Modeling of states of matter under intense laser pulse influences

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Experiments

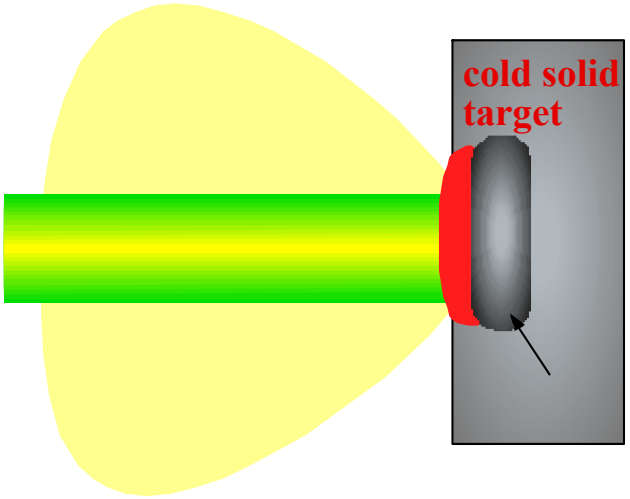
Motivation

The knowledge of the Equation of State (EOS) of strongly compressed materials is very important in astrophysics and in the framework of inertial confinement fusion (ICF). EOS is required for numerical simulations of condensed matter under the action of intense laser pulses. A wide variety of states of matter can be obtained with laser irradiation, showing many interesting phase transitions.

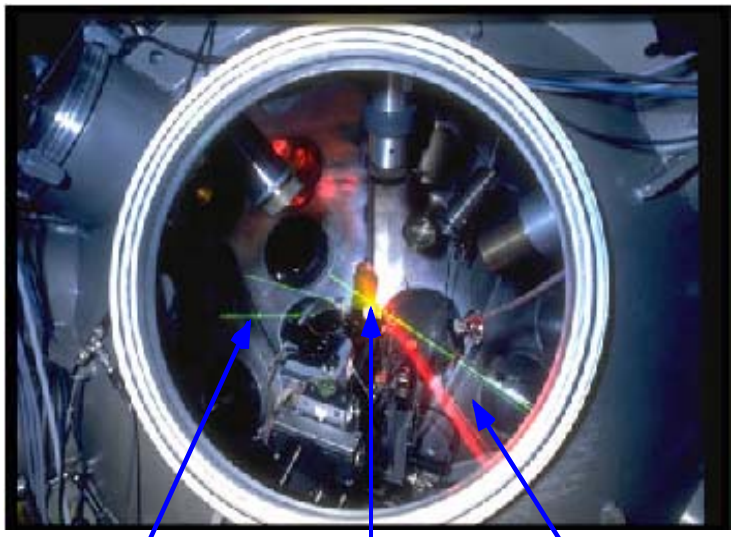
The only way to compress matter to multimegabar pressurs is by shock-waves, whose propagation is described by Rankine–Hugoniot relations. Measuring two of the five (U_p, U_s, E, P, ρ) shock parameters (usually, the shock-wave front velocity, U_s, and the fluid velocity, U_p) one obtains data for caloric EOS, $E = E(P, \rho) = E(P, V)$.

To obtain the full thermodynamic EOS, the temperature should be specified as a function of pressure and specific volume, $T = T(P, V)$. Thus the measurement temperature behind the shock-wave front is an important problem for constructing a full EOS.

Pressure generation with high-energy laser



Target chamber



Ablation pressure

$$P(MBar) = 10\left(\frac{I_L(W/cm^2)}{10^{14}}\right)^{2/3} \lambda(\mu m)^{-2/3}\left(\frac{A}{2Z}\right)^{1/3}$$

beams Target Probe beams

I= 2 10^{13} W/cm² λ =0.53 μm => P = 5 MBar

We use shock to compress matter and measure EOS

Conservation laws:

Mass

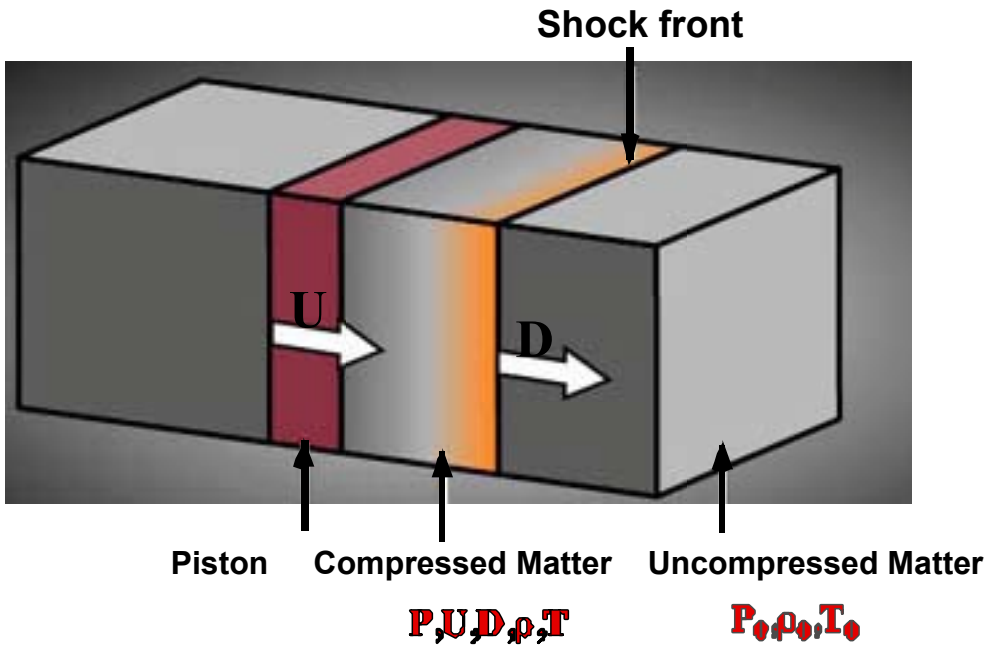
$\rho_o D = \rho\,(D-U)$

Momentum

$\rho_o DU = P-P_o$

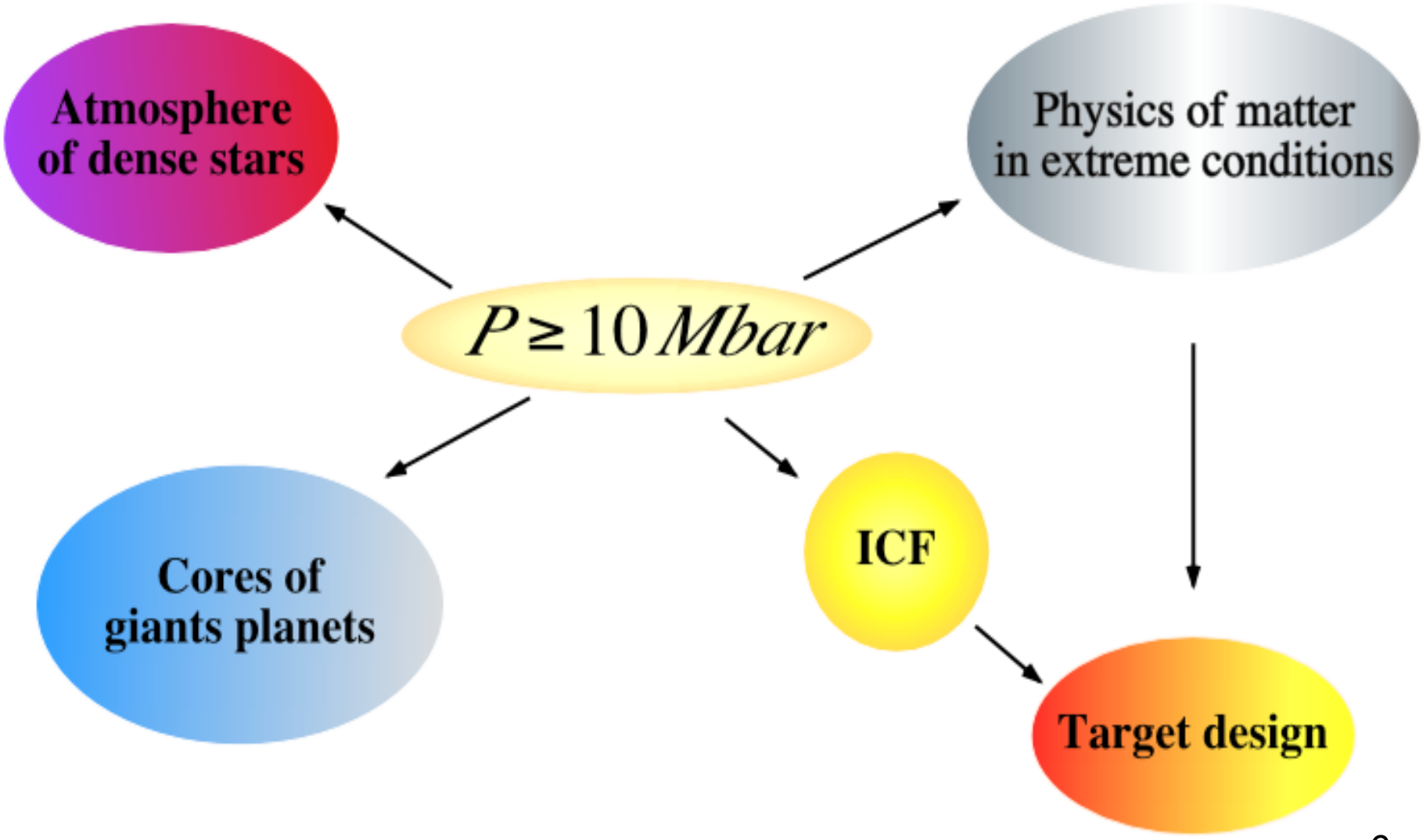
Energy

$\rho_o D(E-E_o+U^2/2) = PU$



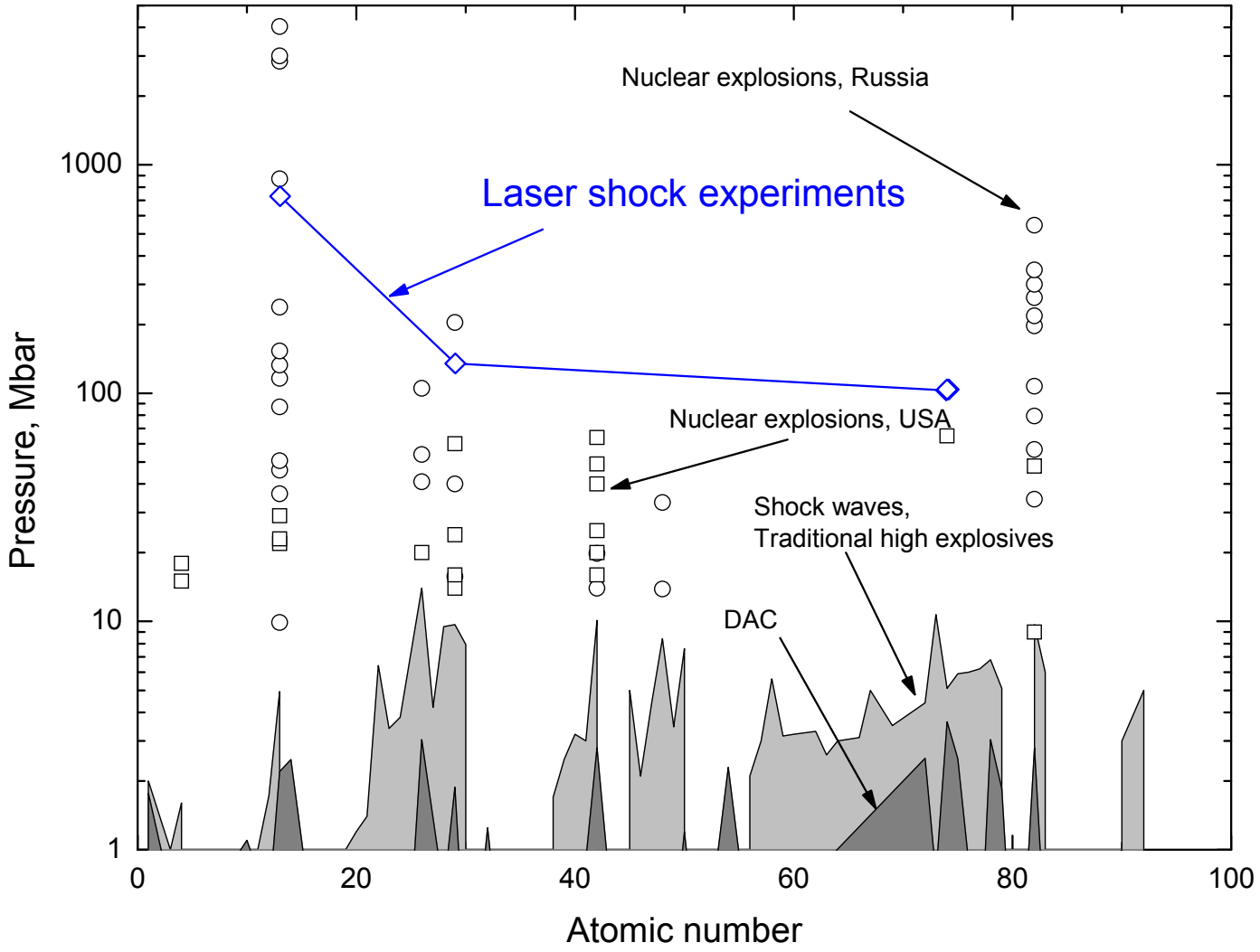
3 equations, 5 unkown parameters ρ, D, U, P, E
Measurement of 2 parameters to get an EOS point.
This point lies on the principal Hugoniot curve (i.e. the ensemble of all states that can be reached with a single shock)

High Pressures in Physics



Previous EOS Study

Measurements have been done with diamond anvil (P≤ 6 Mbar), chemical and nuclear explosions, gas guns, lasers



An Example: Iron

Why is it interesting?

★ Very high Pressures (> 10 Mbars)

- Several experimental points from nuclear explosions theoretical calculations

  Trunin et al., *Physics-Uspekhi,* **37**, 1123 (1994).

- Planetology

  Rocky cores of giant planets
  Impact phenonema (e.g. formation of the earth-moon system)
  Impact of "planetesimals" to form earth core

★ Intermediate pressures (1-5 Mbars)

Fusion point in compressed iron (T~ 6000° K at P~3.3 Mbar)

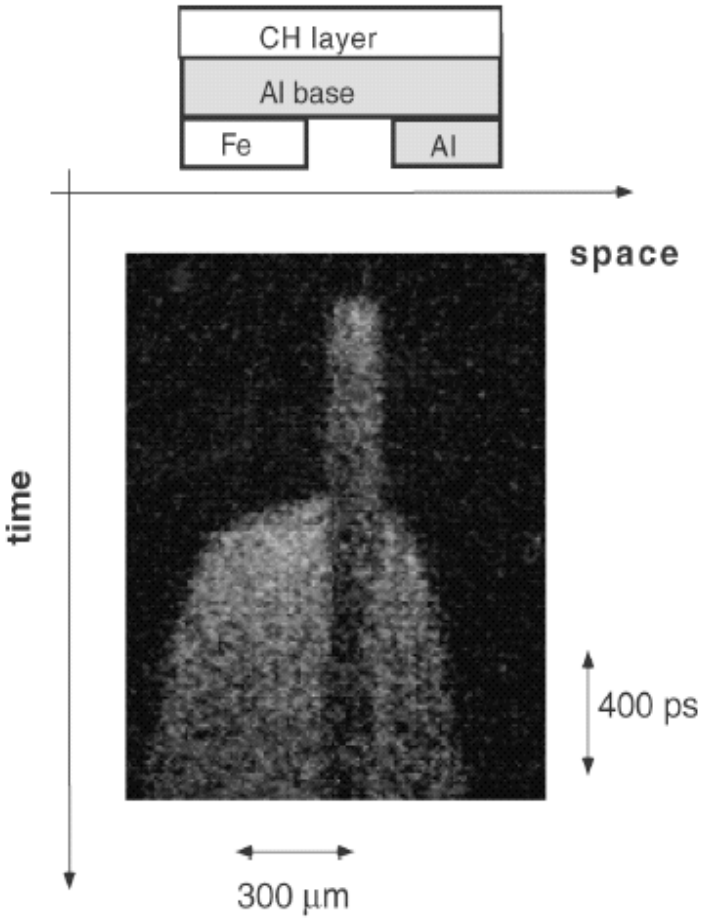
Important issue for terrestrial planets (earth)
Occurs between outer core (liquid) and inner core (solid)

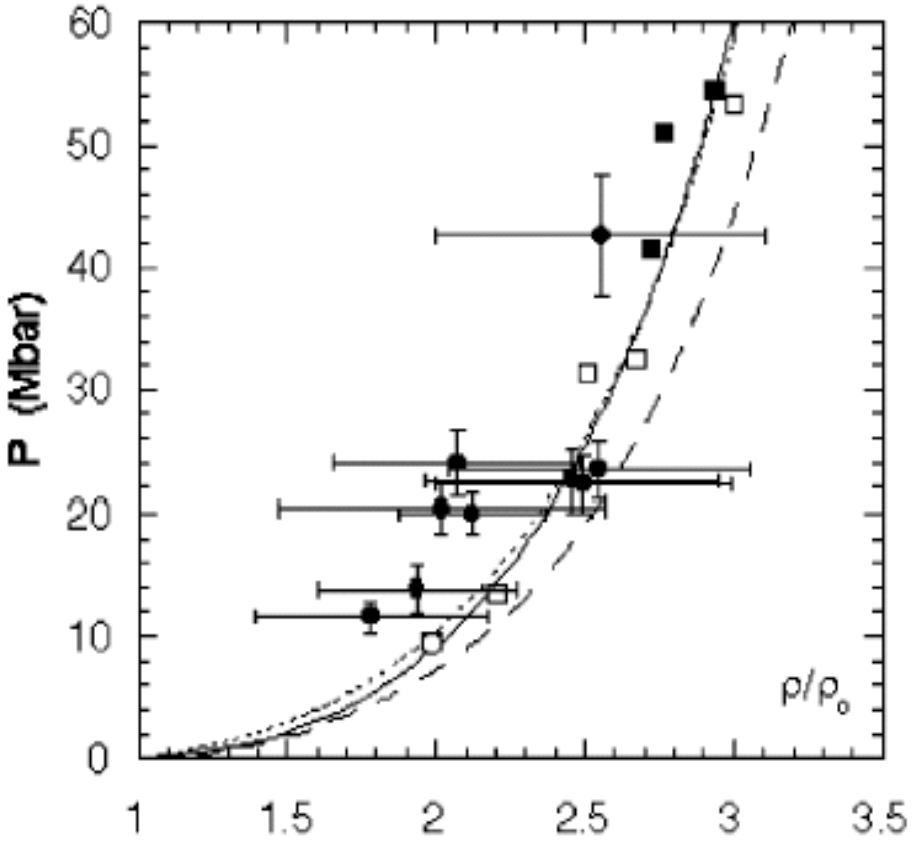
Brown and McQueen, *J. Geophys Res.* **91**, 7485 (1986)
Anderson & Ahrens, *J. Geophys Res.* **99**, 4273 (1994)

Relative EOS measurements for Iron

P > 10 Mbar

EXP ON PHEBUS LASER





D. Batani, A. Morelli, et al. "Equation of State Data for Iron at Pressures beyond 10 Mbar" Vol. 88, N. 23 PHYSICAL REVIEW LETTERS, 10 JUNE 2002

QEOS model, continuous line; the SESAME tables,dashed line and the empirical fit given by Trunin, dotted line. Experimental points correspond to the present work black circles; Altshuler, white squares; Krupnikov, white circles; and Trunin, black squares. Not shown apoint by Trunin at 104.8 Mbar.

How to measure temperature?

