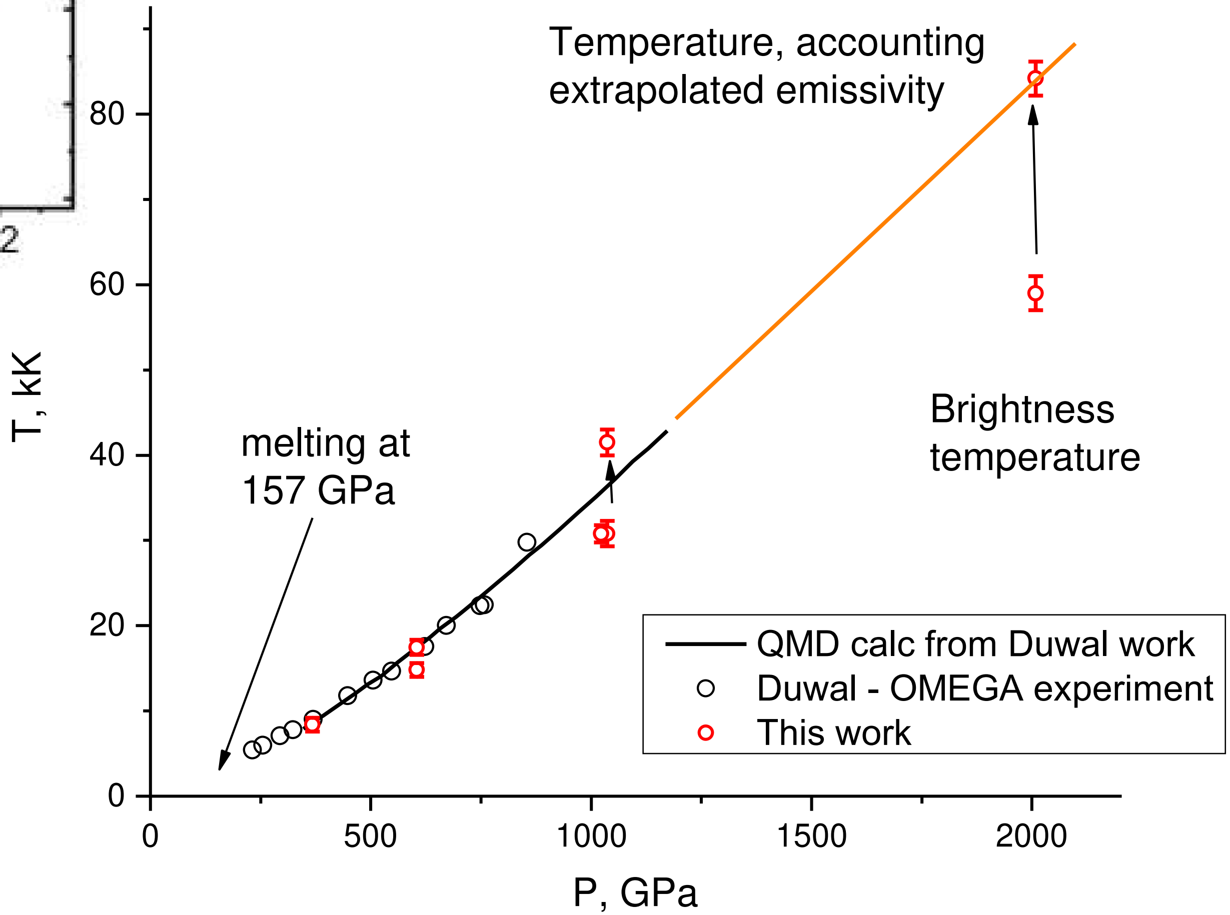
Possible triple point of B1-B2-melt coexistence – 3th point, 410 GPa, 12000K

Shock compression of single-crystal and porous TiO_2 (Rutile)
Highest pressure achieved with modified 2-stage generator is 2008 GPa. It is higher that achieved at Z-machine (850 GPa).



Shock temperature of single-crystal TiO_2. For highest points, taking into account experimental emissivity affect temperature value




Temperature, accounting extrapolated emissivity

melting at 157 GPa

Brightness temperature

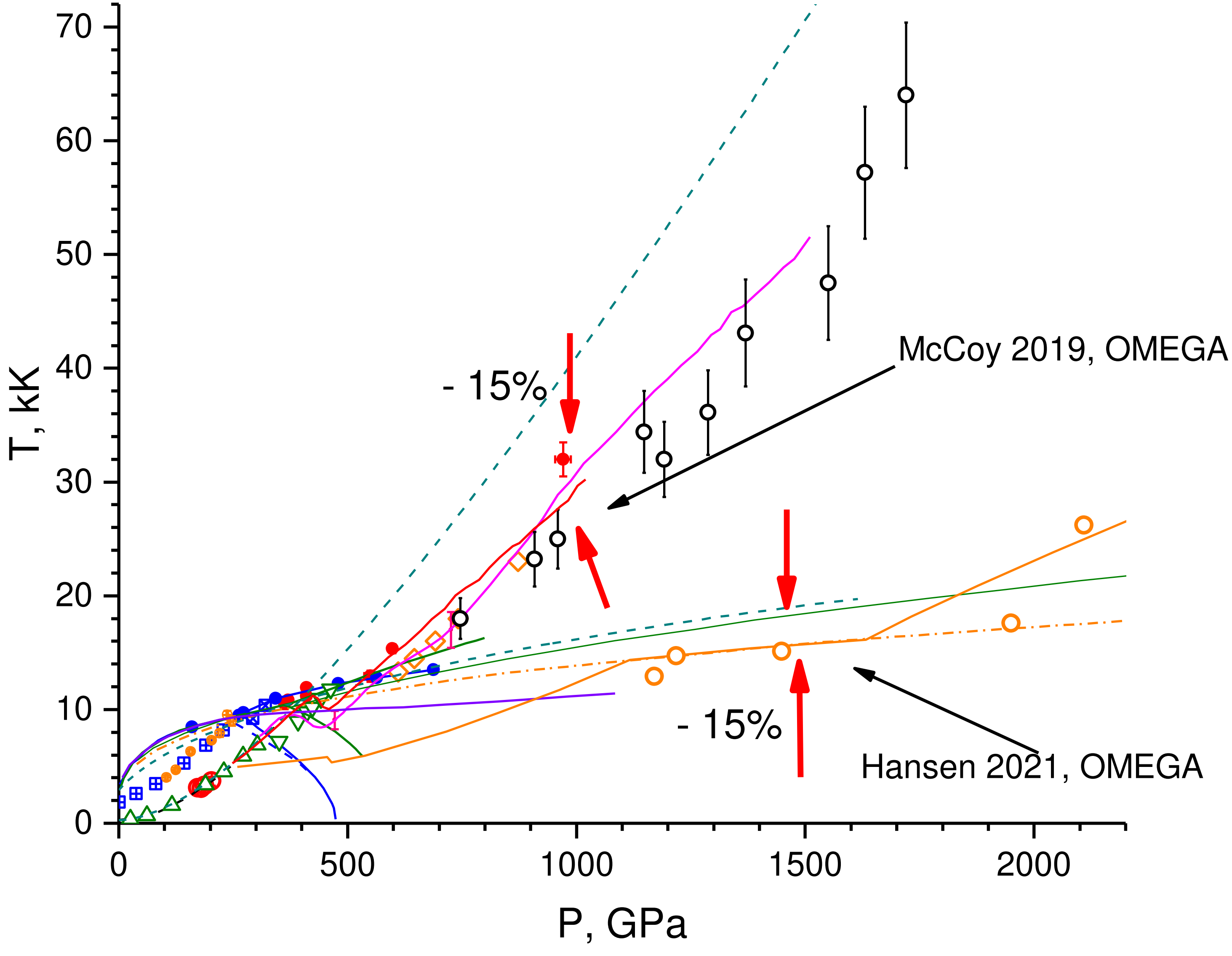
Results:

Al_2O_3 Sapphire:
“Stiff” shock adiabate for pressures > 400 GPa confirmed. Temperature is not in agreement with laser shock measurements. Indication of shock-induced meltting at 500 – 650 GPa and 11000 – 12500 K obtained. In agreement with Ostrik’s (EOS + Lindemann melting law) melting curve.

MgO Periclase:
Shock adiabate is in agreement with Z-machine data except one point near B1-B2 transition. Shock adiabate passing through possible triple point of B1-B2-melt coexistence (410 GPa, 12000 K). B1-B2 boundary at highest pressure, and highest possible temperatures of melting curve. Melting curve is best described by Ostrik (EOS + Lindemann melting law) and QMD-DFT calculation of Militzer. Melting starts at 420 GPa (Boilis), ends at 550 GPa (from temperature measurements) or 600 (from shock compressibility slope)

TiO_2 Rutile:
Record point 2008 GPa, plasma state, fully dissociated, high ionization degree. Shock adiabate is in agreement with Lomonosov KEOS-4 calculations for both single-crystal and porous samples and in good agreement with Trunin 1975 data.
Still no calculation of temperature for 2 TPa, but quite good agreement with QMD-DFT calculations of Duwal 2020