=> Pyrometric Measurements

Need for absolute calibration of diagnostics

- **Brightenss temperature**

  Stefan Boltzman's law $\approx \sigma T^4$

- **Emissivity temperature**

  Emission at a given wavelenghth λ

  Need for relative calibration

- **Spectral temperature**

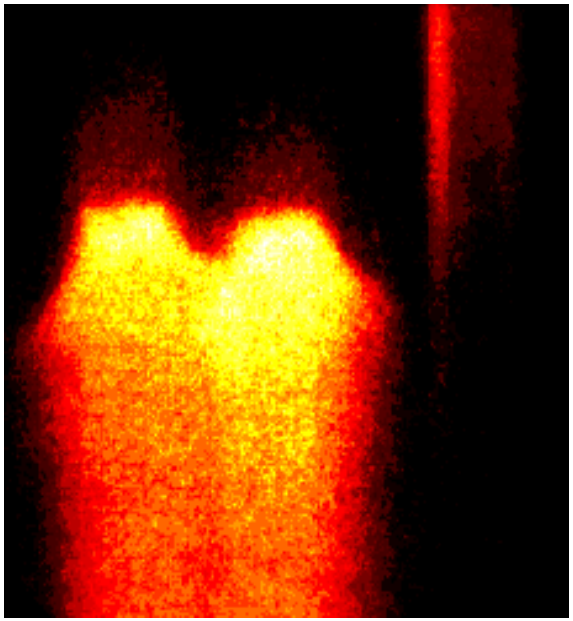
  Fit to a blackbody spectrum

- **Color temperature**

  Emission ratio of in two channels I_b / I_r

TARGET
--> 12 µm Al coated with
1000 ÅAu on laser side

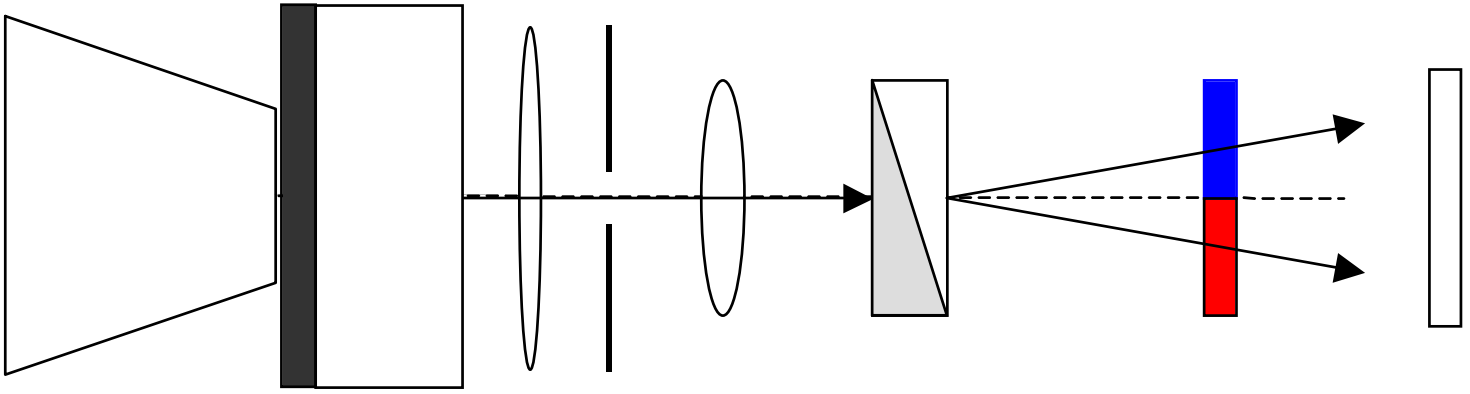
I - 6 10^{13} W/cm^2



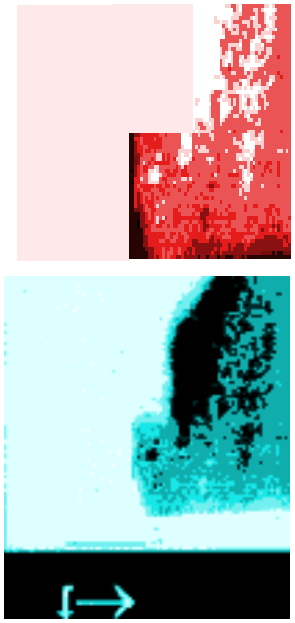
T.Hall, A.Benuzzi, D.Batani, D.Beretta, S.Bossi, B.Faral, M.Koenig, J.Krishnan, M.Mahdieh, Th.Lower "Colour temperature measurement in laser driven shock waves" **Physical Review E**, 55, R6356 (1997).

D.Batani, A.Benuzzi, M.Koenig, I.Krasyuk, P.Pashinin, A.Semenov, I.Lomonosov, V.Fortov "Problems of measurement of dense plasma heating in laser shock wave compression" **Plasma Physics Controlled Fusion**, 41, 93 (1999).

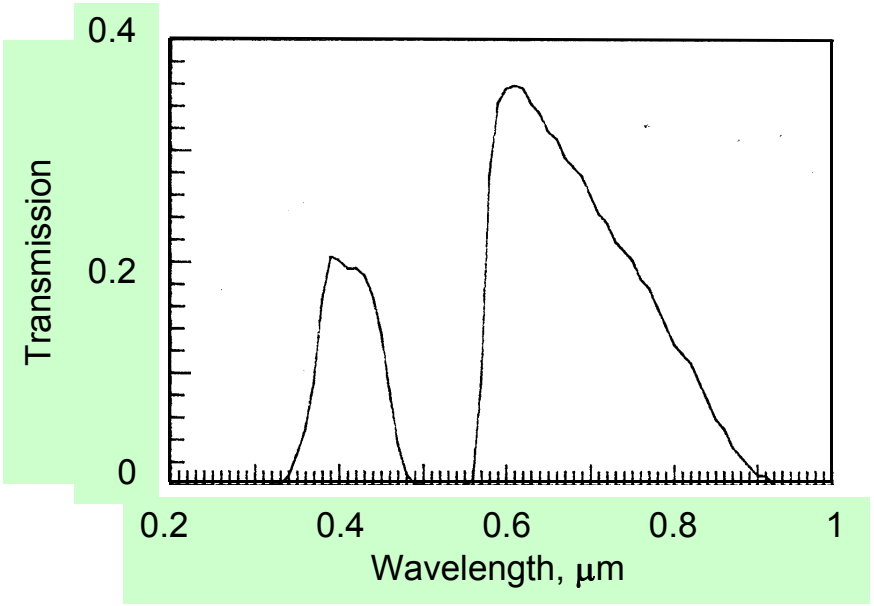
A scheme of the experiment set-up to measure light signals in the “red” and “blue” channels

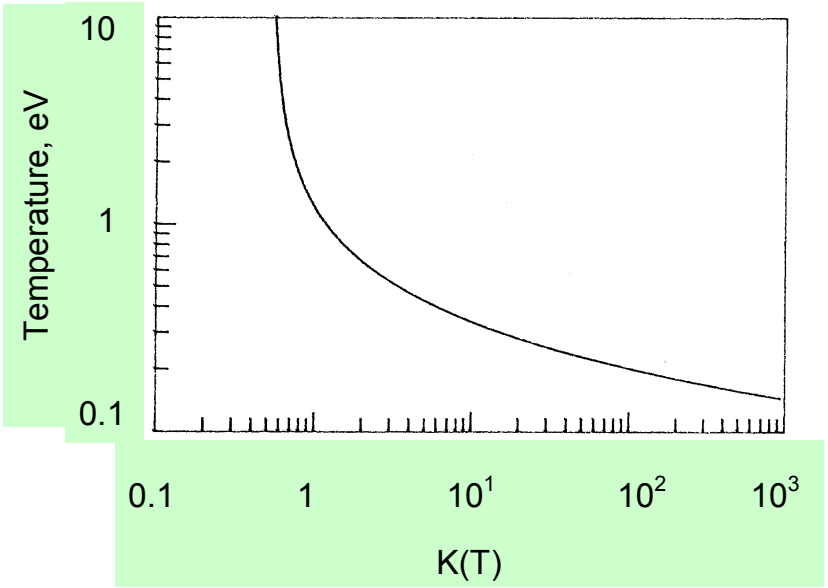


laser beam target glass lenses beam splitter optical filters slit of the streak camera



Characteristics of two-channel pyrometer





- **To the left**: spectral range sensitivity of each channel $g_{blue}(\lambda)$ and $g_{red}(\lambda)$.
- **To the right**: the curve a result of calculation based on relation:

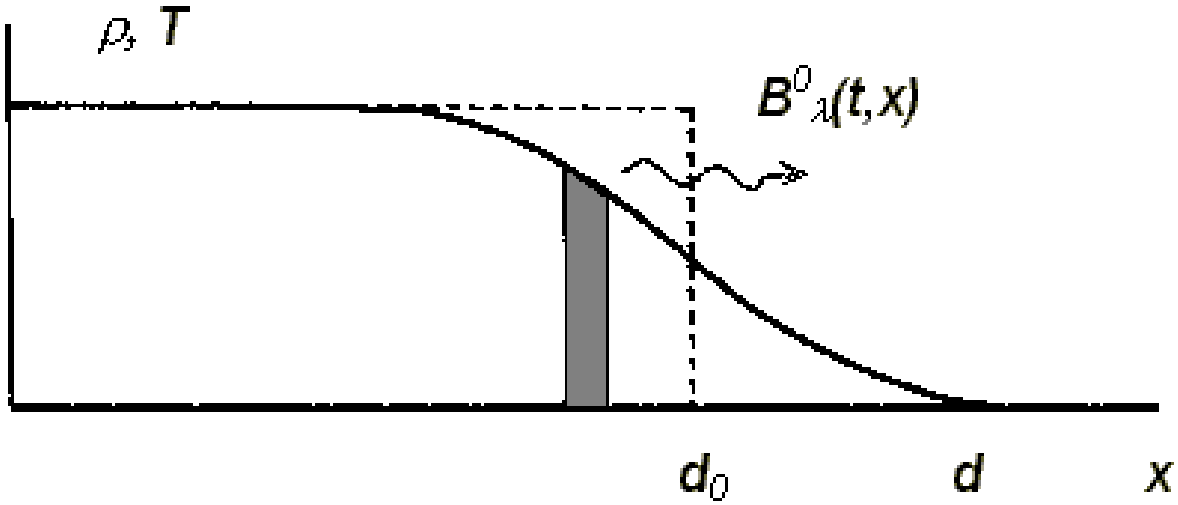
$$\left(\int g_{red} B_\lambda d\lambda\right) / \left(\int g_{blue} B_\lambda d\lambda\right) = \mathbf{K}(\mathbf{T}^*)$$

Problems of optical measurements

- In the case of metals, direct optical measurement of the temperature of matter behind the shock-wave front is complicated by the material released by the rarefaction wave that follows the shock breakout at the solid surface.

- This rarefying material forms a cold optically-thick layer, which screens the luminescence of the high-temperature bulk.

Numerical modeling of light emission with calculation *T* and ρ profiles at consecutive times



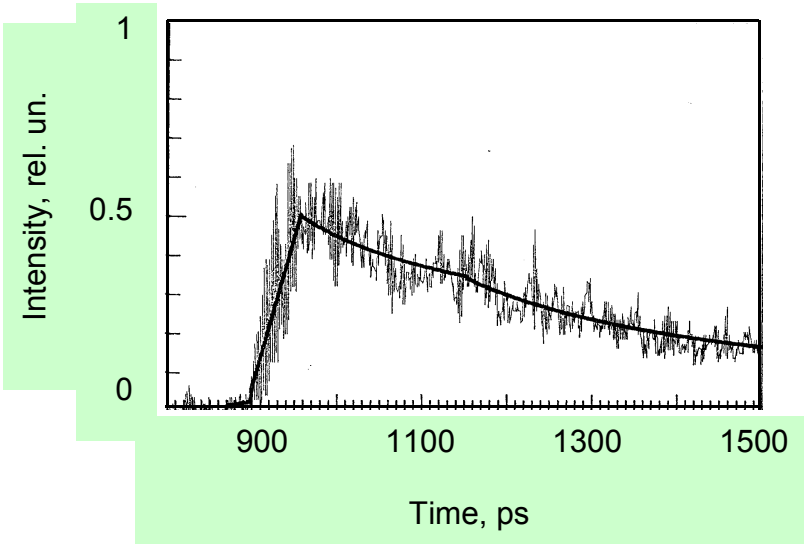
$$B_\lambda = \int_0^d dx\ B_\lambda^0(T(x,t))\tilde{\chi}_\lambda(x,t)\exp(-\int_0^x \tilde{\chi}_\lambda(\xi,t)d\xi)$$

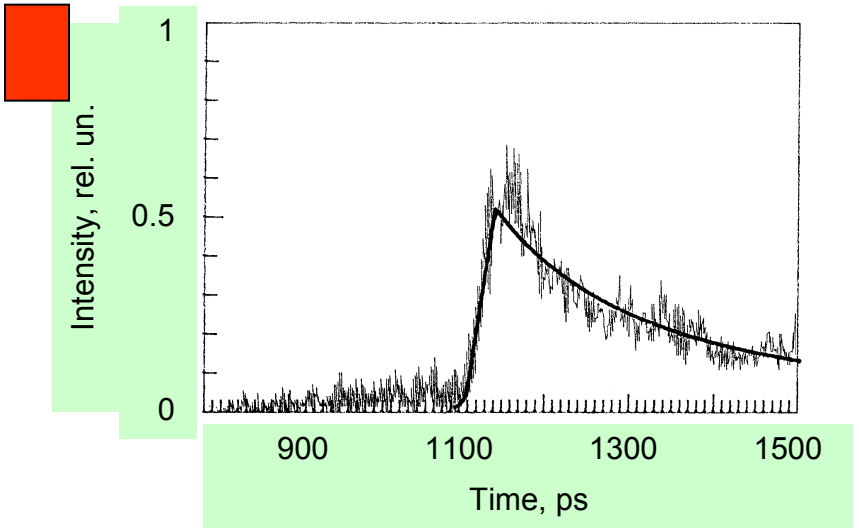
$$B_\lambda^0 = \frac{2hc^2}{\lambda^5}\frac{1}{\exp(hc\ /\ \lambda kT) - 1}$$

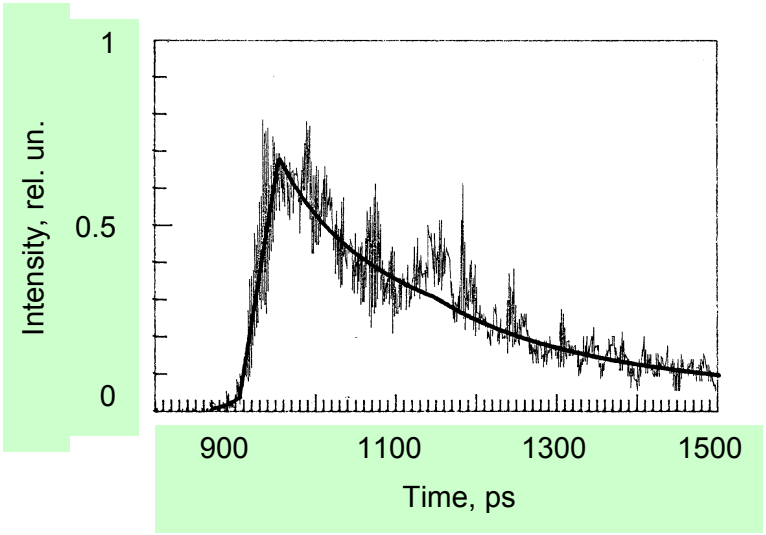
Kramers-Unsold formula for absorption coefficient: $\frac{1}{\chi_\lambda}[\text{мкм}] = \frac{1.2\cdot 10^{-3}}{\lambda^3 \rho T}\exp\left(\frac{5.99 - \frac{1.24}{\lambda}}{T}\right)$

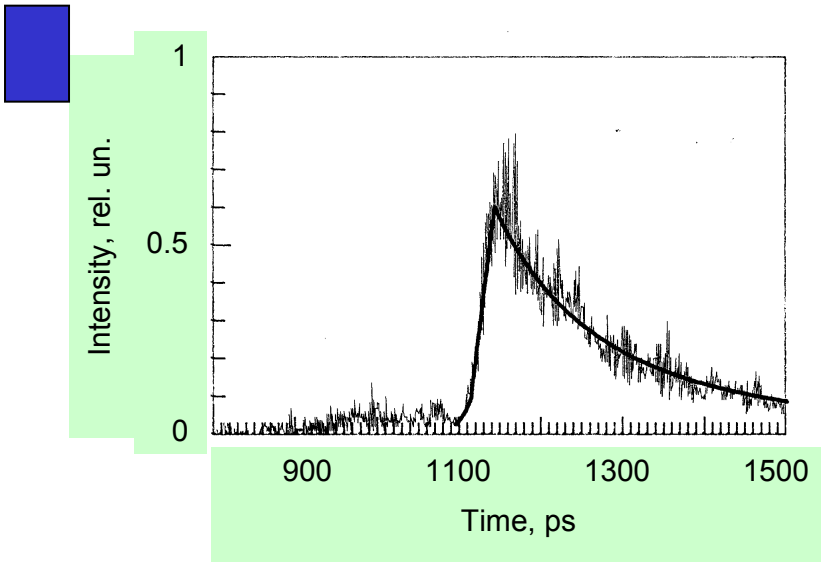
$$(\int g_{red} B_\lambda d\lambda)/(\int g_{blue} B_\lambda d\lambda) = \mathrm{K(T^*)} \neq (\int g_{red} B_\lambda^0 d\lambda)/(\int g_{red} B_\lambda^0 d\lambda)$$

The observed “red” and “blue” emission on a rear side of the target (to the left- base surface; and to the right- step surface)