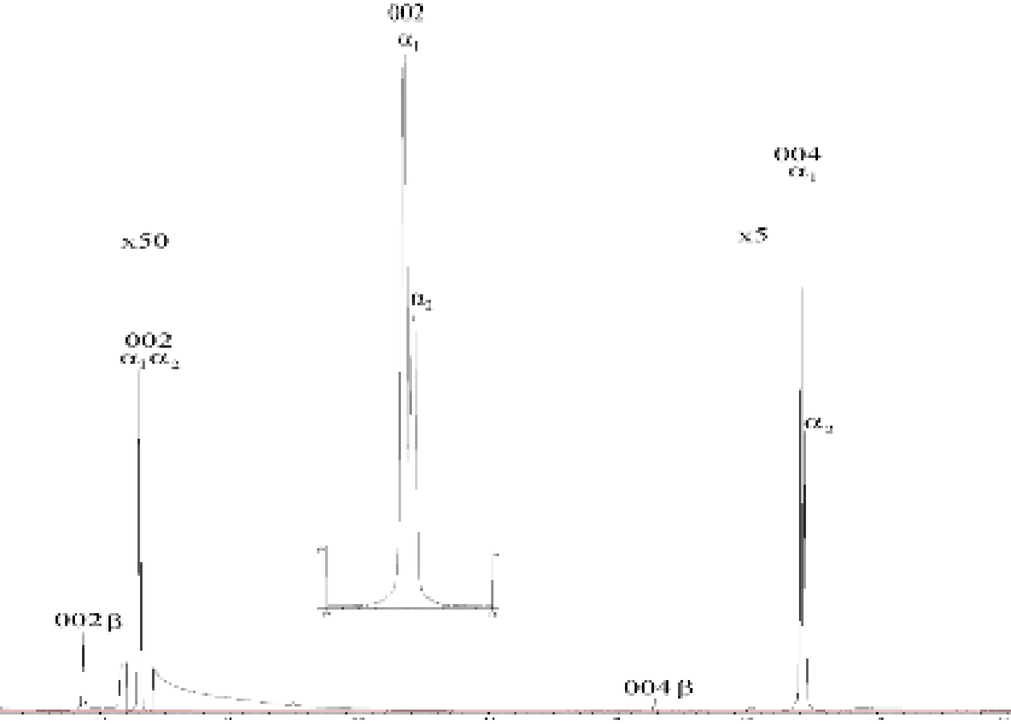
Результаты: Занижение температур стрик-пирометром ОМЕГА



Исходные монокристаллы имели размер 10x10x1 мм, ориентация 100

Кристаллы были характеризованны рентгеновской дифрактометрией и взвешиванием в воде

Вывод – монокристаллы отличного качества, плоскость 100 идеально параллельна поверхности.



Параметр решетки оксида магния рассчитанный по α1 отражениям *a*=4,211±0,002 Å (для длины волны α1, излучения принято значение 1,54051 Å).

Плотность, рассчитанная из этих параметров ρα=3,587±0.005 г/см^3,

Взвешивание в воде – 3.583г/см^3, справочная плотность 3.584г/см^3

МАХОВСКИЙ КУМУЛЯТИВНЫЙ ГЕНЕРАТОР УДАРНОГО СЖАТИЯ

Дмитрий Николаев

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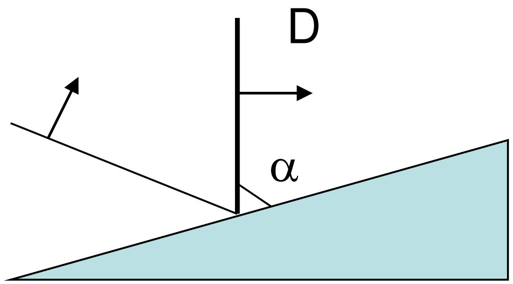
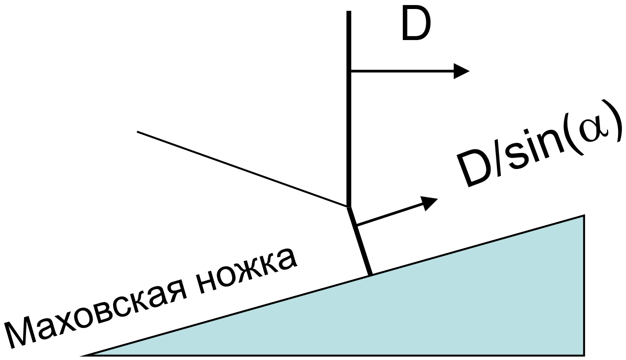
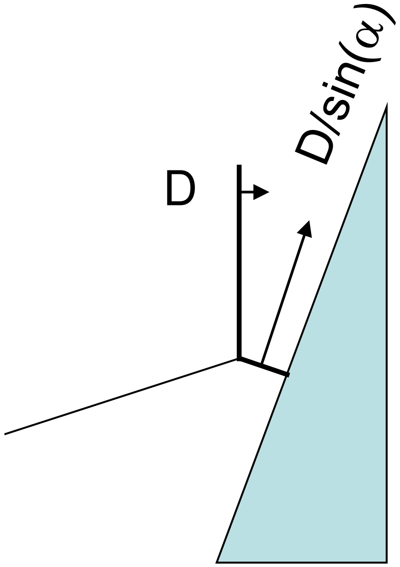
Нерегулярное (Маховское) отражение ударной волны от клина



Регулярное отражение



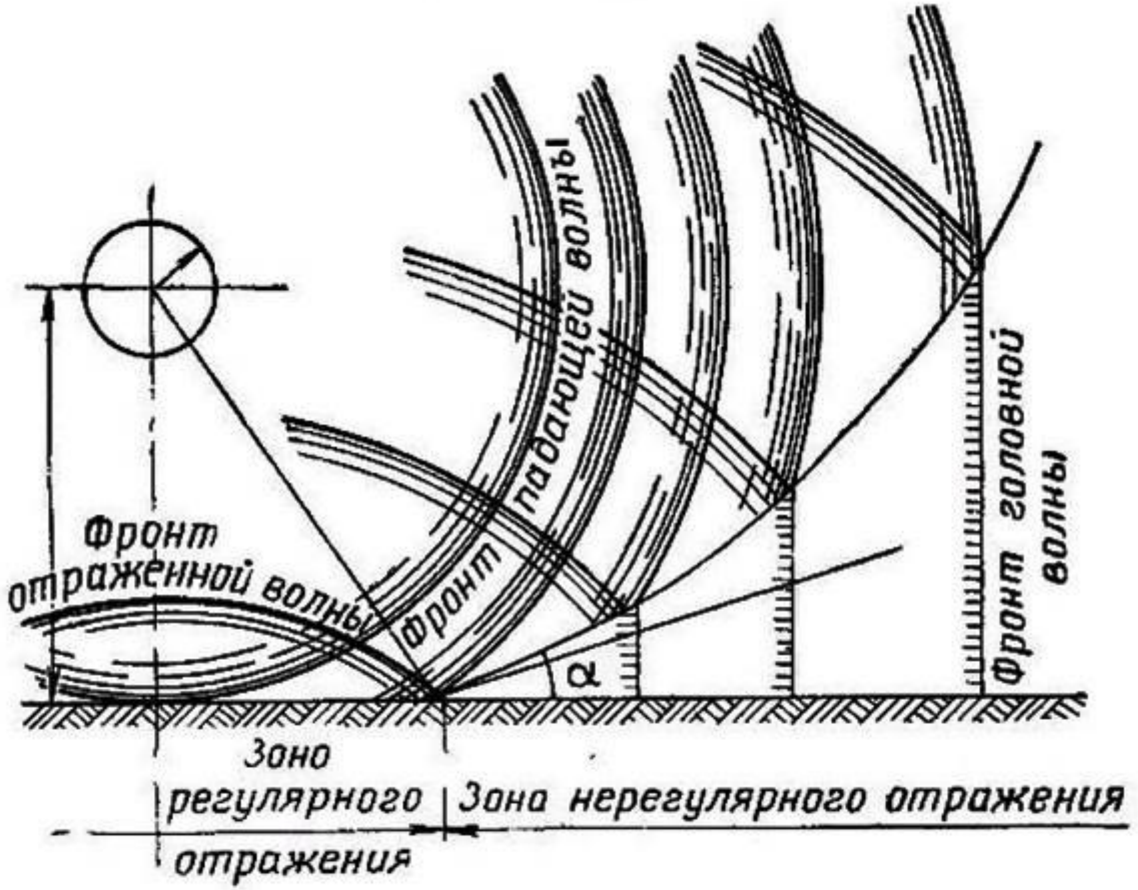
Нерегулярное отражение



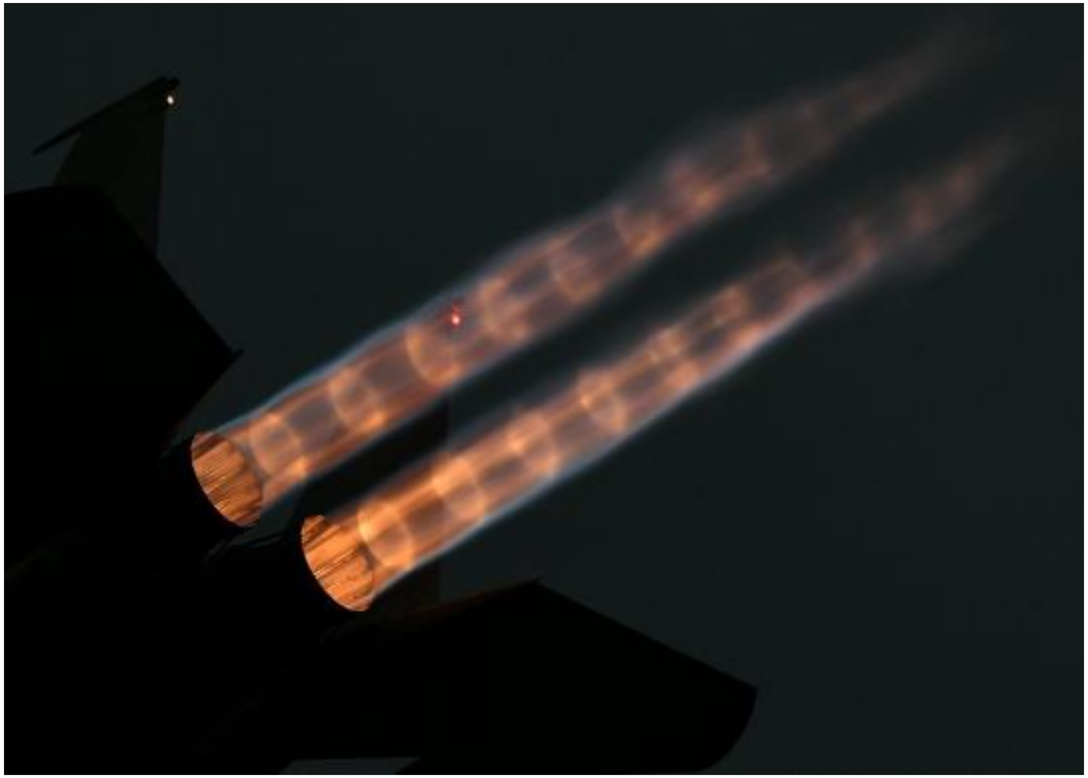
Уменьшаем угол –
увеличиваем скорость

Маховская конфигурация при взаимодействии ударной волны от воздушного взрыва с поверхностью земли