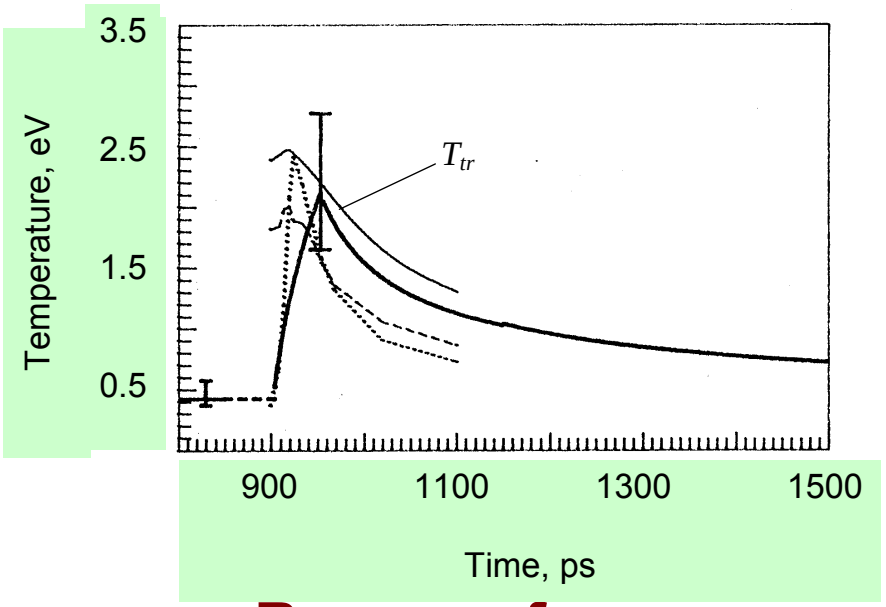




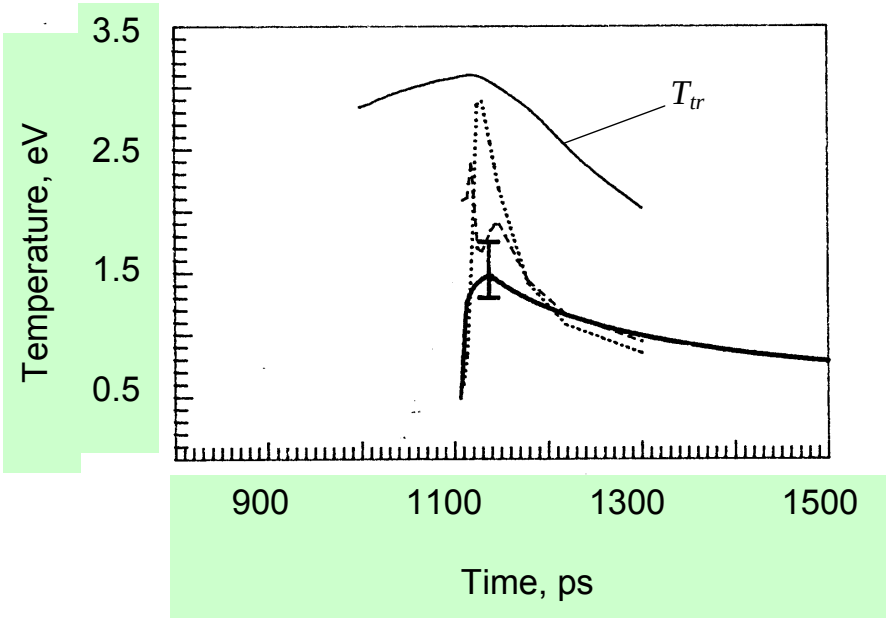




The measured and calculated temporal evolution of the temperature



Base surface



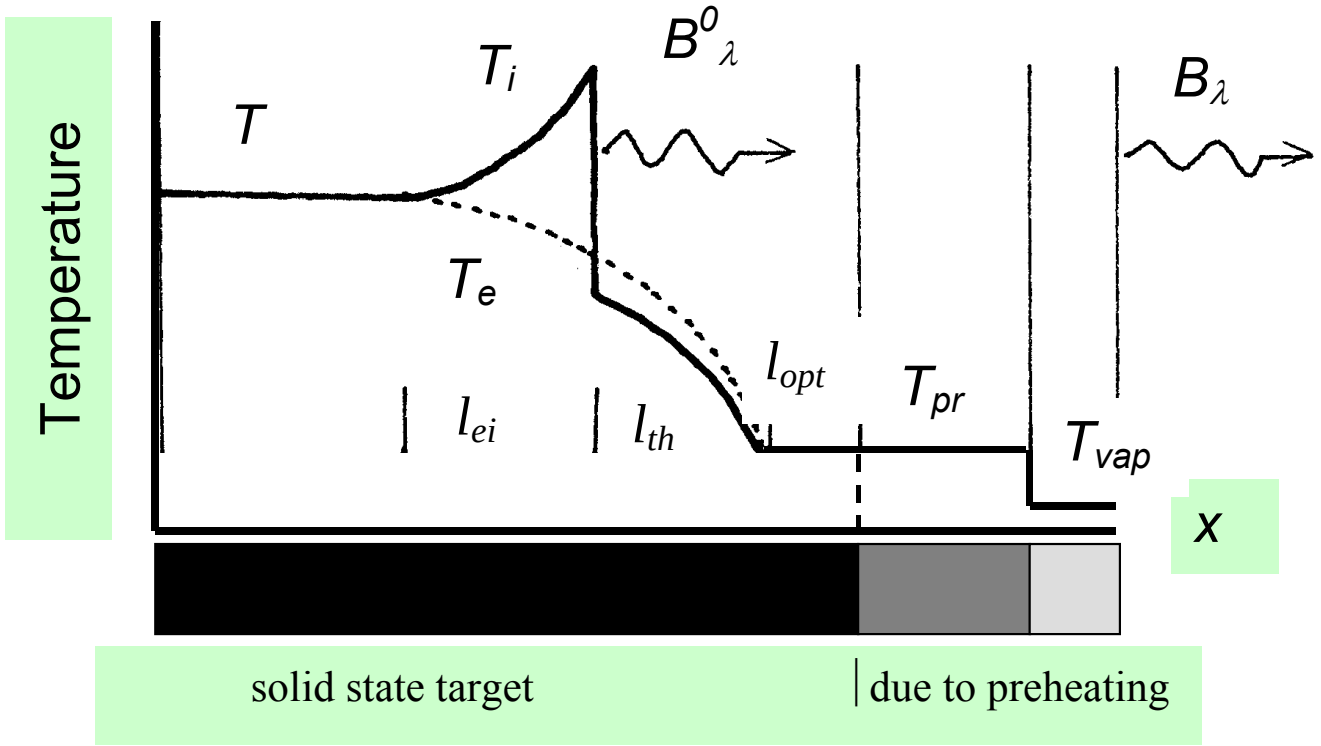
Step surface

- Solid thick line – Experimental results
- Solid slim line – Temperature from hydro simulations
- Dotted line – Semiempirical model for the opacity calculation
- Dash line – Kramers-Unsold formula for the opacity calculation

(Preheating temperature 0.45 eV)

Schemes of shock-wave front structure

(target is in case of preheating)



T_i and T_e ion and electron temperatures

T_{pr}- preheating temperature

T_{vap} – evaporated matter temperature

$l_{ei} = t_{ei}D$ – e-i relaxation zone,

l_{th} – electron thermal conductivity zone,

l_{opt} – optical depth

Rise time of optical signal in case of cold and preheated metal target

On base of structure of the shock-wave front* in aluminum cold target, estimation shows that the rise time of optical signals which equal to $(l_{ei} + l_{th} + l_{opt})/D$ does not exceed **1 ps**.

Experimental value of rise time of optical signals on base surface is **52.5 ps**.

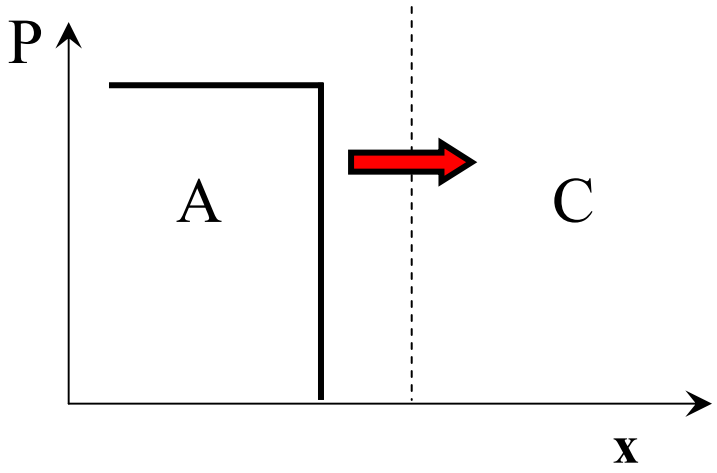
According to the numerical calculations made for the case of target preheating (0.45 eV) the total rise time of optical signals is estimated at **50 ps**.

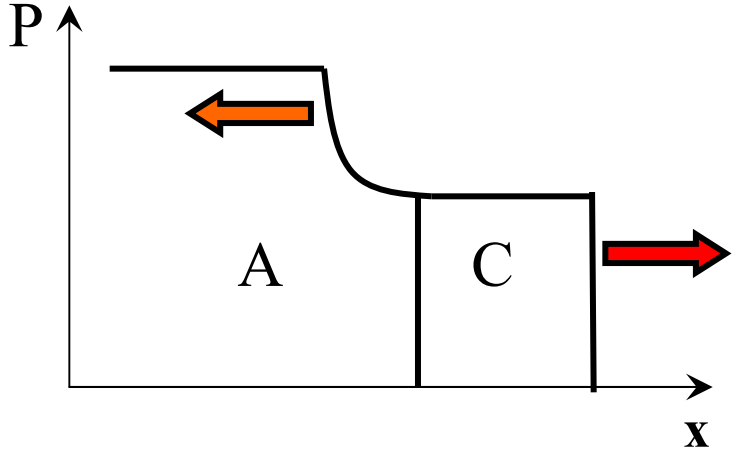
* Ya.B. Zel'dovich and Yu.P. Raizer. 1967 *Physics of Shock Waves and High Temperature Hydrodynamic Phenomena* (Academic Press, New York).

Another approach to EOS: studying the release of materials

- **The presence of a second (transparent) layer behind the shocked material avoids vaporization. Release is limited to a pressure determined by impedance mismatch conditions**
- **This allows maintaining the pressure and the density of the material under study.**
- **When the shock reaches the second material (of lower density) an unloading wave is reflected back in the first material while a shock wave travels in the transparent material.**
- **On the contrary unloading into vacuum (i.e. to zero pressure) brings to an expansion and possibly vaporization of the material, which is no longer characterized by a single value of density and temperature.**

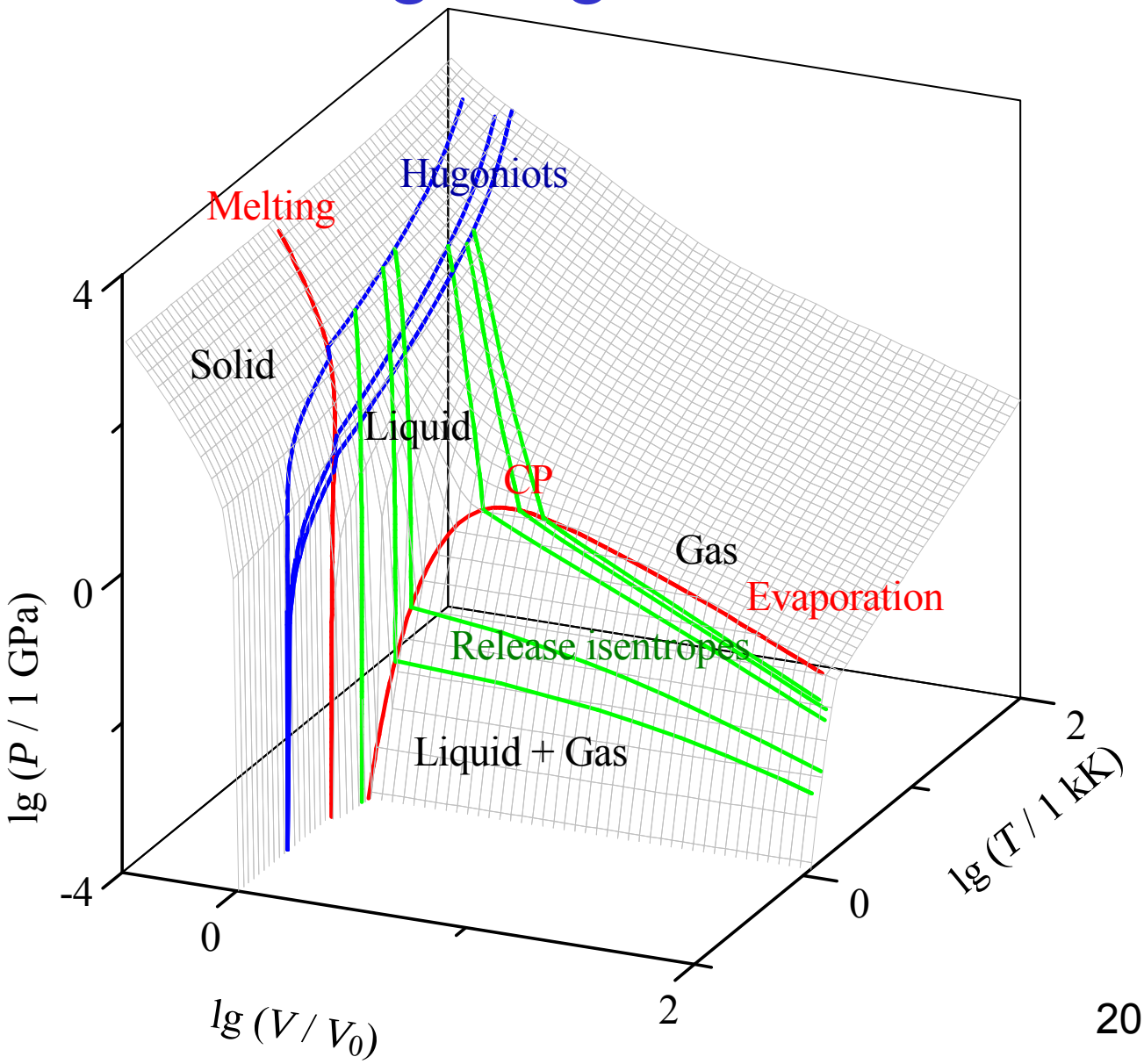
From high density to low density





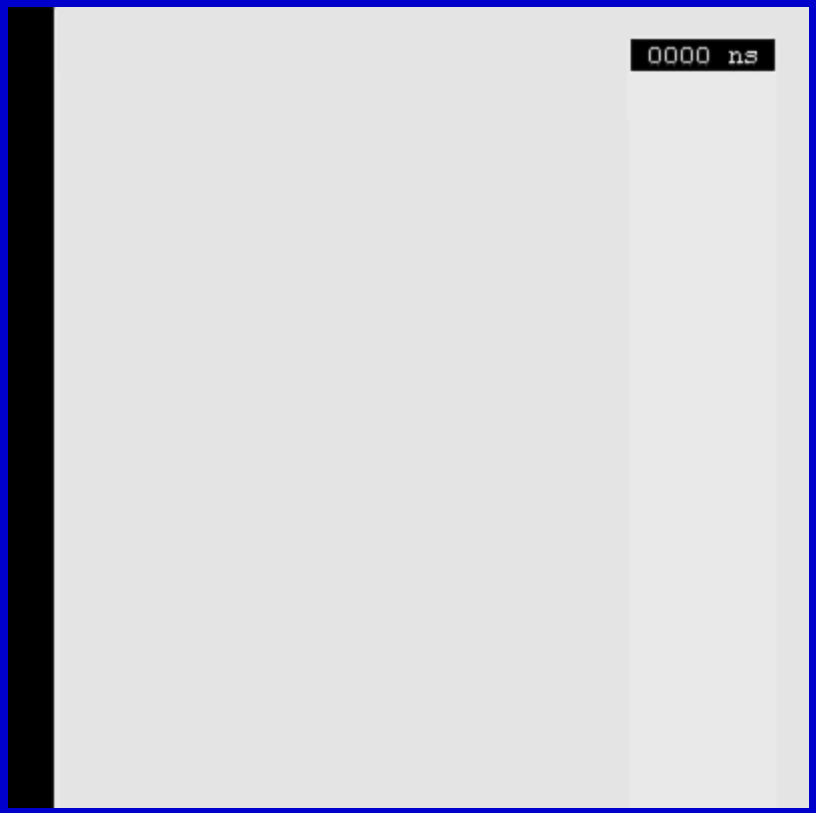
EOS on release of materials is even less known than EOS along Hugoniot

Pressure versus Volume and Temperature for Zinc



Equation of State

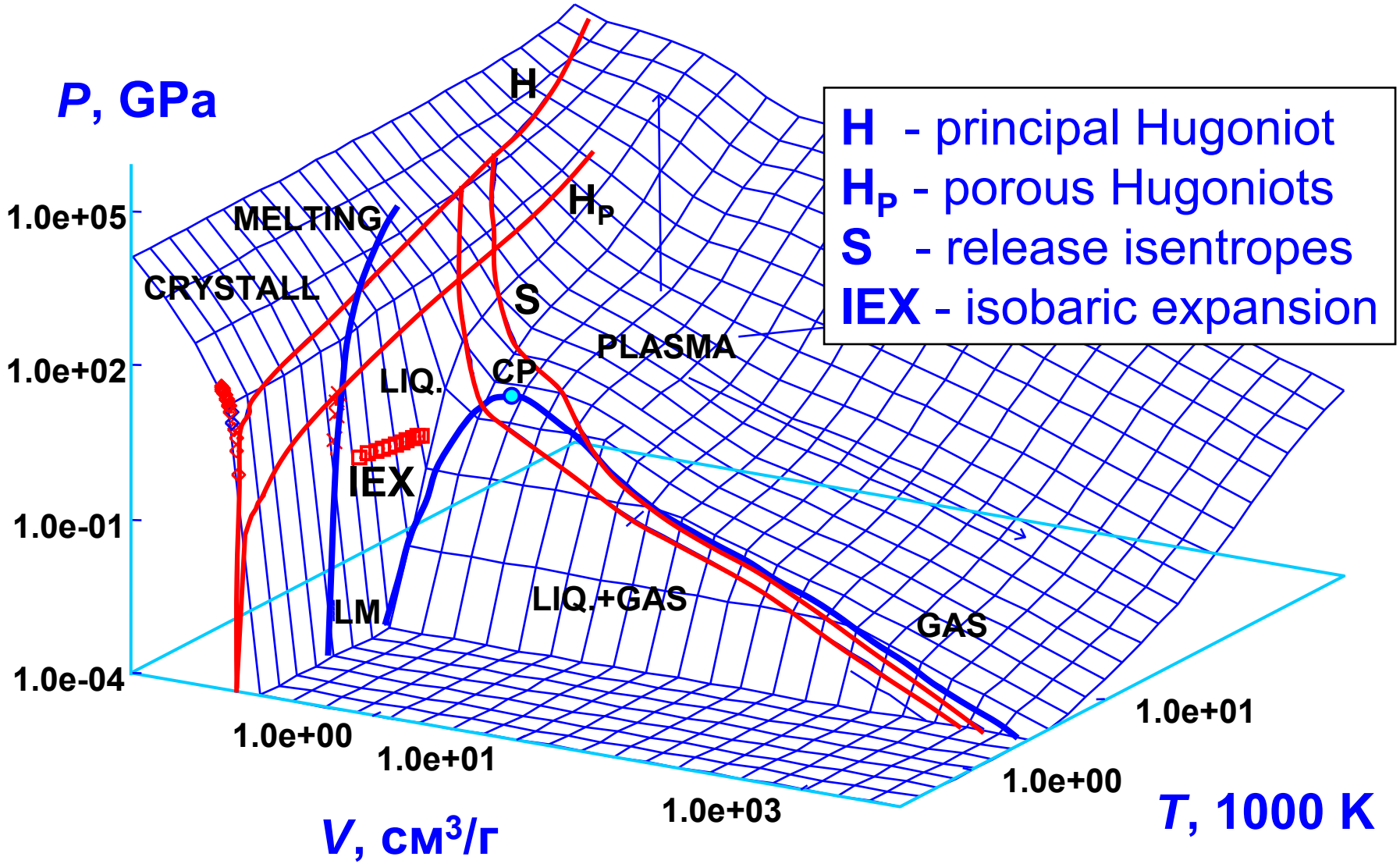
Modeling of Laser-Matter Interaction



Images of the shockwave in the ambient gas (at normal conditions) and the ejected material after irradiation of the aluminum target with pulse parameters:

τ_L = 20 ns,
R = 0.96,
λ_{opt} = 200 nm,
I_L = 5x10^8 W/cm^2,
t_0 = τ_L
r_L = 300 mm

Experimental Data Available at High Energy Densities



Multiphase Equations of State

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Solid phase. Elastic component (EOS at T = 0 K)

at $V < V_{0c}$:

$$F_c(V) = 3V_{0c}\sum_{i=1}^{2}\frac{a_i}{i}\left(\sigma_c^{i/3}-1\right) - 3V_{0c}\sum_{i=1}^{3}\frac{b_i}{i}\left(\sigma_c^{-i/3}-1\right) + b_0 V_{0c}\ln\sigma_c$$

at $V > V_{0c}$:

$$F_c(V) = V_{0c}\left[A\left(\sigma_c^m/m - \sigma_c^n/n\right) + B\left(\sigma_c^l/l - \sigma_c^n/n\right)\right] + E_{sub}$$

at $V = V_{0c}$:

$$F_c(V_{0c}) = F_{0c}$$

$$P_c(V_{0c}) = -dF_c/dV = 0$$

$$B_c(V_{0c}) = -VdP_c/dV = B_{0c}$$

$$B_c'(V_{0c}) = dB_c/dP_c = B_{0c}'$$

$$B_c''(V_{0c}) = -d(V\,dB_c/dV)/dB_c = B_{0c}''$$

$$\sigma_c = V_{0c}/V$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Solid phase. Thermal lattice components

$$F_a(V,T) = F_a^{acst}(V,T) + \sum_{\alpha=1}^{3(\nu-1)} F_{a\alpha}^{opt}(V,T)$$

$$F_a^{acst}(V,T) = \frac{RT}{\nu}\left[3\ln\left(1-e^{-\theta^{acst}/T}\right) - D\left(\theta^{acst}/T\right)\right] - \beta_{acst}\frac{T^2/\theta^{acst}}{e^{\theta^{acst}/T}-1}$$

$$F_{a\alpha}^{opt}(V,T) = \frac{RT}{\nu}\ln\left(1-e^{-\theta_\alpha^{opt}/T}\right) - \beta_{opt\alpha}\frac{T^2/\theta_\alpha^{opt}}{e^{\theta_\alpha^{opt}/T}-1}$$

$$D(x) = \frac{3}{x^3}\int_0^x \frac{t^3 dt}{e^t - 1}$$

$$\frac{\theta^{acst}(V)}{\theta_0^{acst}} = \frac{\theta_\alpha^{opt}(V)}{\theta_{0\alpha}^{opt}} = \sigma^{2/3}\exp\left\{(\gamma_0 - 2/3)\frac{\sigma_n^2 + \ln^2\sigma_m}{\sigma_n}\operatorname{arctg}\left[\frac{\sigma_n \ln\sigma}{\sigma_n^2 - \ln(\sigma/\sigma_m)\ln\sigma_m}\right]\right\}$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Fluid phase. Elastic component (EOS at T = 0 K)

at $V < V_{m0}$:

$$F_c^{(l)}(V) = F_c^{(s)}(V) + 3RT_{m0}\frac{2\sigma_m^2}{1+\sigma_m^3}\left[\frac{3A_m}{5}\left(\sigma_m^{5/3}-1\right)+C_m\right]$$

at $V_{m0} < V < V_{cr}$:

$$F_c^{(l)}(V) = F_c^{(s)}(V) + V_{m0}\sum_{i=1}^{7}\frac{a_{mi}}{\alpha_{mi}}\left(\sigma_m^{\alpha_{mi}}-1\right)+E_{m0}$$

$$\sigma_m = V_{m0}/V$$

at $V_{cr} < V$:

$$F_c^{(l)}(V) = F_c^{(s)}(V) + 3V_{cr}\sigma_v\sum_{i=1}^{3}\frac{b_{mi}}{i}\left(\sigma_v^{i/3}-1\right)$$

$$\sigma_v = V_{cr}/V$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Fluid phase. Thermal atomic components

$$F_a(V,T) = C_a(V,T)T\ln\left(1-e^{-\theta^{liq}/T}\right) + 3RT\,\frac{B_m}{D_m + \left(\theta^{liq}/T\right)^{\alpha_m}}$$

$$C_a(V,T) = \frac{3}{2}R\left[2 - \frac{1}{1+\theta^{liq}/T}\right]$$

$$\theta^{liq}(V,T) = T_{sa}\sigma^{2/3}\left[\theta_l(V) + \frac{1-\theta_l(V)}{1+\sqrt{T_{ca}\sigma_m^{2/3}/T}}\right]$$

$$\frac{\theta_l(V)}{\theta_{0l}} = \exp\left\{(\gamma_{0l} - 2/3)\frac{B_l^2 + D_l^2}{B_l}\,\mathrm{arctg}\left(\frac{B_l\ln\sigma}{B_l^2 + D_l(\ln\sigma + D_l)}\right)\right\}$$

Equation of State Model

General form

$$F(V,T) = F_c(V) + F_a(V,T) + F_e(V,T)$$

Thermal electron component is from Ref. [A. V. Bushman, V. E. Fortov, G. I. Kanel', A. L. Ni, *Intense Dynamic Loading of Condensed Matter* (Taylor & Francis, Washington, 1993).]

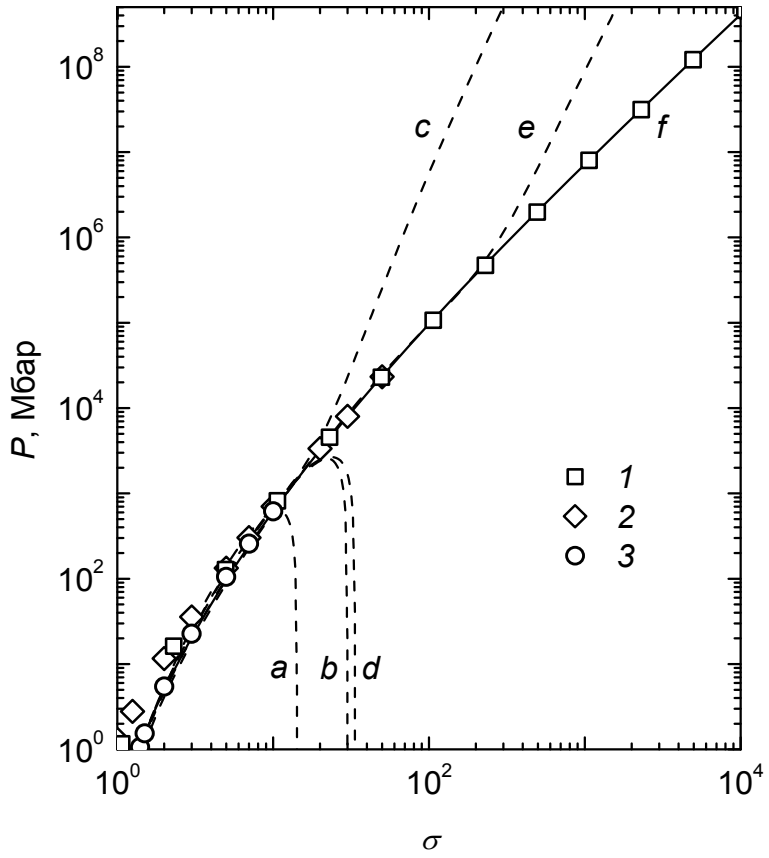
$$F_e(V,T) = -C_e(V,T)T\ln\left\{1 + \frac{B_e(T)T}{2C_{ei}}\sigma^{-\gamma_e(V,T)}\right\}$$

$$C_e(V,T) = \frac{3R}{2}\left\{Z + \frac{\sigma_z T_z^2(1-Z)}{(\sigma+\sigma_z)(T^2+T_z^2)}\right\}\exp(-\tau_i(V)/T) \qquad C_{ei} = \frac{3RZ}{2}$$

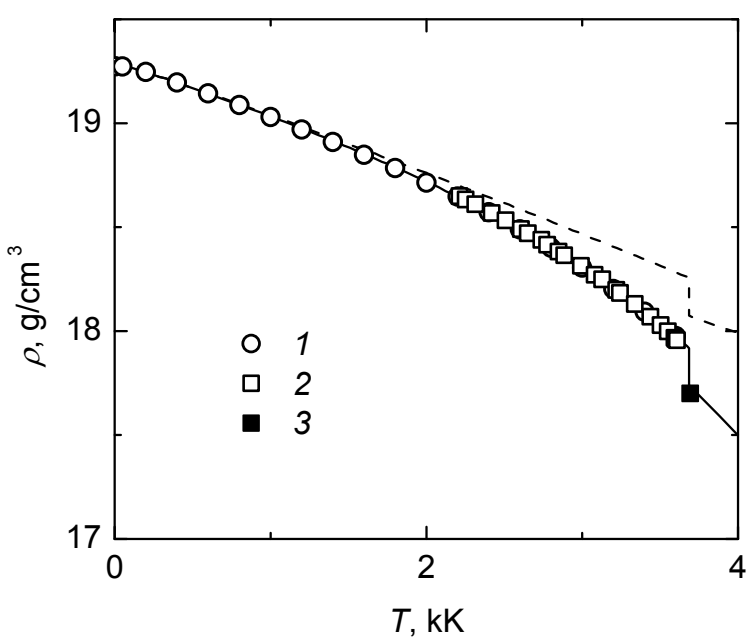
$$B_e(T) = \frac{2}{T^2}\int_0^T\int \beta(\tau)d\tau dT \qquad \beta(T) = \beta_i + (\beta_0 - \beta_i + \beta_m T/T_b)\exp(-T/T_b)$$

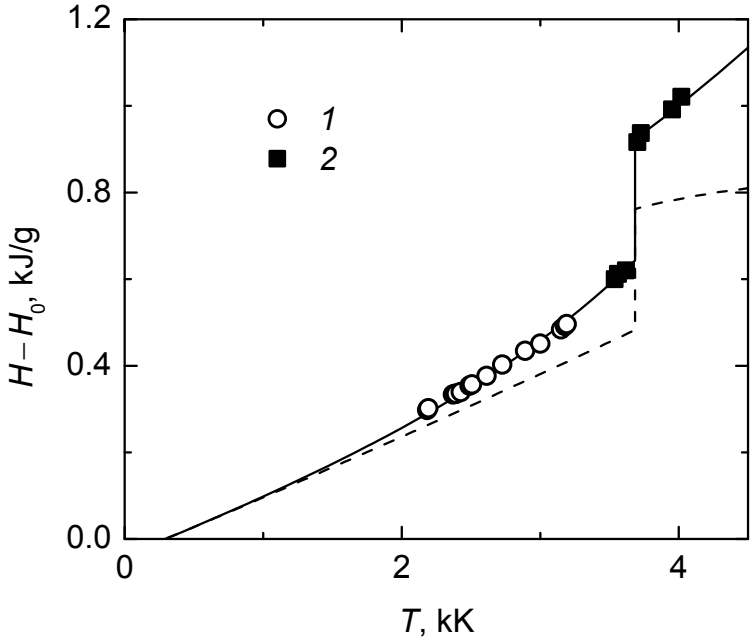
$$\tau_i(V) = T_i\exp(-\sigma_i/\sigma) \qquad \gamma_e(V,T) = \gamma_{ei} + (\gamma_{e0} - \gamma_{ei} + \gamma_m T/T_g)\exp(-T/T_g)$$

Copper at T = 0 K

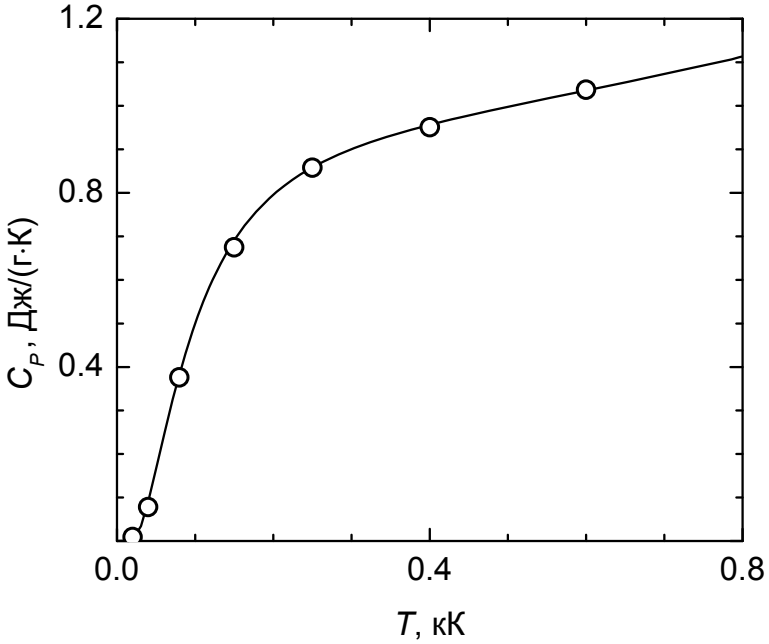


Tungsten at P = 1 bar

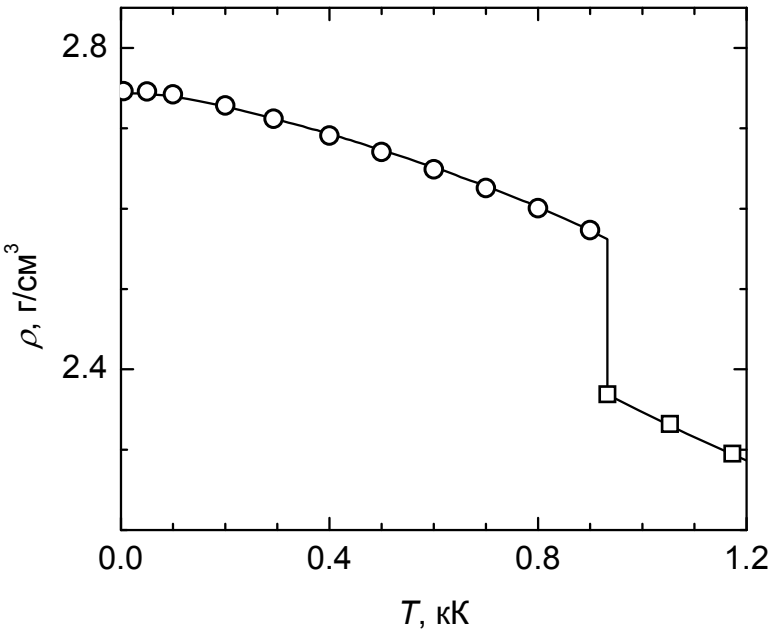




Aluminum at P = 1 bar

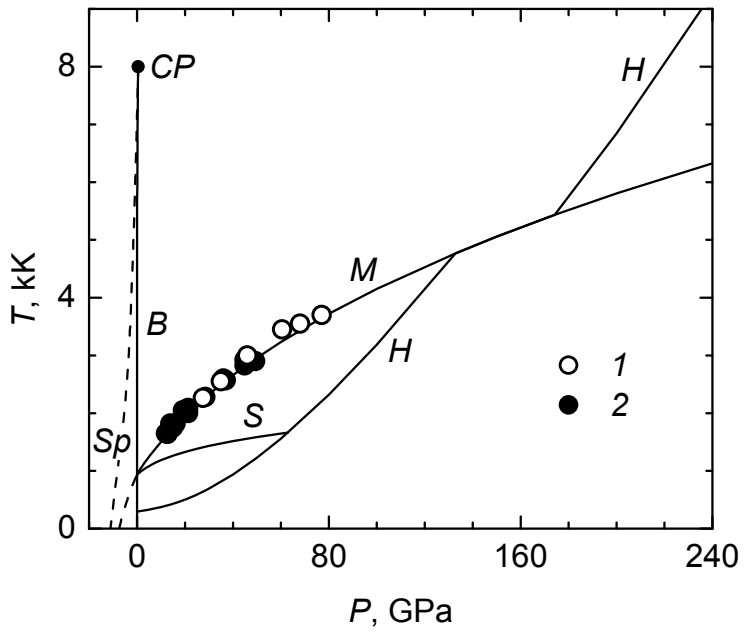


Specific heat capacity of the solid phase under normal pressure

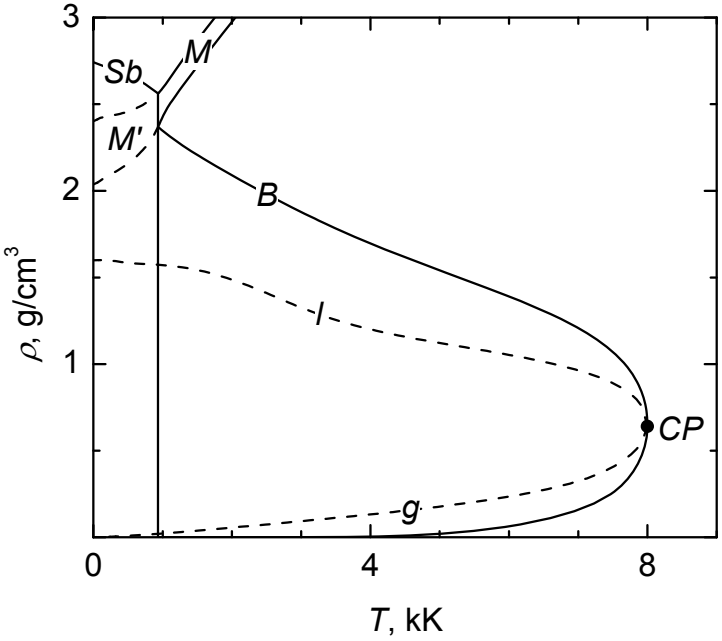


Thermal expansion of the solid and liquid phases

Aluminum Phase Diagram

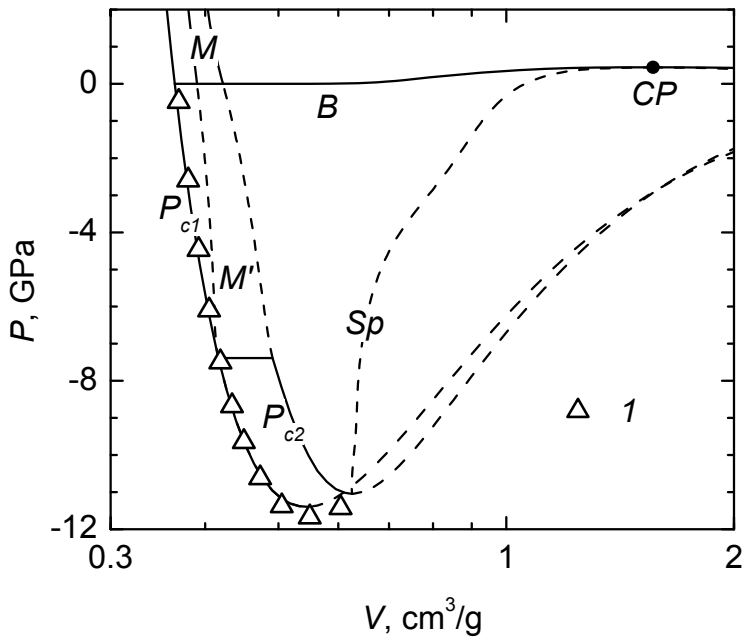


1 - Boehler & Ross 1997
2 - Hanstrom & Lazor 2000

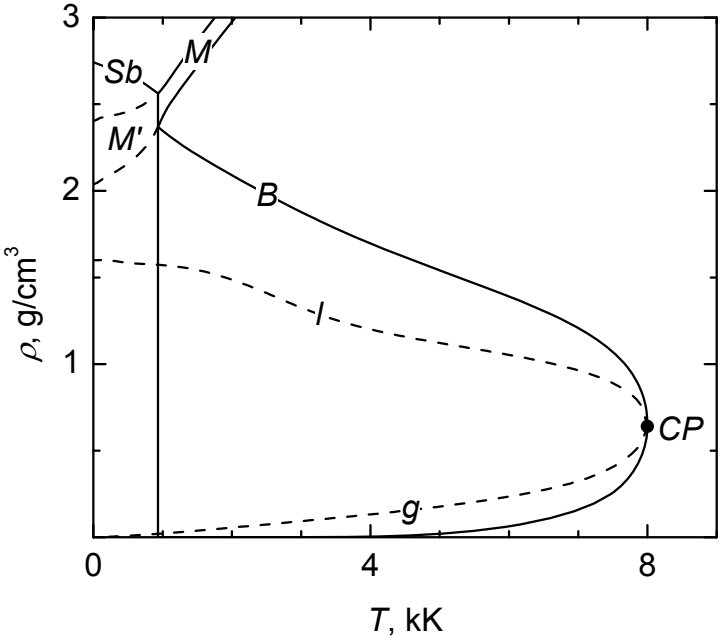


Density-Temperature Diagram

Aluminum Phase Diagram



1 - Sinko & Smirnov 2002

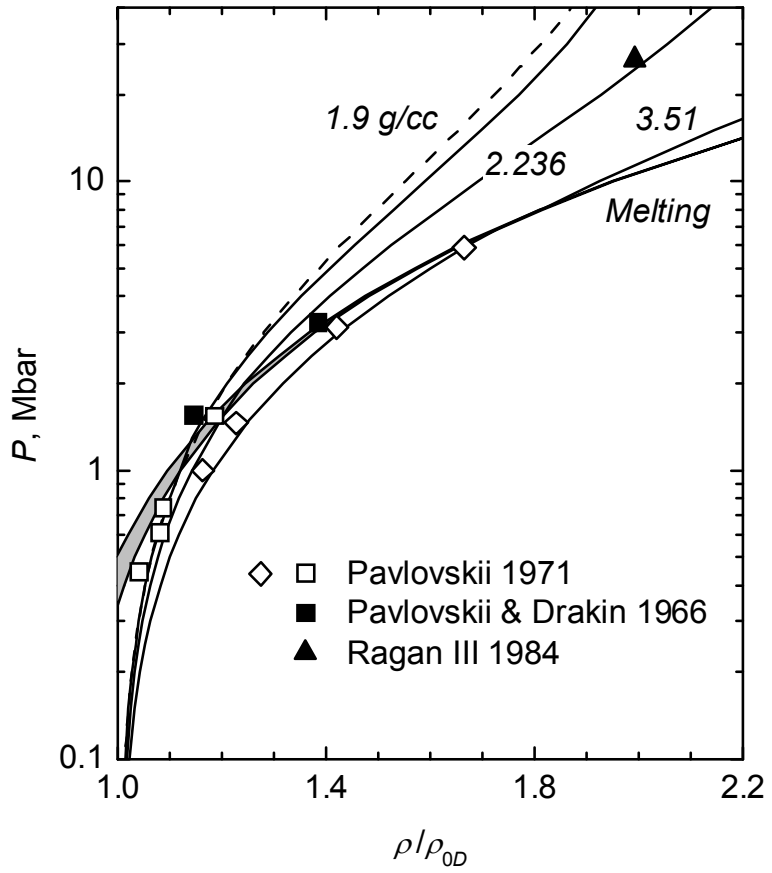


Density-Temperature Diagram

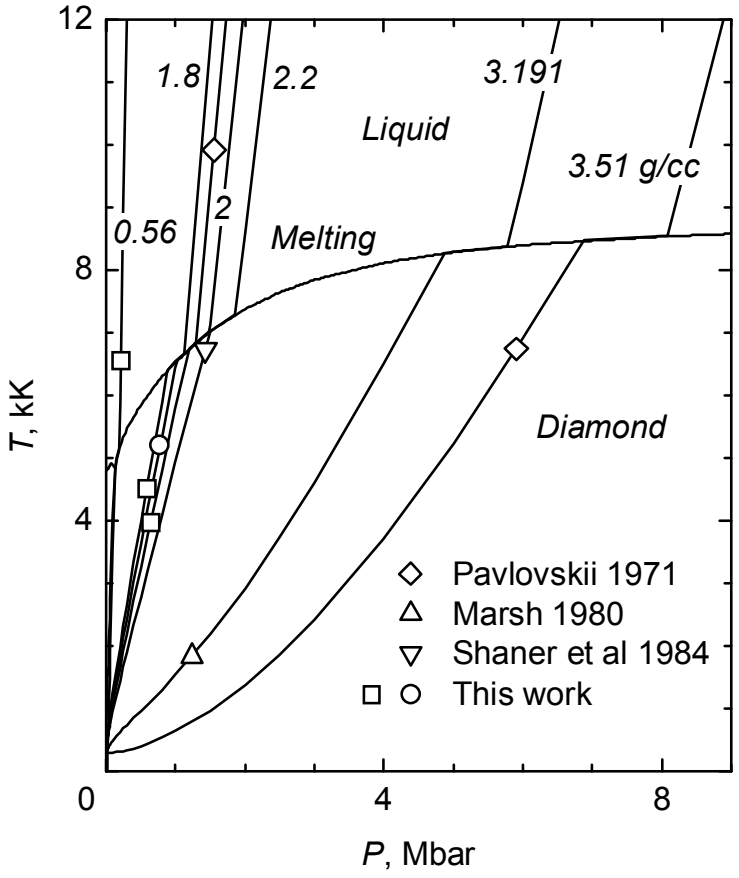
Critical point (CP) parameters are from Ref. [V. E. Fortov, A. N. Dremin, A. A. Leont'ev, *Teplofiz. Vys. Temp.* **13**(5), 1072 (1975)]