Схема формирования ударной волны

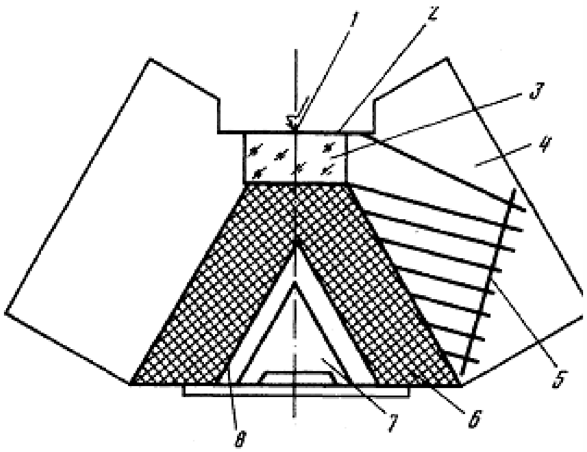


Образование Маховского диска в осесимметричном сходящемся потоке (истечение из реактивного сопла)



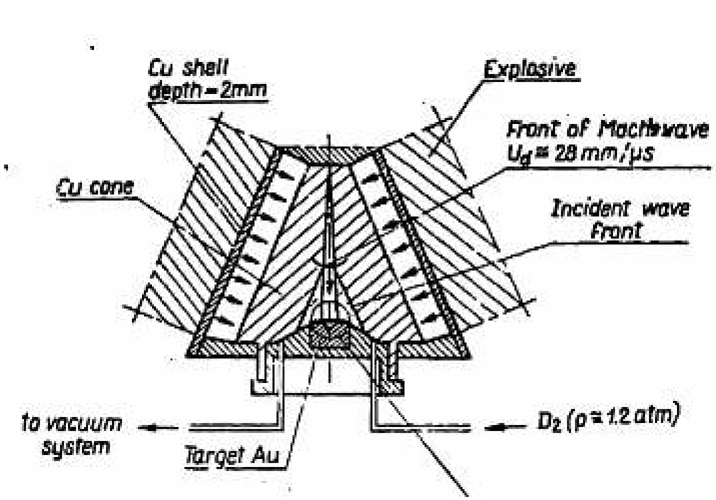
Идея: воспроизвести тоже самое, но в твердом теле

Предложенные в 80-х годах схемы генераторов высокого давления, использующих схождение конической ударной волны.