Equation of State for Carbon

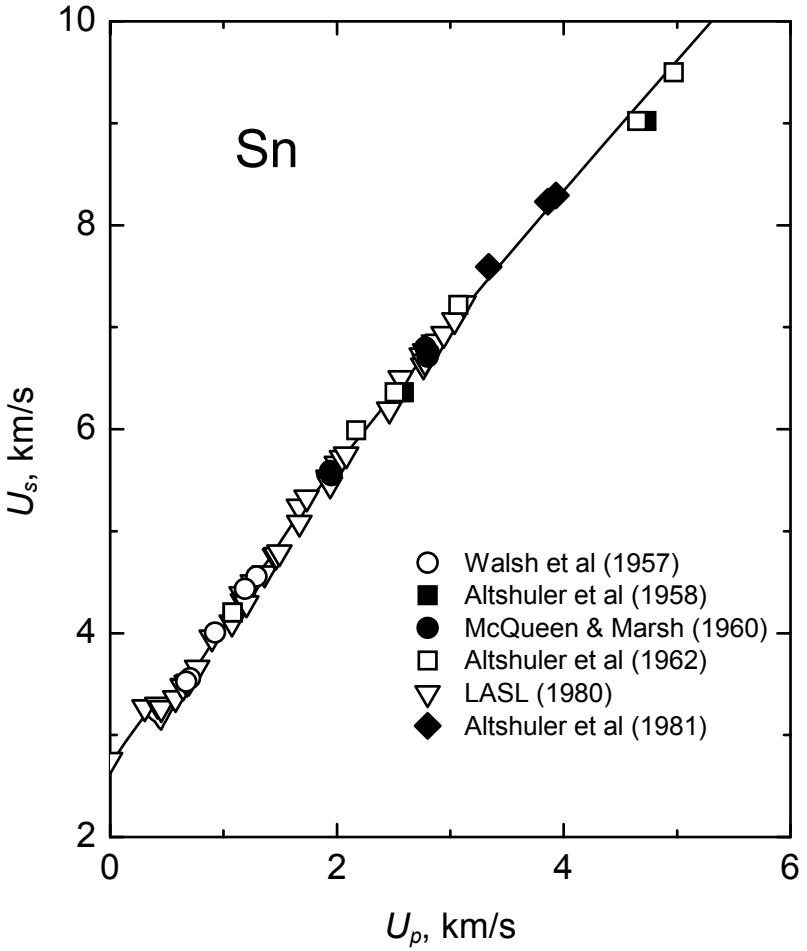
Shock Hugoniots of Diamond



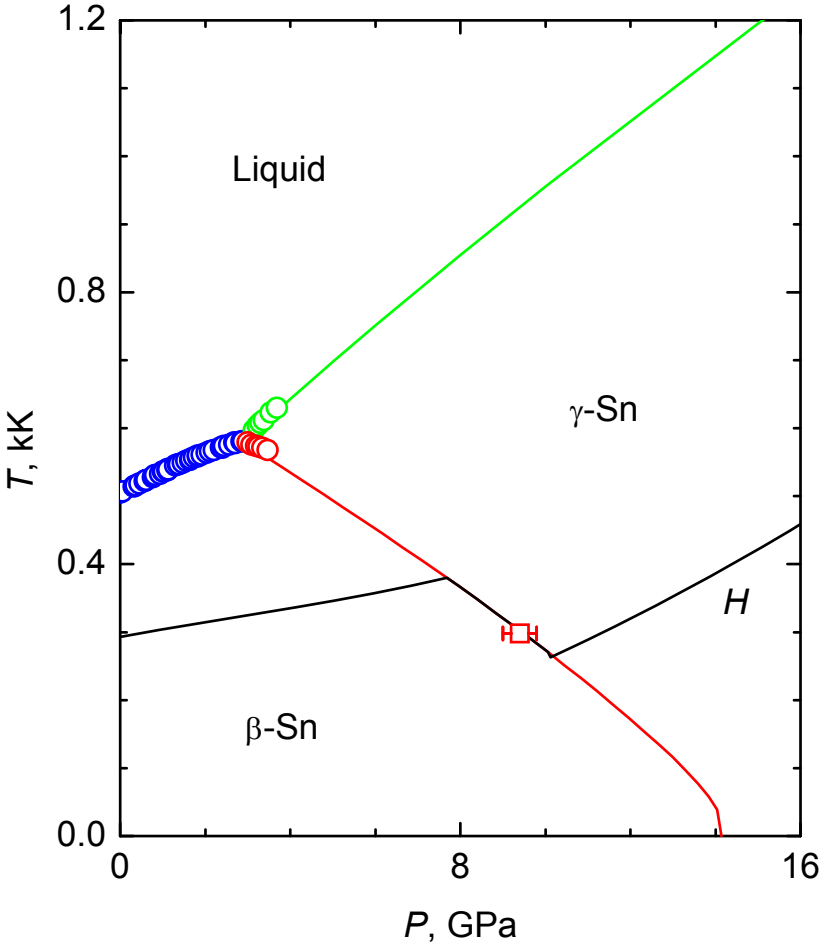
Carbon Phase Diagram

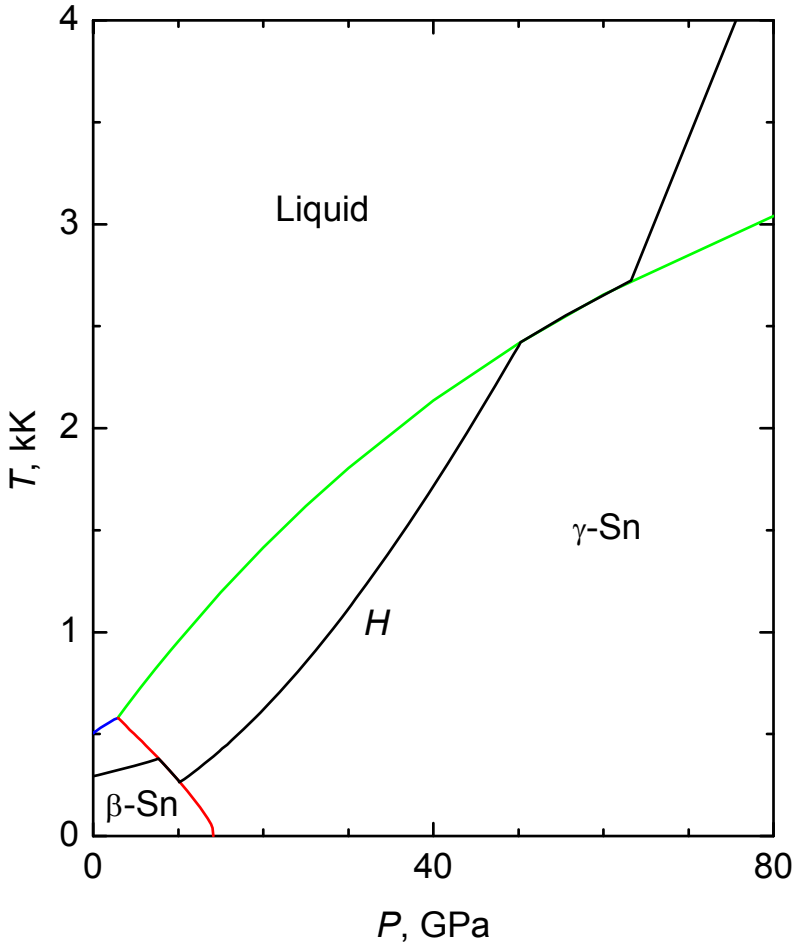


Hugoniot of Tin

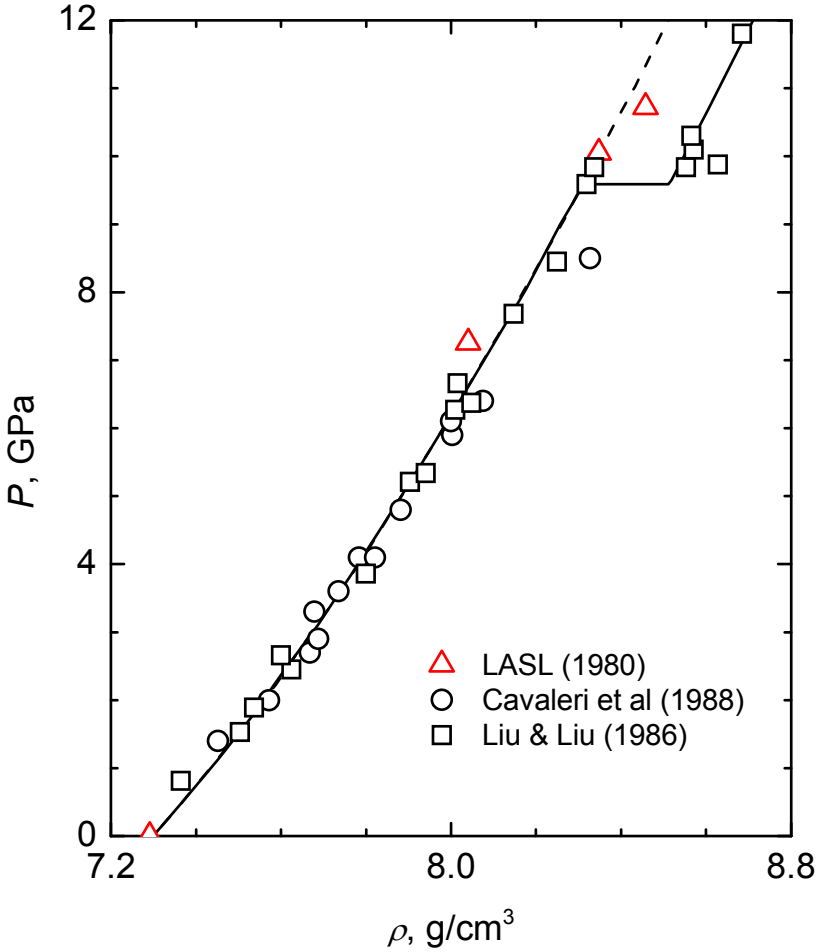


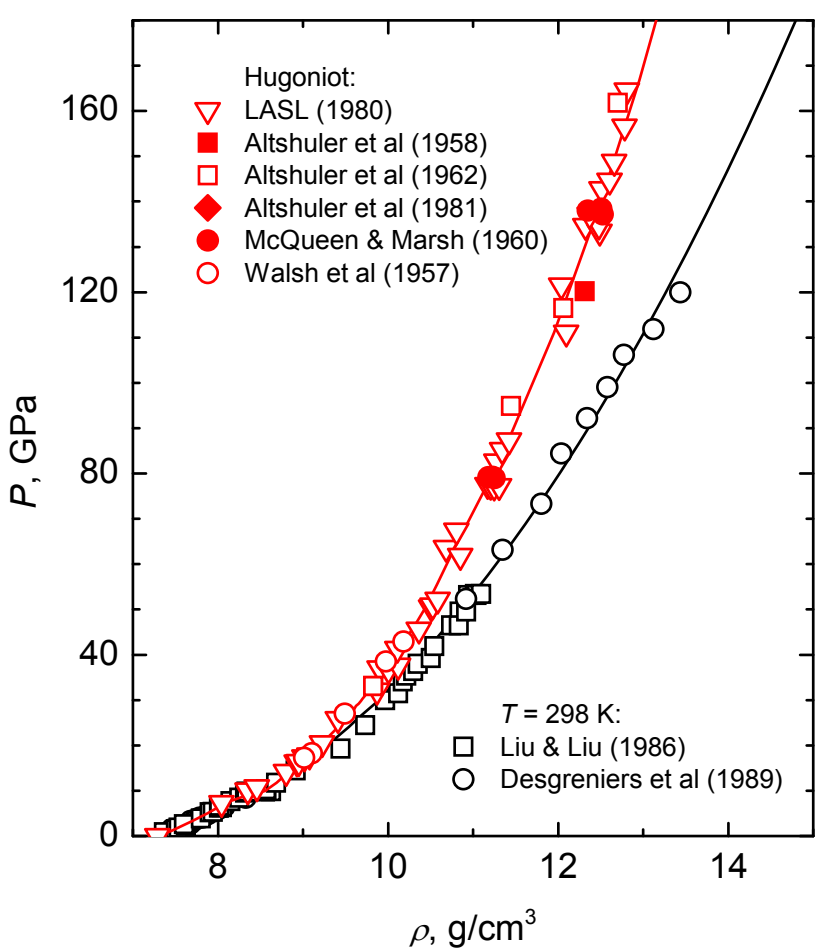
Phase Diagram of Tin



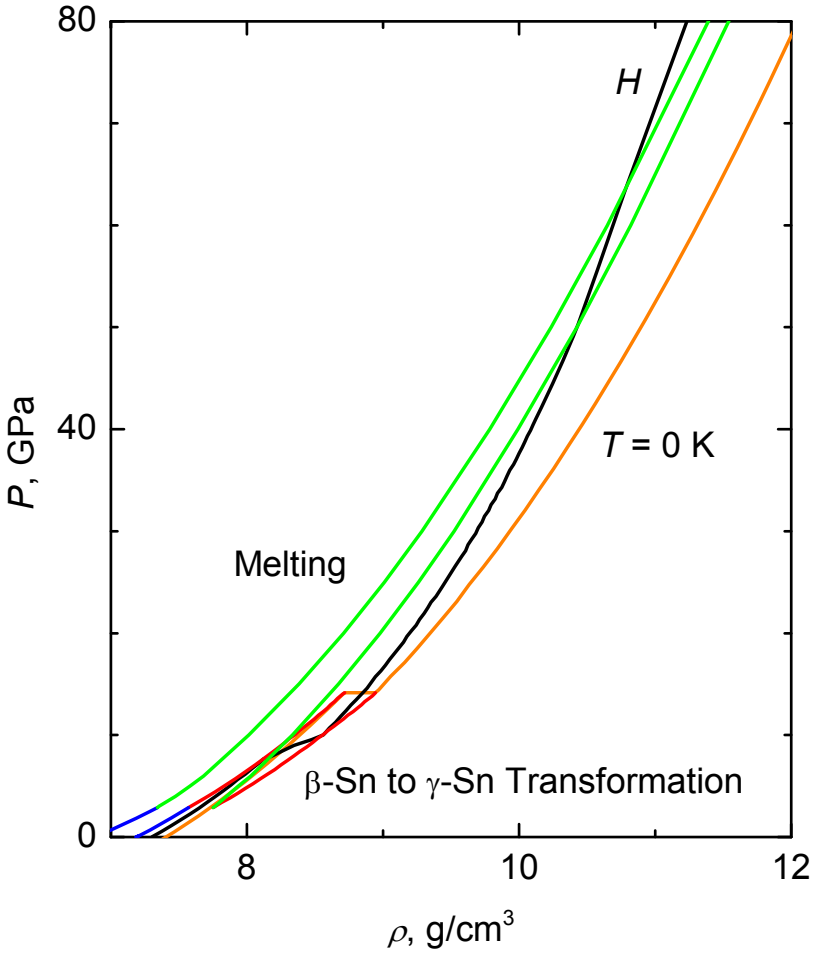


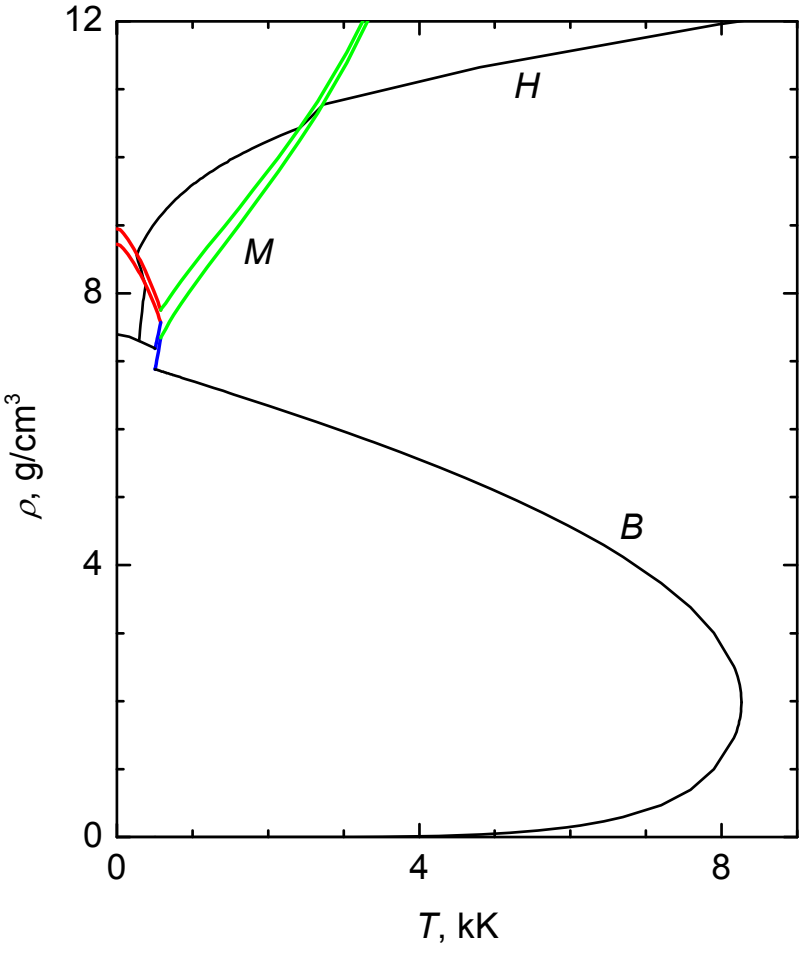
T = 298 K & Hugoniot of Tin



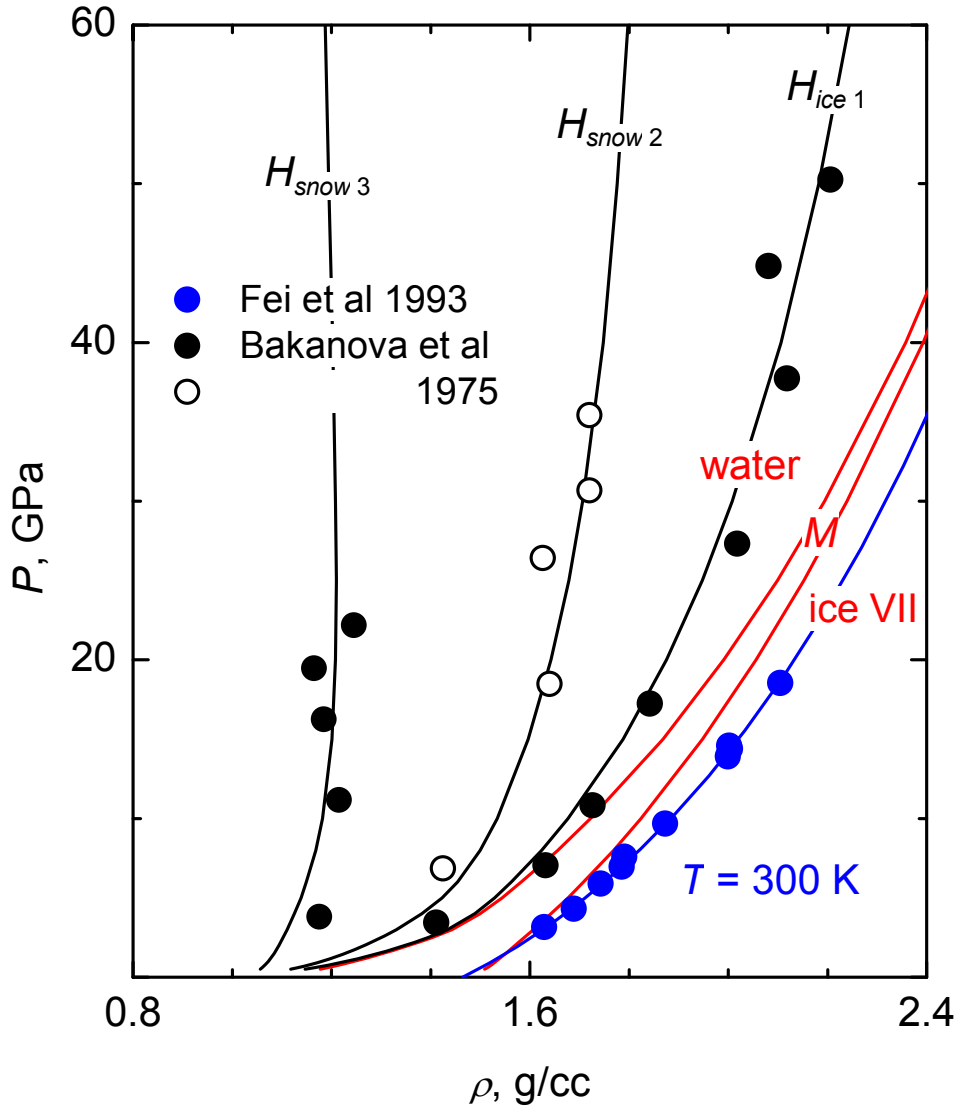