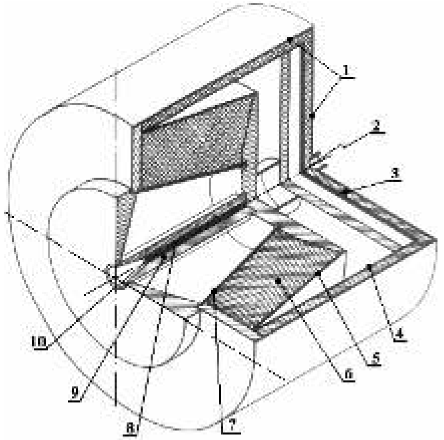
До 600 ГПа в меди

B. Glushak, A. Zharkov, et al. ZETP 96, 1301 (1989)



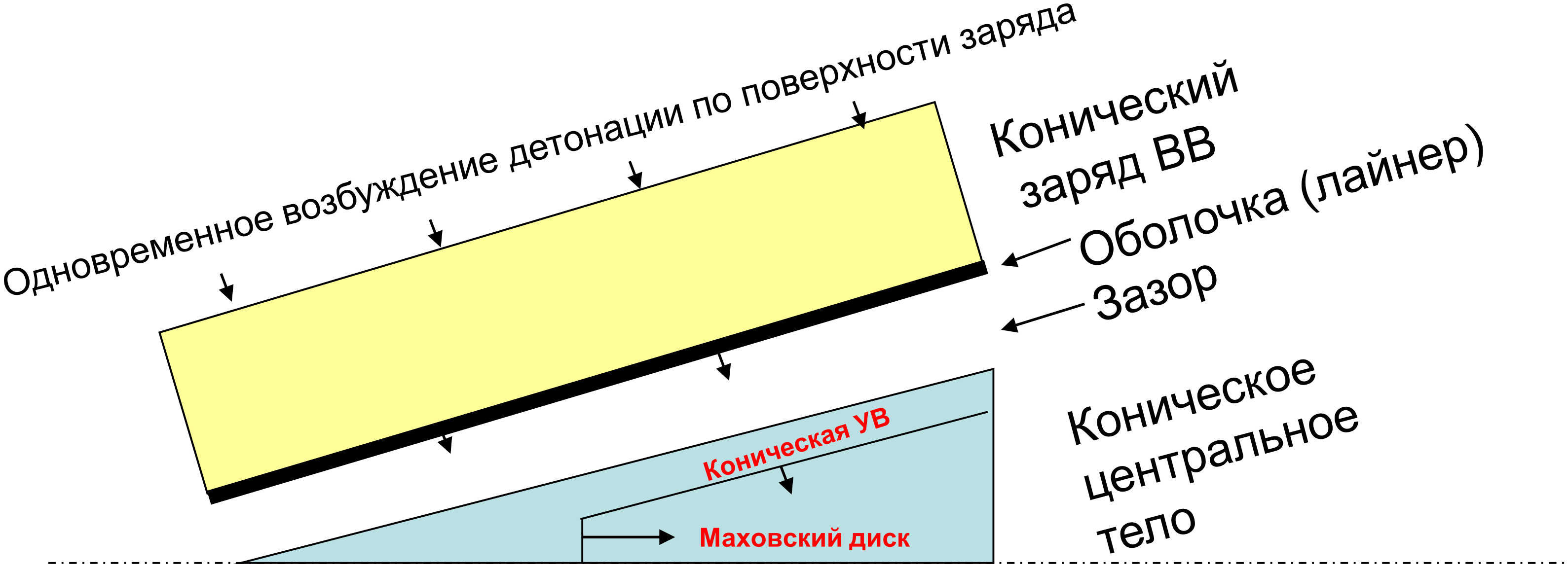
100 - 1000 ГПа в меди

H. Derentowicz, J.App.Mech.Tech.Phys, v 30, Iss 1, p. 21, 1989



1650 ГПа в железе

Жарков А.П., Крюков Б.П. Физика экстремальных состояний вещества, 2004



Одновременное возбуждение детонации по поверхности заряда

Конический заряд ВВ

Оболочка (лайнер)

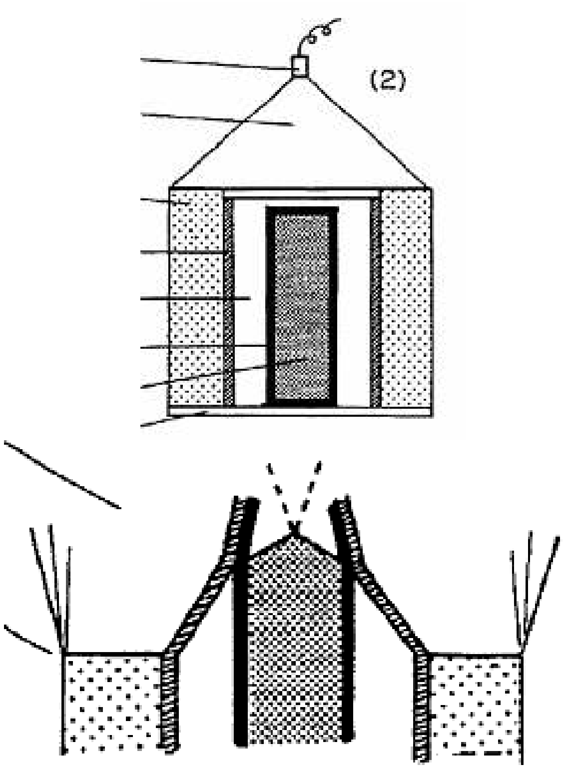
Зазор

Коническое центральное тело

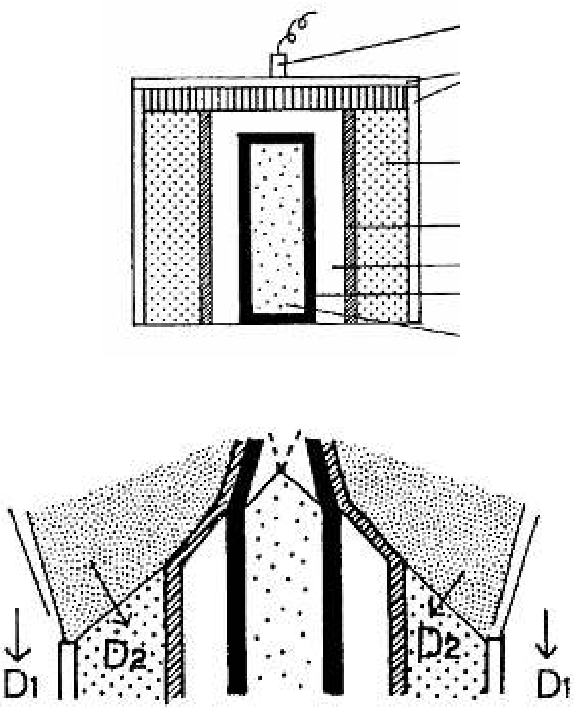
Коническая УВ

Маховский диск

Метание лайнера скользящей детонацией в цилиндрической геометрии: обжатие ампул сохранения (ударный синтез)



Плоская детонация
D ≈ 8 км/с

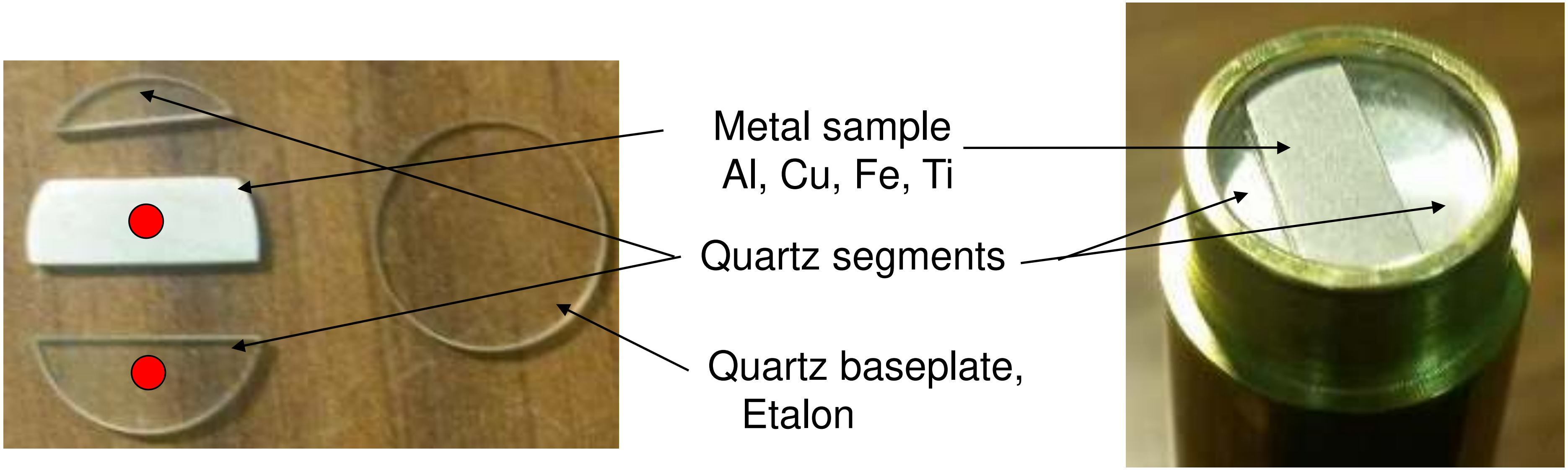


Навязанная детонация
$D_1 \leq 9.6$ км/с (CL-20)

При достаточных параметрах УВ в центральном цилиндре можно сгенерировать Маховский диск.
По-видимому, 9.6 км/с – предел скорости детонации. **Необходима детонационная разводка**

Иллюстрации из обзора S.Fujiwara, Shock compression technology and material science, pp.7-21, 1992
Ссылки на Ададуров et al., 1967, Morris et al., 1984, Гогуля et al., 1981, Воскобойников et al., 1987, Мартынов et al., 1986

Study of Hugoniot of metals. Sapphire window was used.