Phase Diagram of Tin



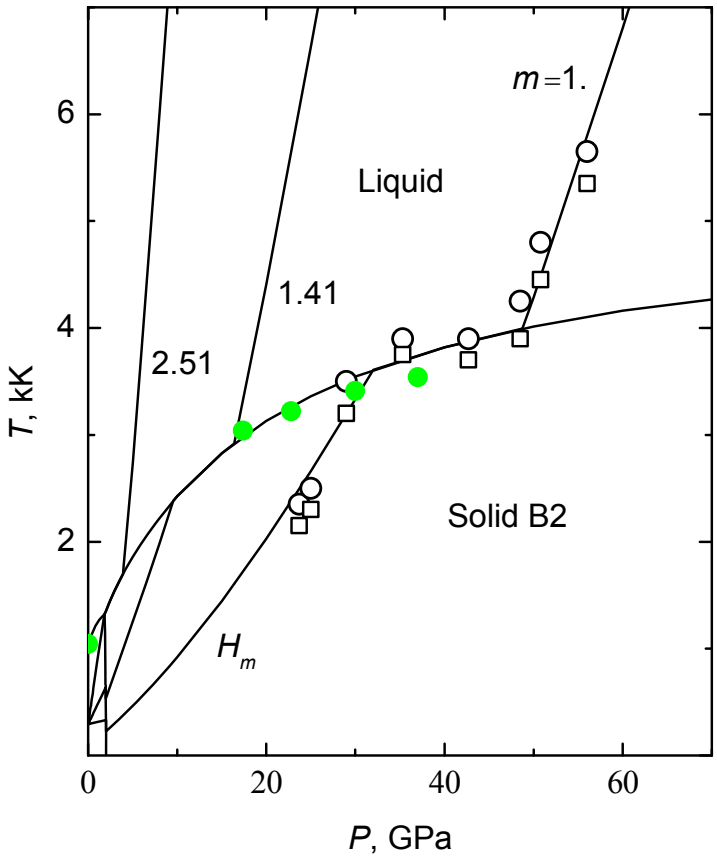


Water Diagram of States

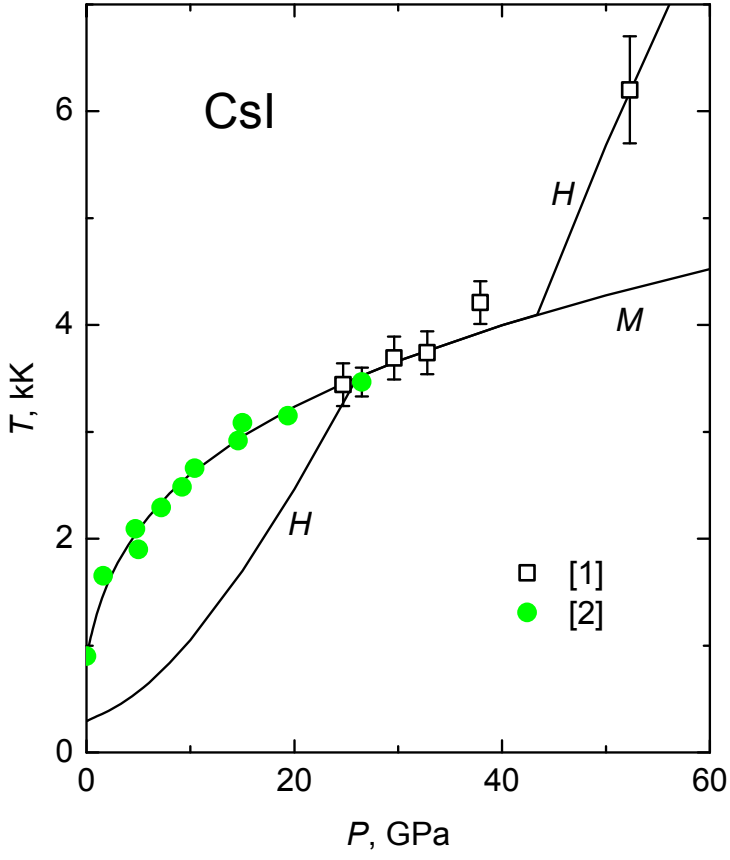


Phase Diagrams of KCl and CsI

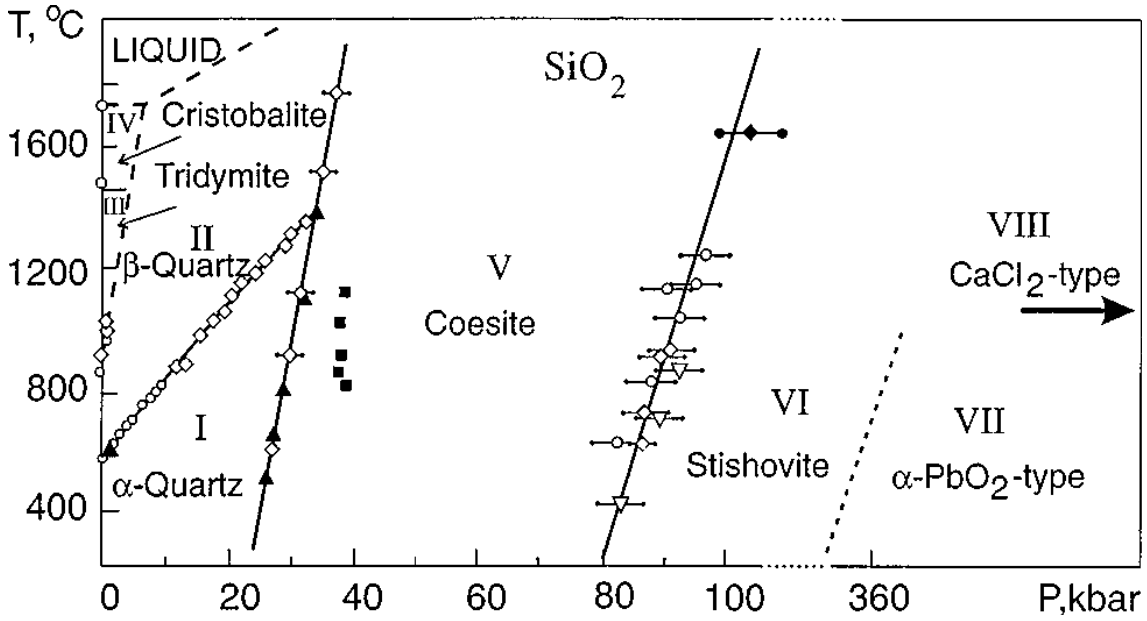
KCL



CsI

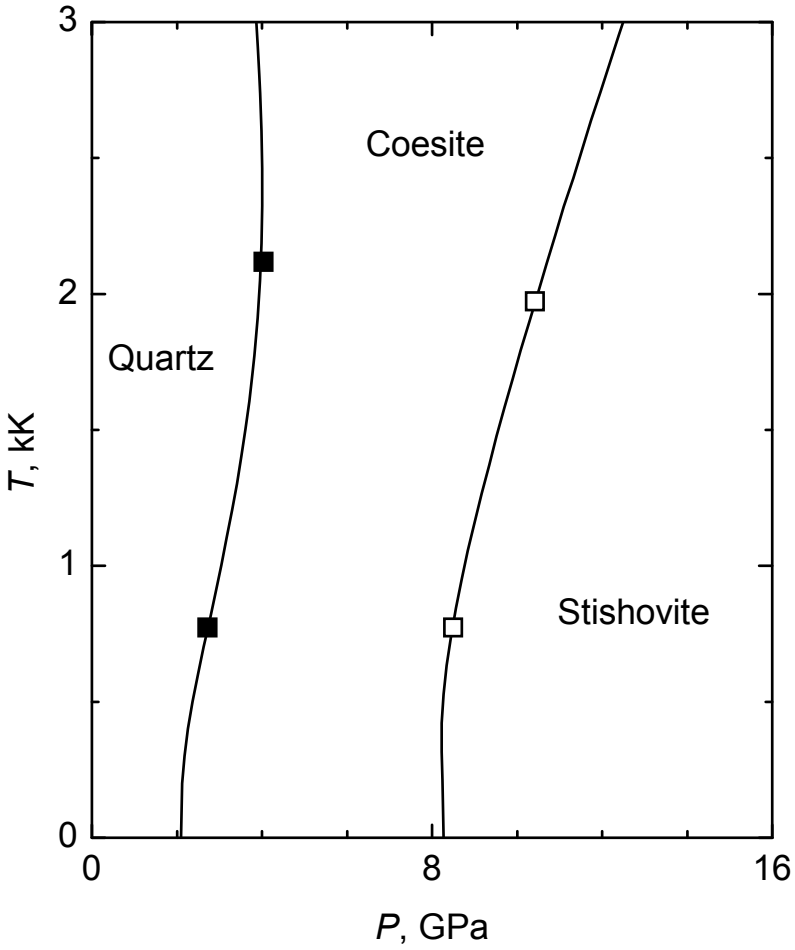


Phase Diagram of Silica

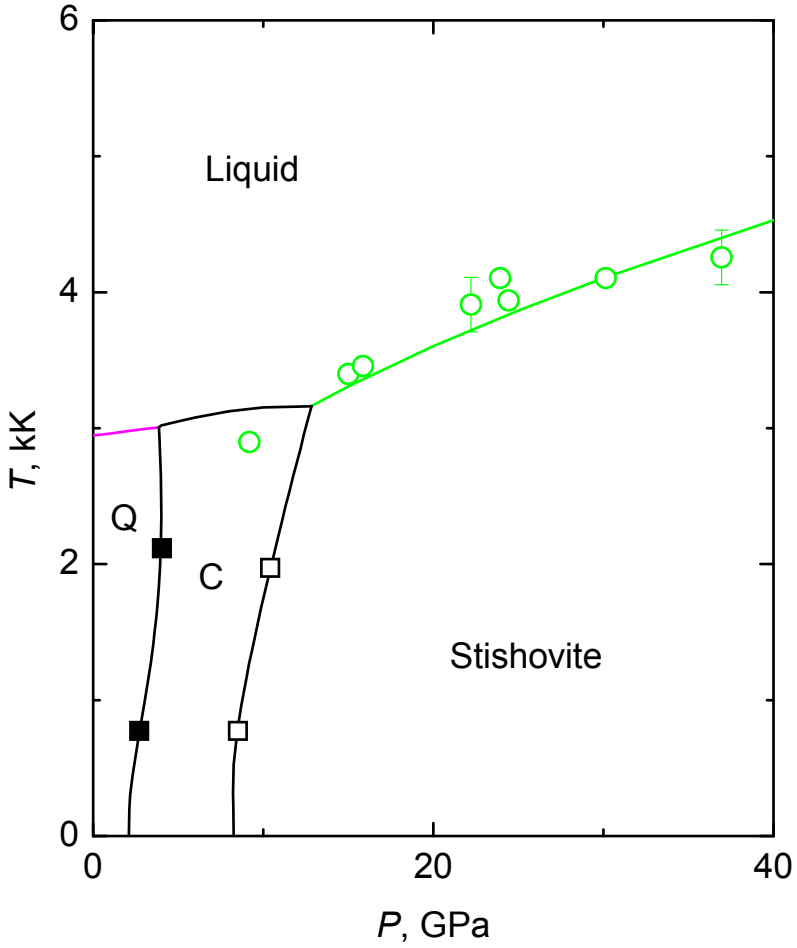


V. P. Dmitriev et al // Phys. Rev. B. 1998. V. 58. P. 11911.

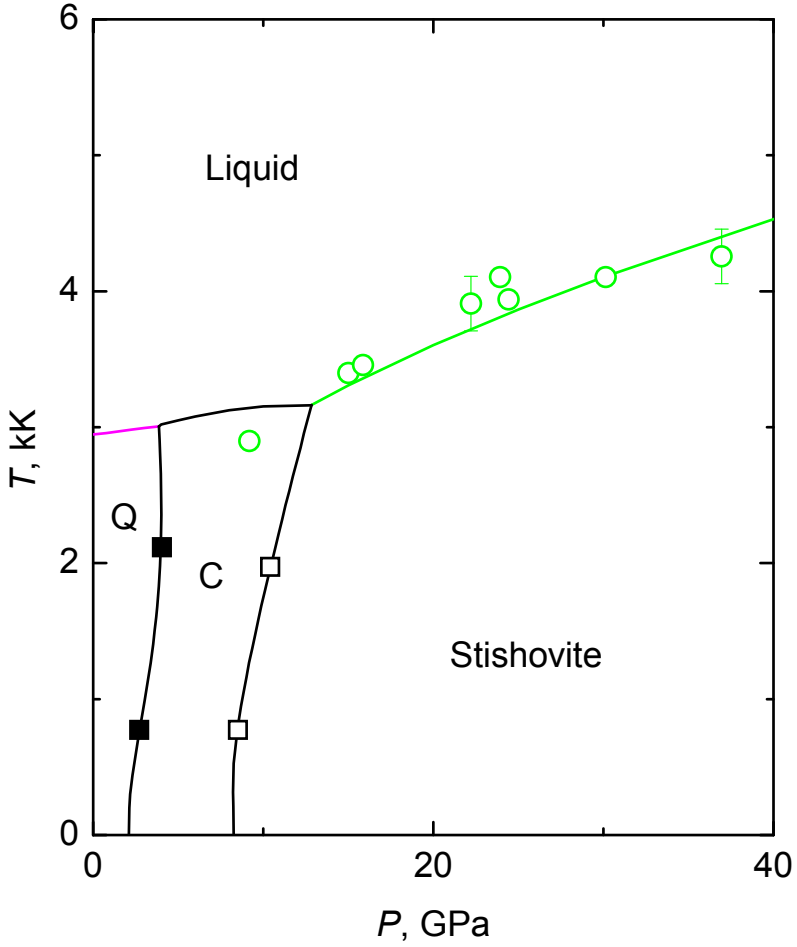
Phase Diagram of System Quartz–Coesite–Stishovite

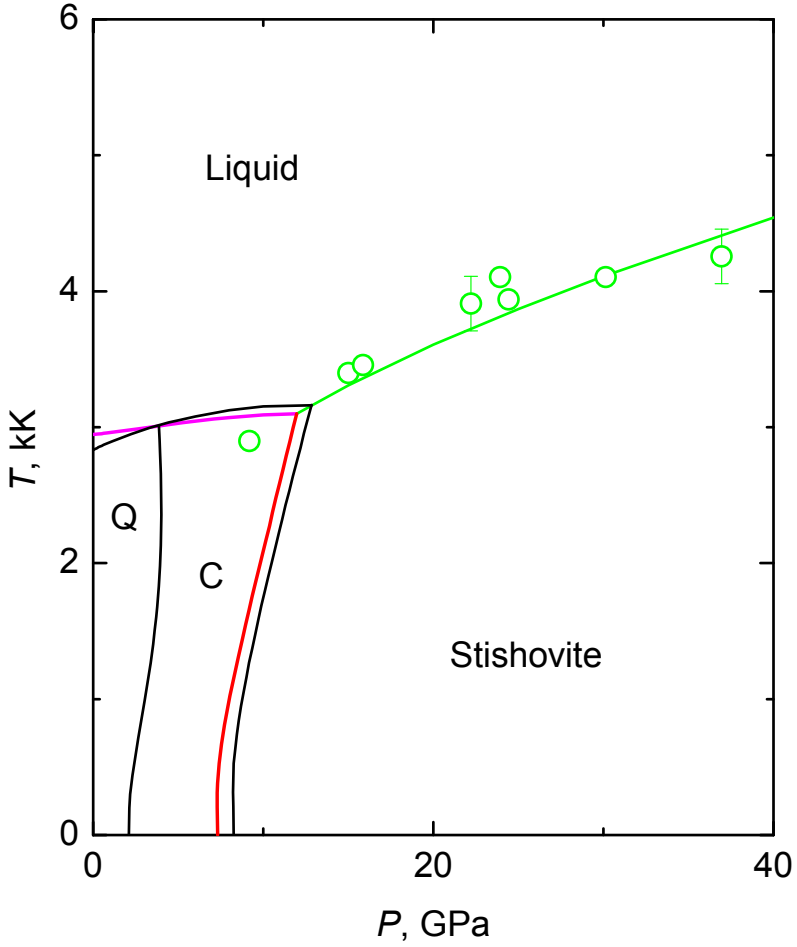


Phase Diagram of System Quartz–Coesite–Stishovite–Liquid

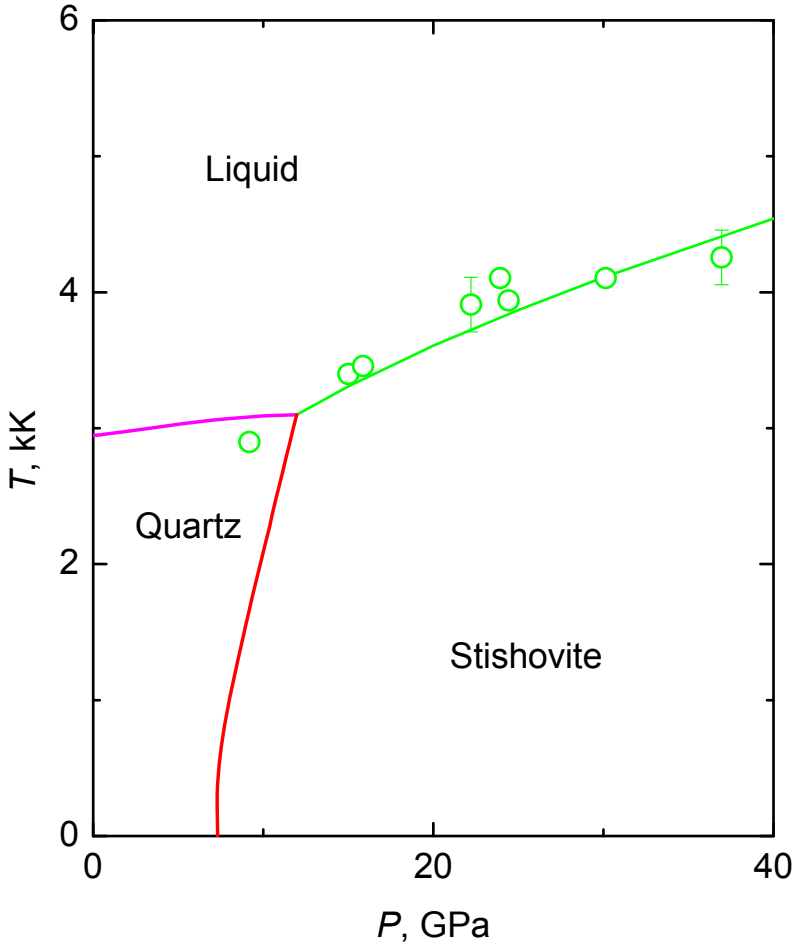


Phase Diagram of System Quartz–Coesite–Stishovite–Liquid

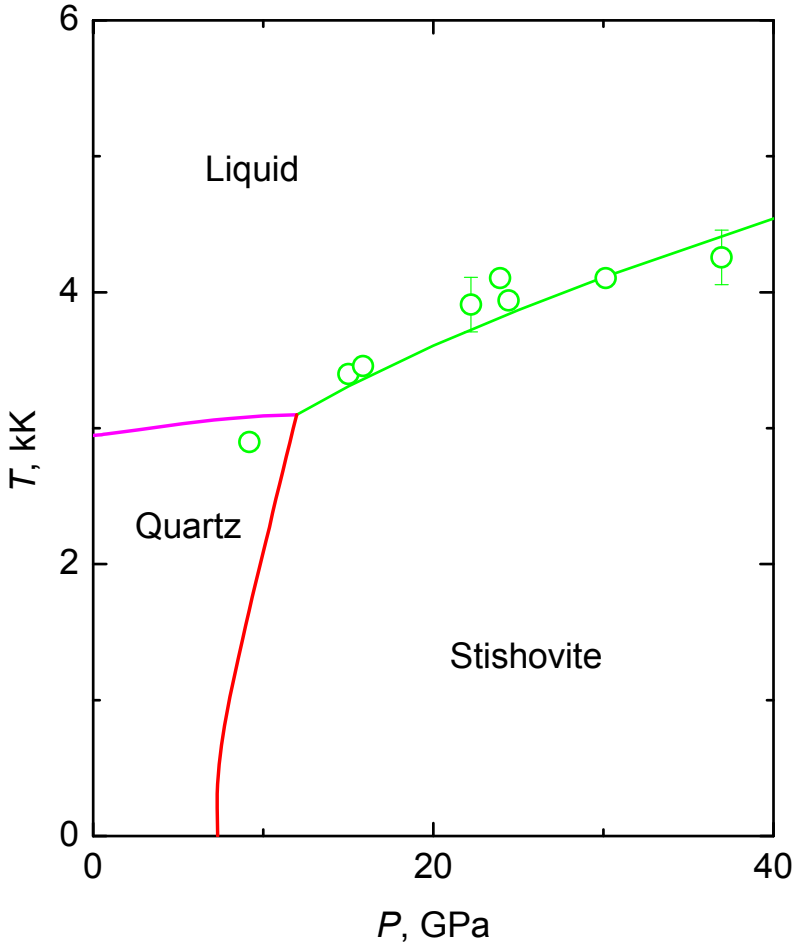


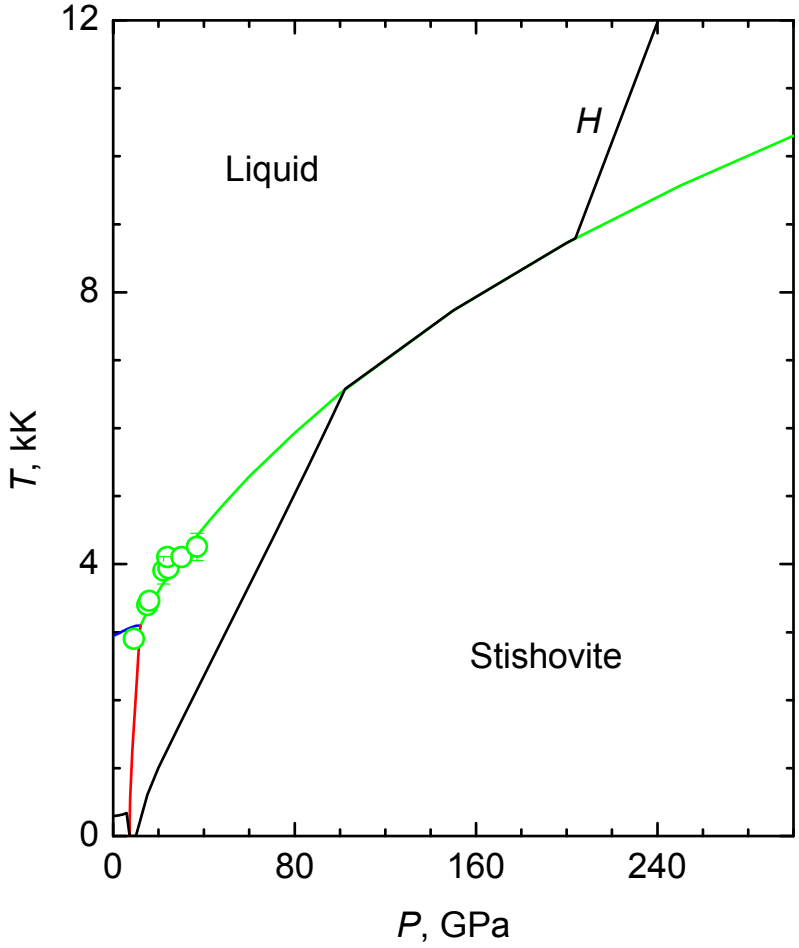


Phase Diagram of System Quartz–Stishovite–Liquid

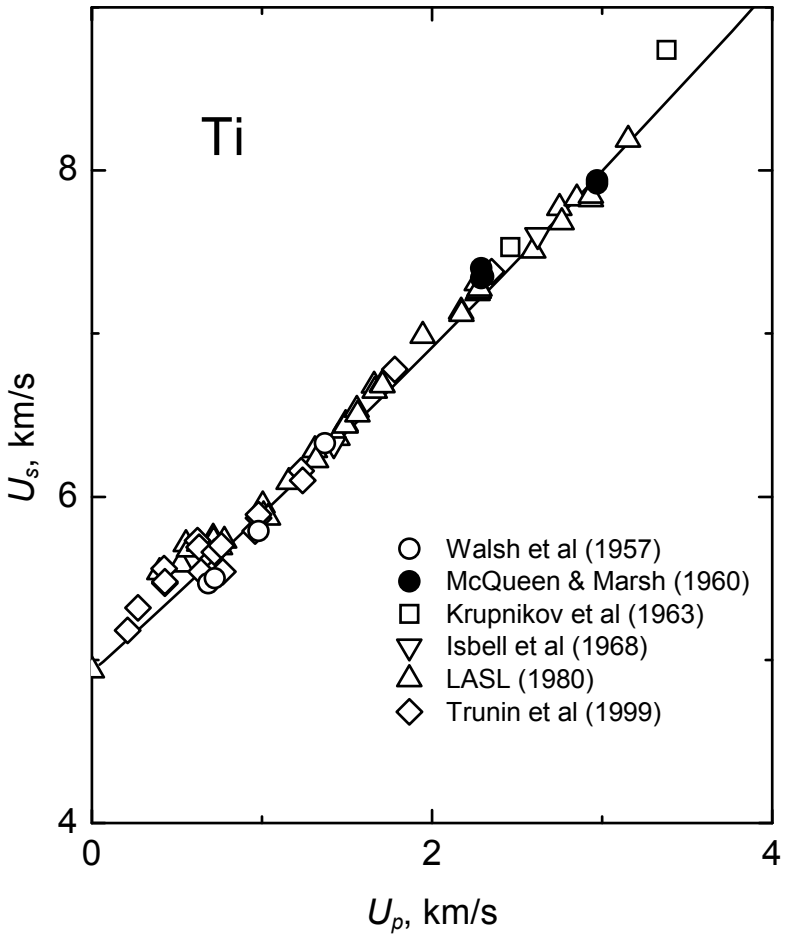


Phase Diagram of System Quartz–Stishovite–Liquid

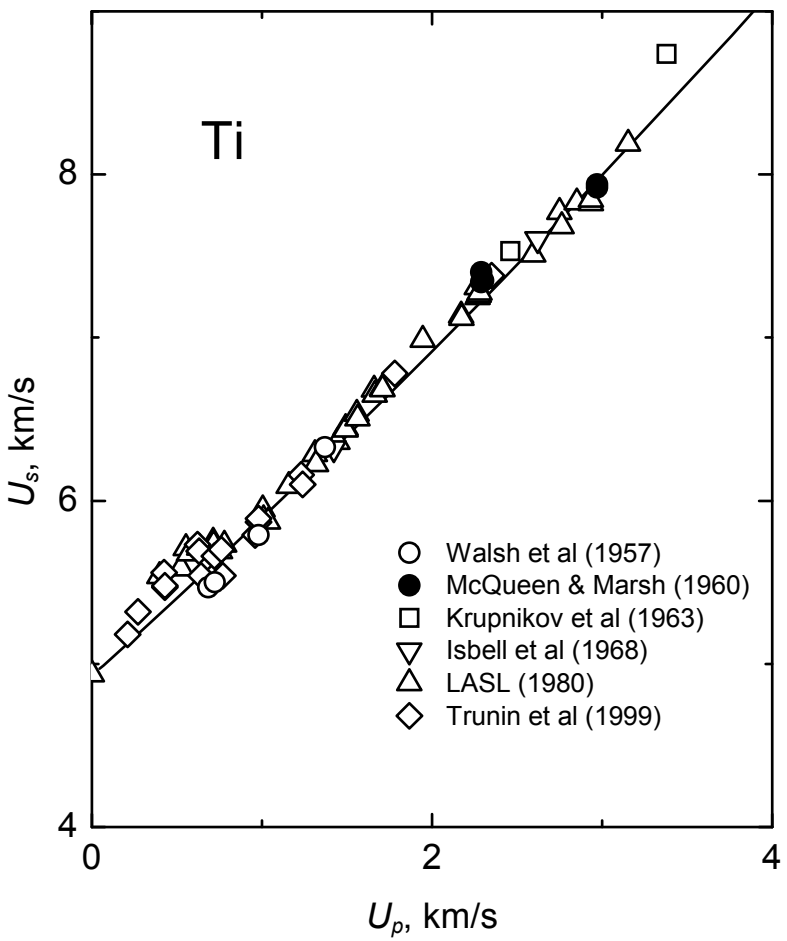


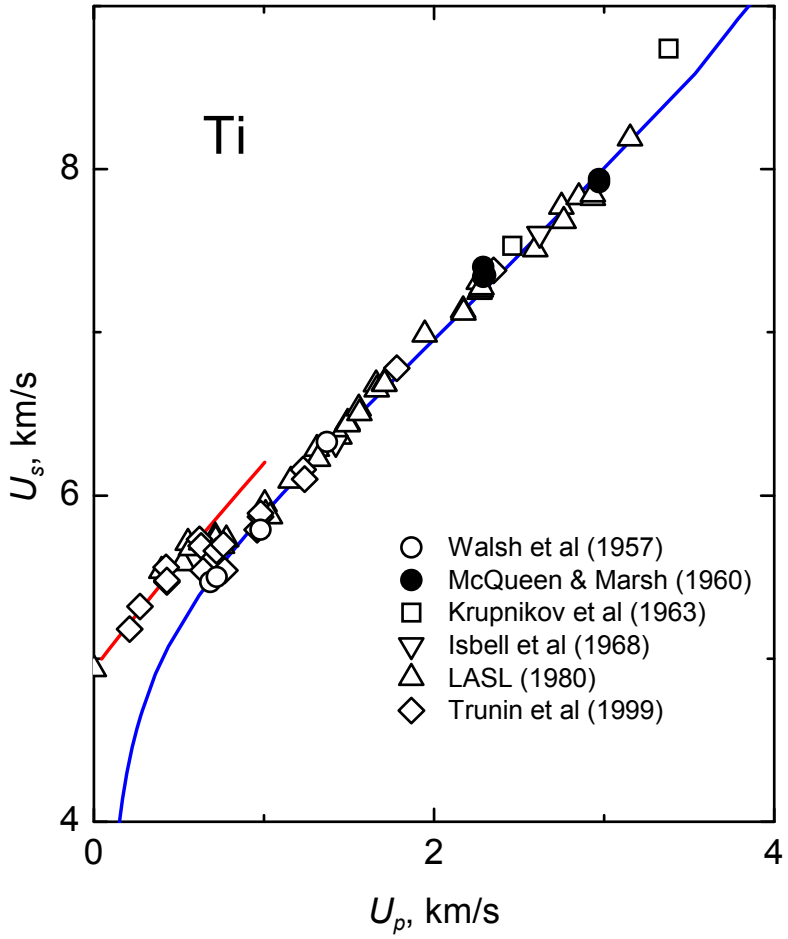


Hugoniot of Titanium

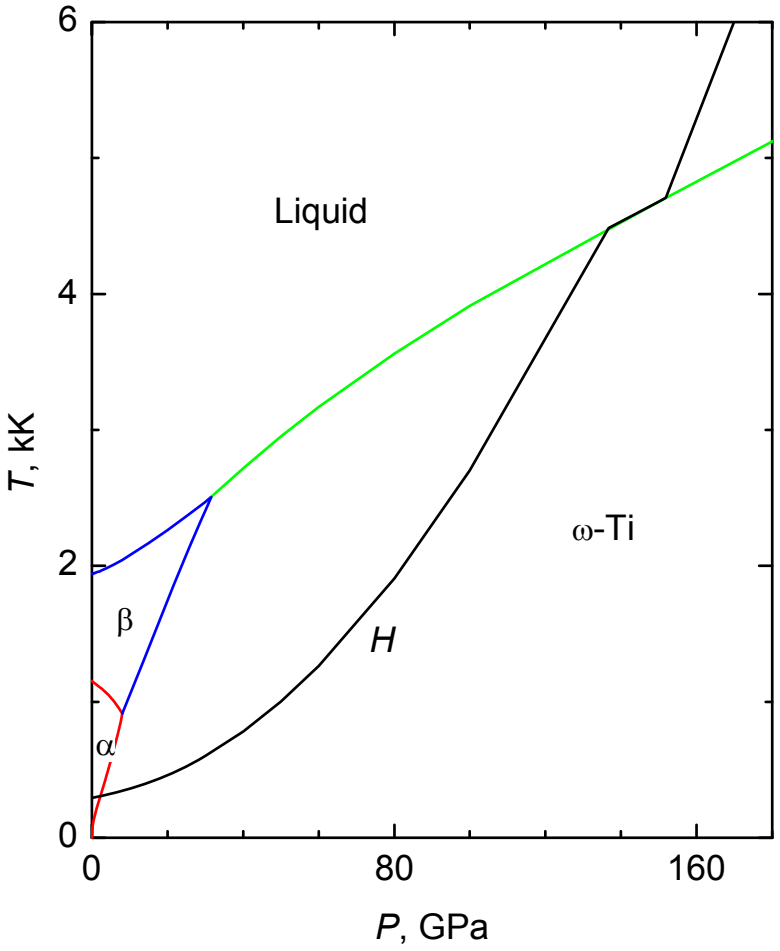


Hugoniot of Titanium



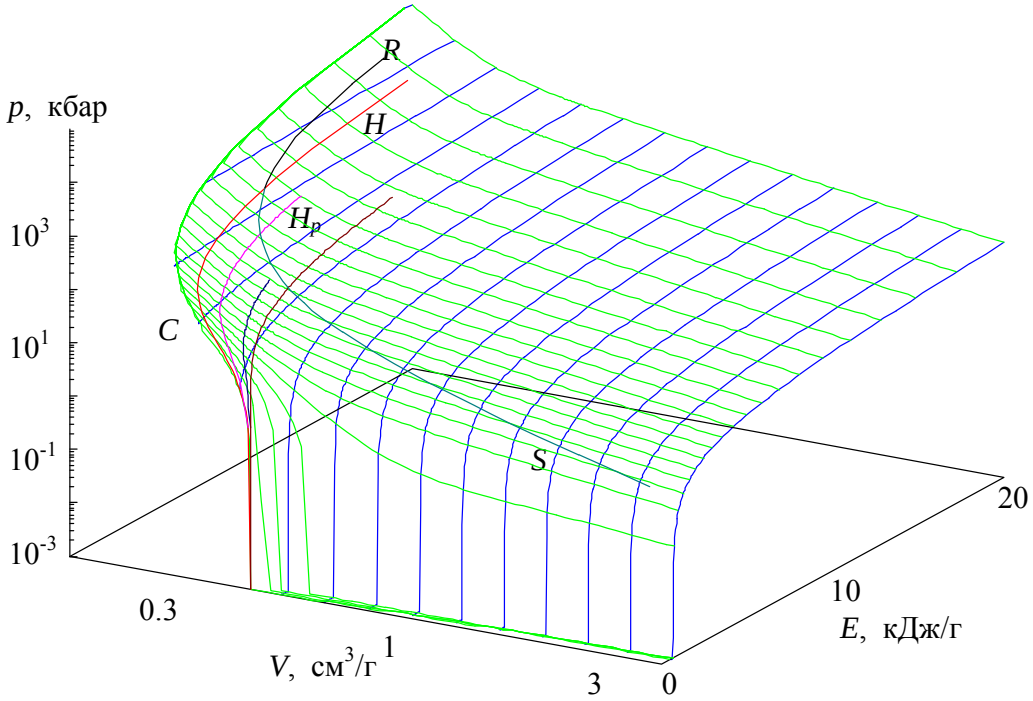


Phase Diagram of Titanium



Caloric Equations of State

Pressure–Volume–Internal Energy Surface for Polytetrafluoroethylene



C — cold curve at *T* = 0 K, *H* & H_p — principal and porous Hugoniots,
R — double shock compression curve, S — release isentrope

Caloric Equation of State Model
$E = E(V, P)$ or $P = P(V, E)$

General form

$$P(V,E) = P_c(V) + \frac{\Gamma(V,E)}{V}(E - E_c(V))$$

Thermal component (according to Bushman & Lomonosov 1989)

$$\Gamma(V,E) = \gamma_i + \frac{\gamma_c(V) - \gamma_i}{1 + \sigma_c^{-2/3}(E - E_c(V))/E_a}$$

$$\gamma_c(V) = 2/3 + (\gamma_{0c} - 2/3)\frac{\sigma_n^2 + \ln^2 \sigma_m}{\sigma_n^2 + \ln^2(\sigma/\sigma_m)}$$

$$\sigma = V_0/V$$

Equation of State Model

General form

$$P(V,E) = P_c(V) + \frac{\Gamma(V,E)}{V}(E - E_c(V))$$

Elastic component (EOS at T = 0 K)

at $V < V_{0c}$:

$$F_c(V) = 3V_{0c}\sum_{i=1}^{2}\frac{a_i}{i}\left(\sigma_c^{i/3} - 1\right) - 3V_{0c}\sum_{i=1}^{3}\frac{b_i}{i}\left(\sigma_c^{-i/3} - 1\right) + b_0 V_{0c}\ln\sigma_c$$

at $V > V_{0c}$:

$$F_c(V) = V_{0c}\left[A\left(\sigma_c^m/m - \sigma_c^n/n\right) + B\left(\sigma_c^l/l - \sigma_c^n/n\right)\right] + E_{sub}$$

at $V = V_{0c}$:

$$F_c(V_{0c}) = 0$$

$$P_c(V_{0c}) = -dF_c/dV = 0$$

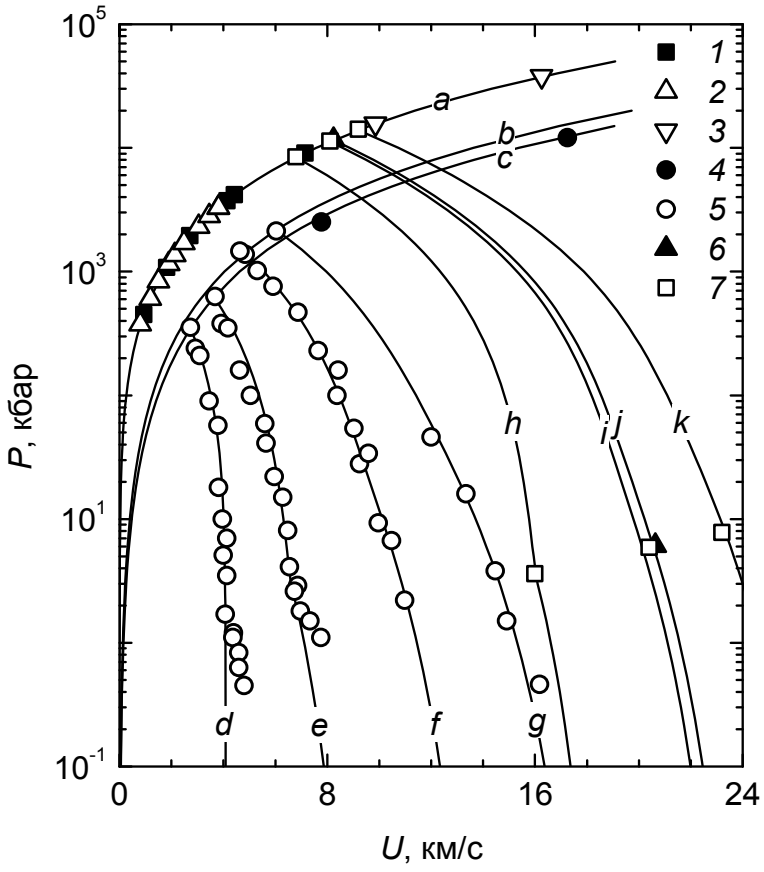
$$B_c(V_{0c}) = -VdP_c/dV = B_{0c}$$

$$B_c'(V_{0c}) = dB_c/dP_c = B_{0c}'$$

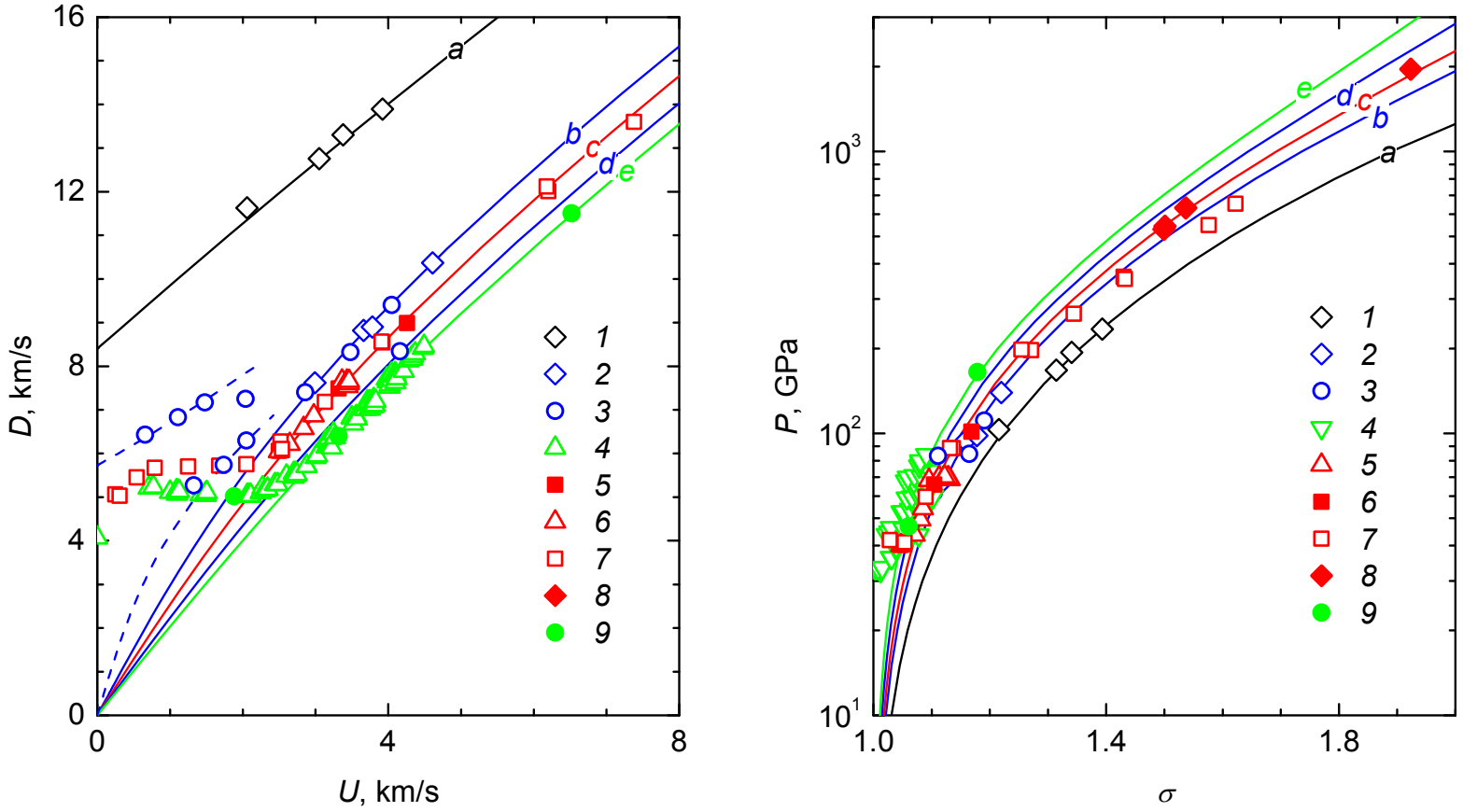
$$B_c''(V_{0c}) = -d(V\,dB_c/dV)/dB_c = B_{0c}''$$

$$\sigma_c = V_{0c}/V$$

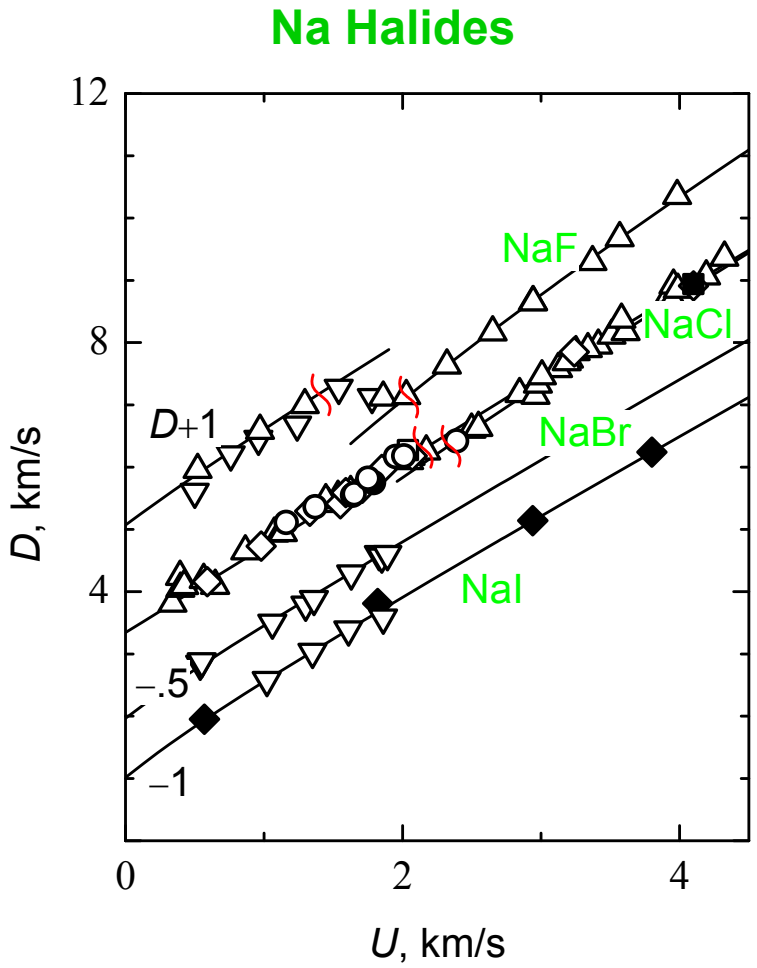
Equation of State for Copper

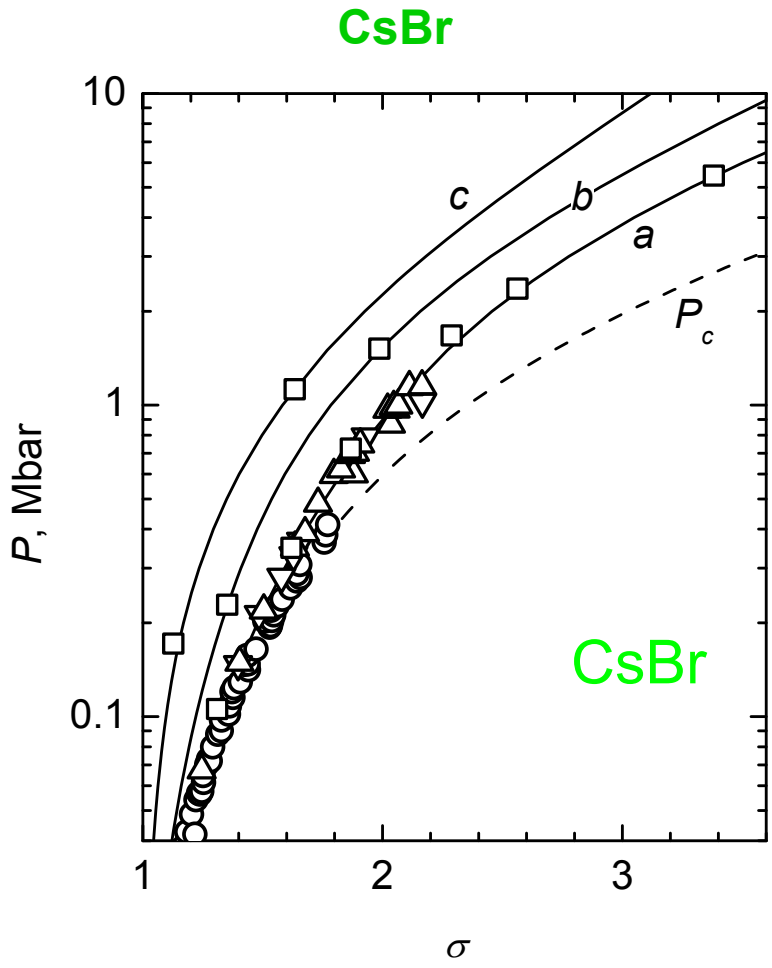


Equation of State for Stishovite

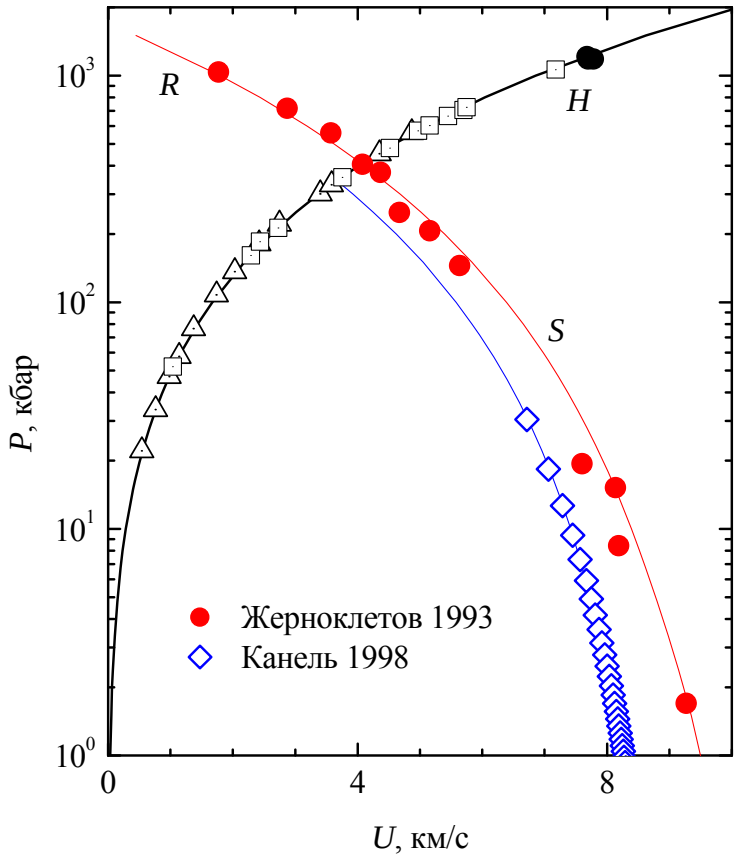


Equations of State for Alkali Halides

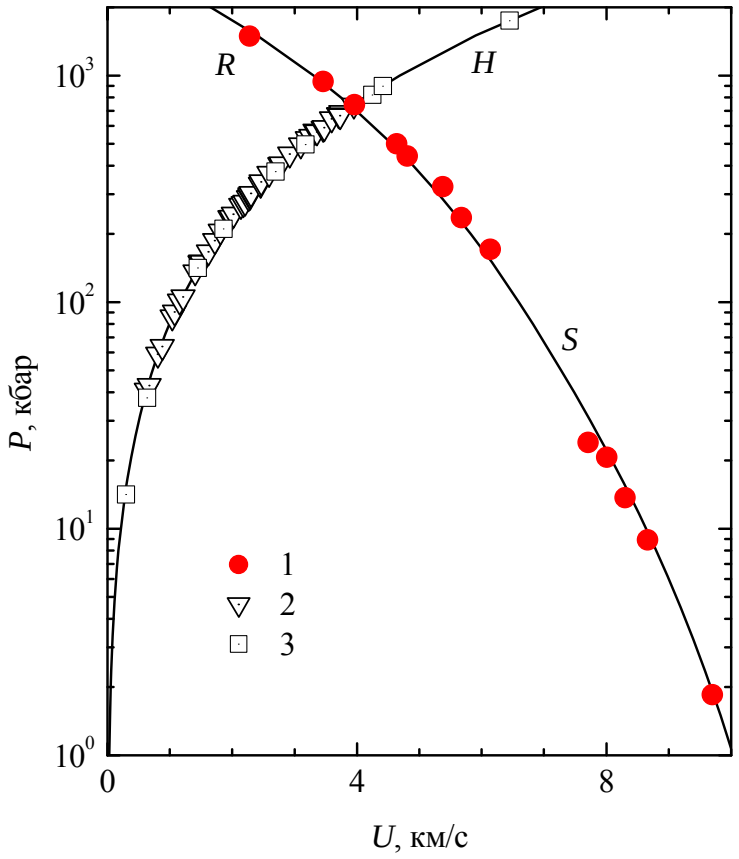




Shock Hugoniots & Release Isentropes

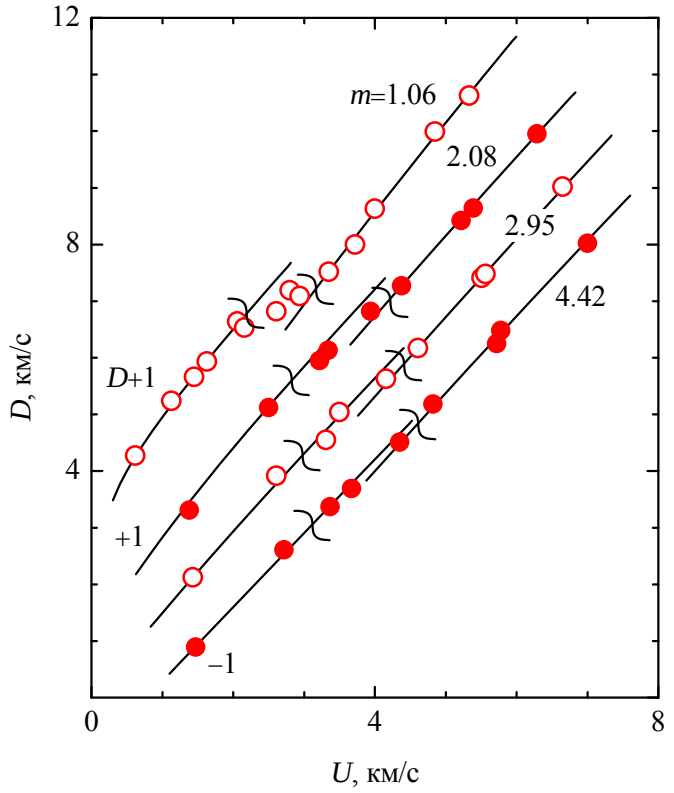


Polymethylmethacrylate

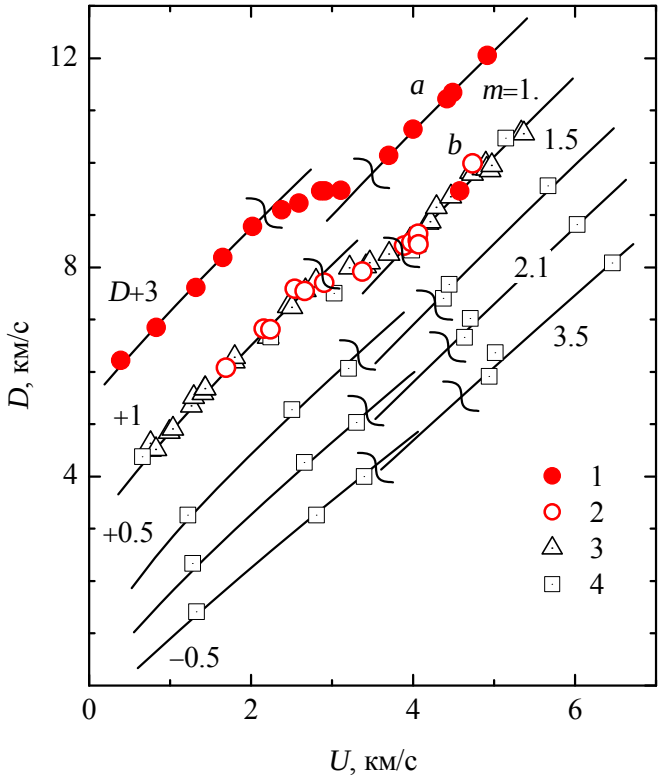


Polytetrafluoroethylene

Shock Hugoniots of Aromatic Polymers

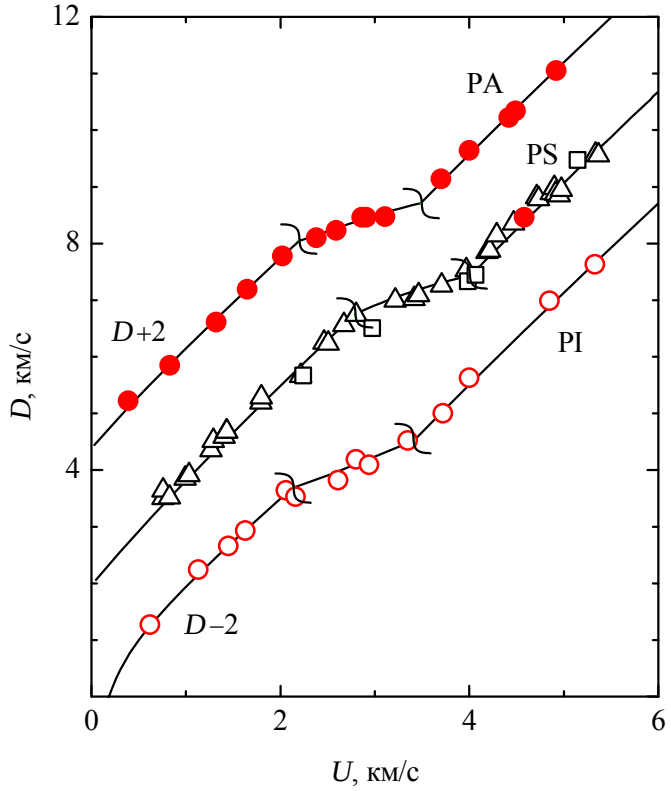


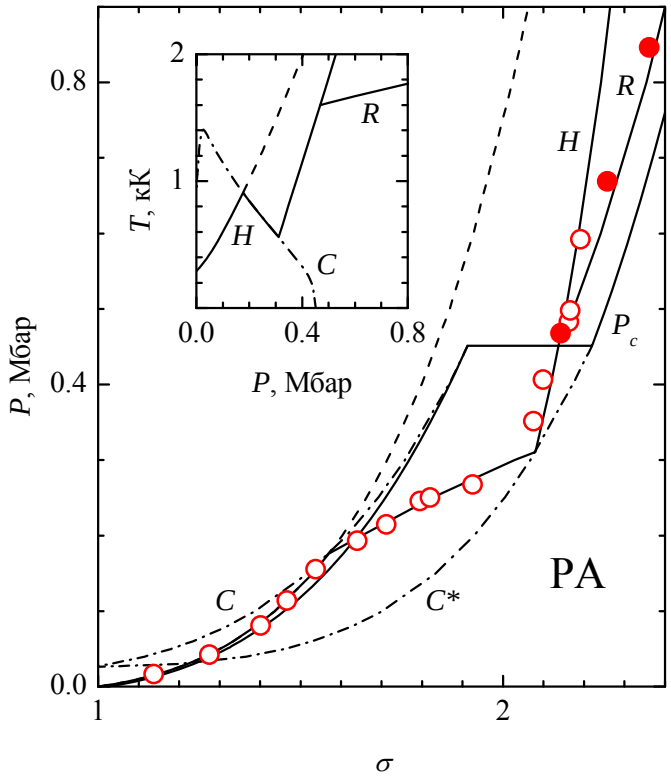
Polyimide



***a* — Polyamide,**
***b* — Polystyrene**

Shock Hugoniots of Polyamide (PA), Polystyrene (PS) & Polyimide (PI)





Thank You