Metal sample
Al, Cu, Fe, Ti

Quartz segments

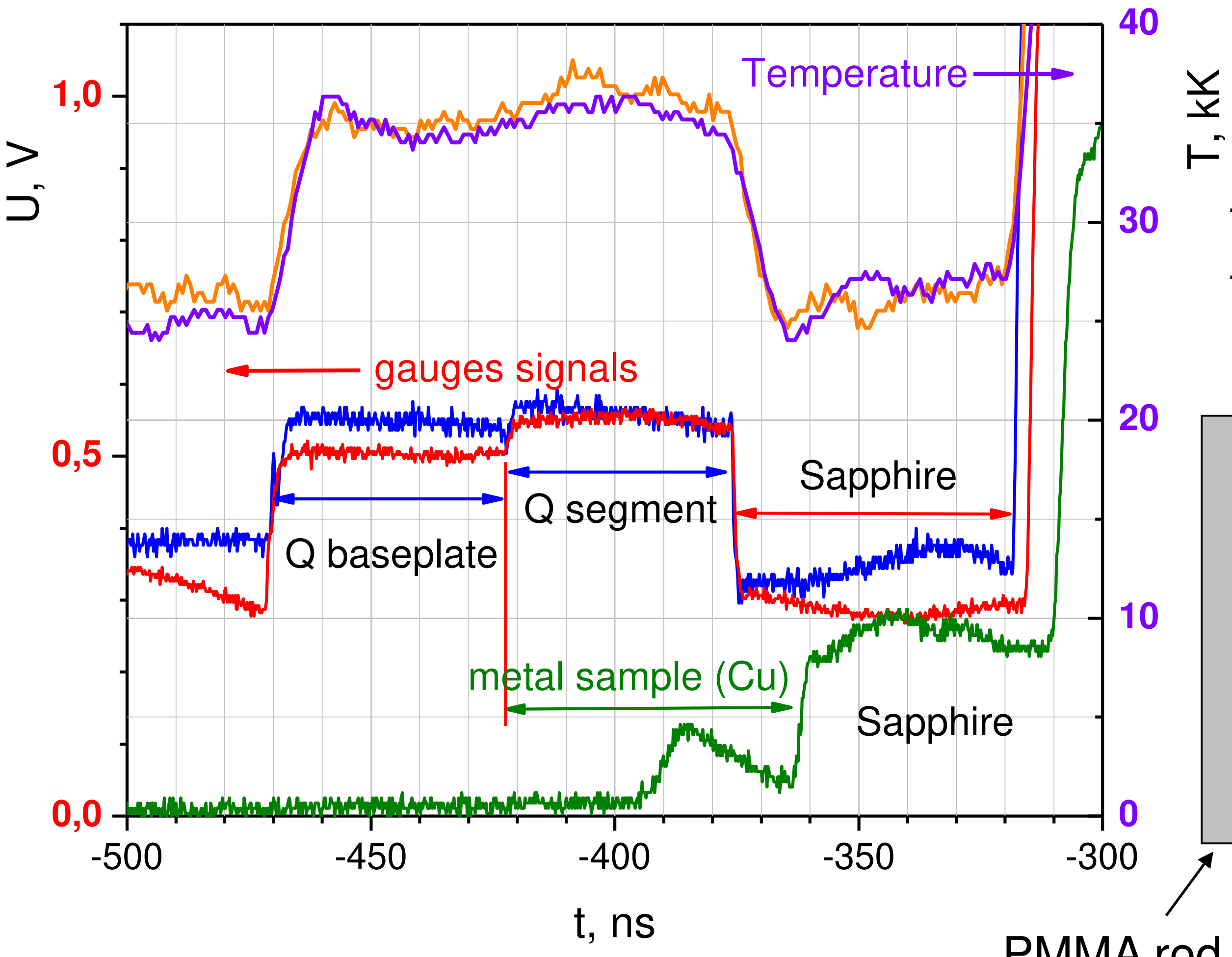
Quartz baseplate,
Etalon

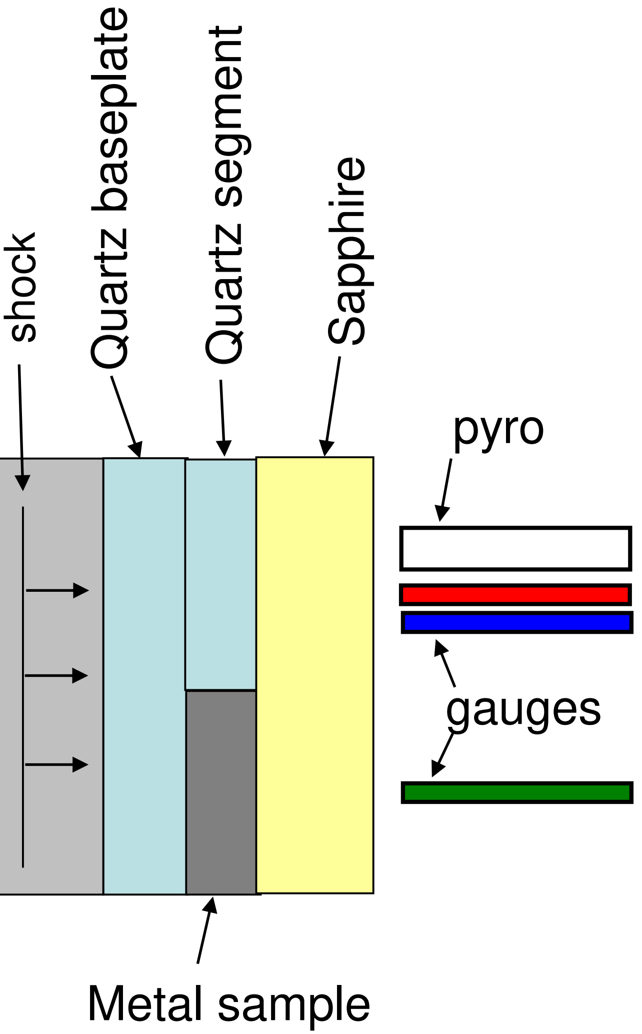
Optical pyrometer was used to register the brightness temperature in 2 points

Wave velocities was measured in Quartz, metal and Sapphire

Measuring of wave velocities in quartz ethalon and metal sample > **compressibility of metal**

Additional info from fast optical gauges: velocity of shock in Sapphire. We can get the **compressibility of Sapphire!**





Результаты: температура ударного сжатия и кривая плавления

1. Две нижние точки – фаза B1. QMD-DFT Расчет Дежарли неправильно описывает превращение B1-B2
2. Ударная адиабата в P-T по-видимому, проходит через тройную точку B1-B2-жидкость
3. Измерения 2012 года на Омеге (McWilliams) дают заниженную температуру. Интерпретация скачка как переход B1-B2 неверна. Правильная интерпретация – Boilis 2016: это плавление
4. Плавление начинается при 420 ГПа (Boilis), заканчивается при 550 ГПа (наша точка)
5. Лучше всего плавление описывается QMD-DFT-расчетом Шабриана и Милицера. Так же плавление B2 фазы хорошо описывается расчетом А.Острика, хотя на ударной адиабате нет признаков B1-B2 превращения. Это может быть связано с п.2: ударная адиабата проходит через тройную точку B1-B2-жидкость
6. В экспериментах по двукратному сжатию (Hansen 2021) кривая плавления занижена по температуре по сравнению с расчетом милицера. Так же, занижена температура однократного сжатия в McCoy 2019 по сравнению с нашей точкой 970 ГПа. Величина занижения – 15%. Дополнение к п. 3 (там занижение на 9%). Стрик-пирометр на установке ОМЕГА занижает температуру?