Investigation of equations of state and phase transitions of substances at high energy densities with PHELIX

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EMMI GSI PHELIX Petawatt High-Energy Laser for Heavy Ion Experiments IHED JIHT RAS

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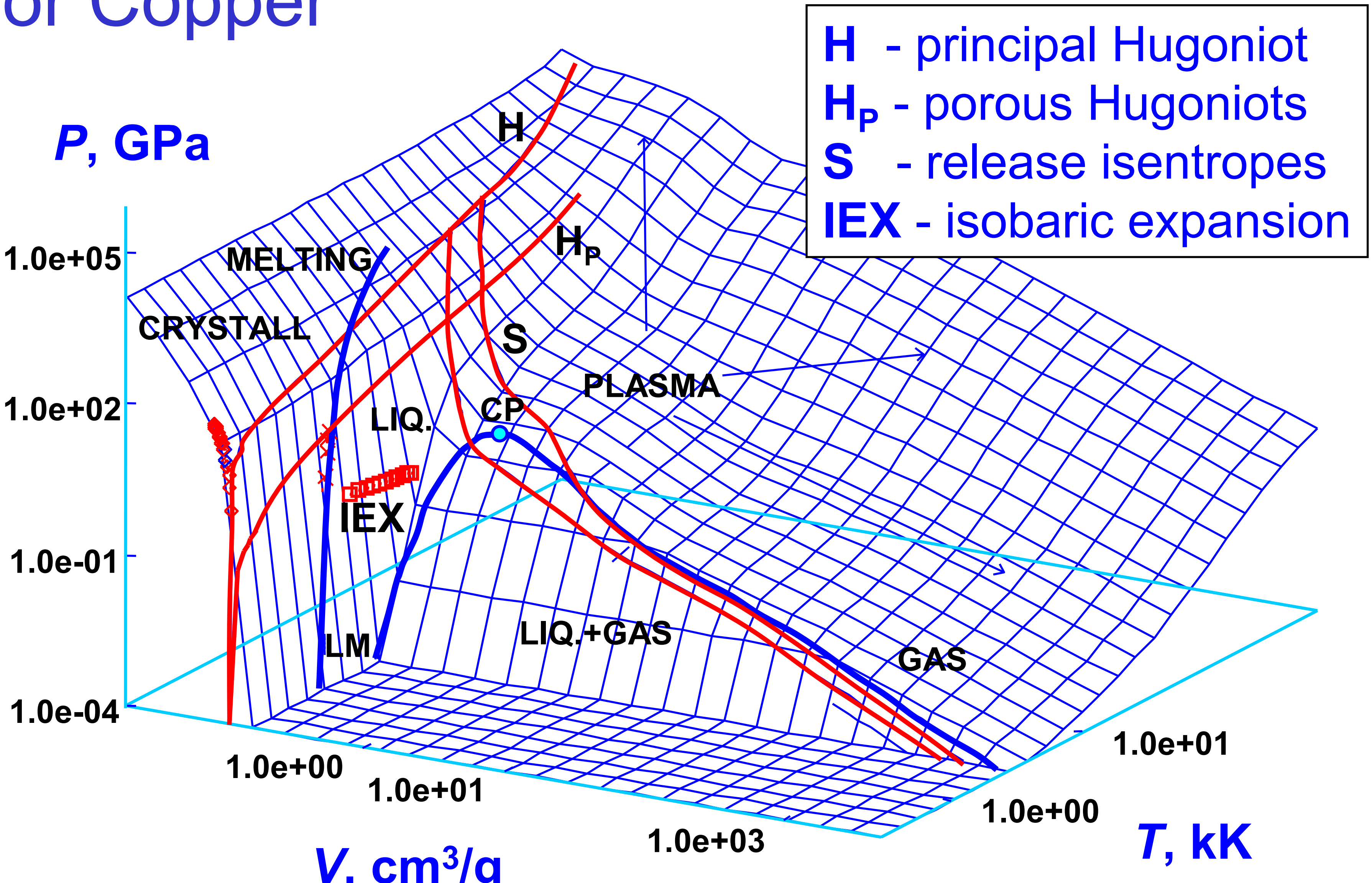
May 14-15, 2009, Moscow, Russia

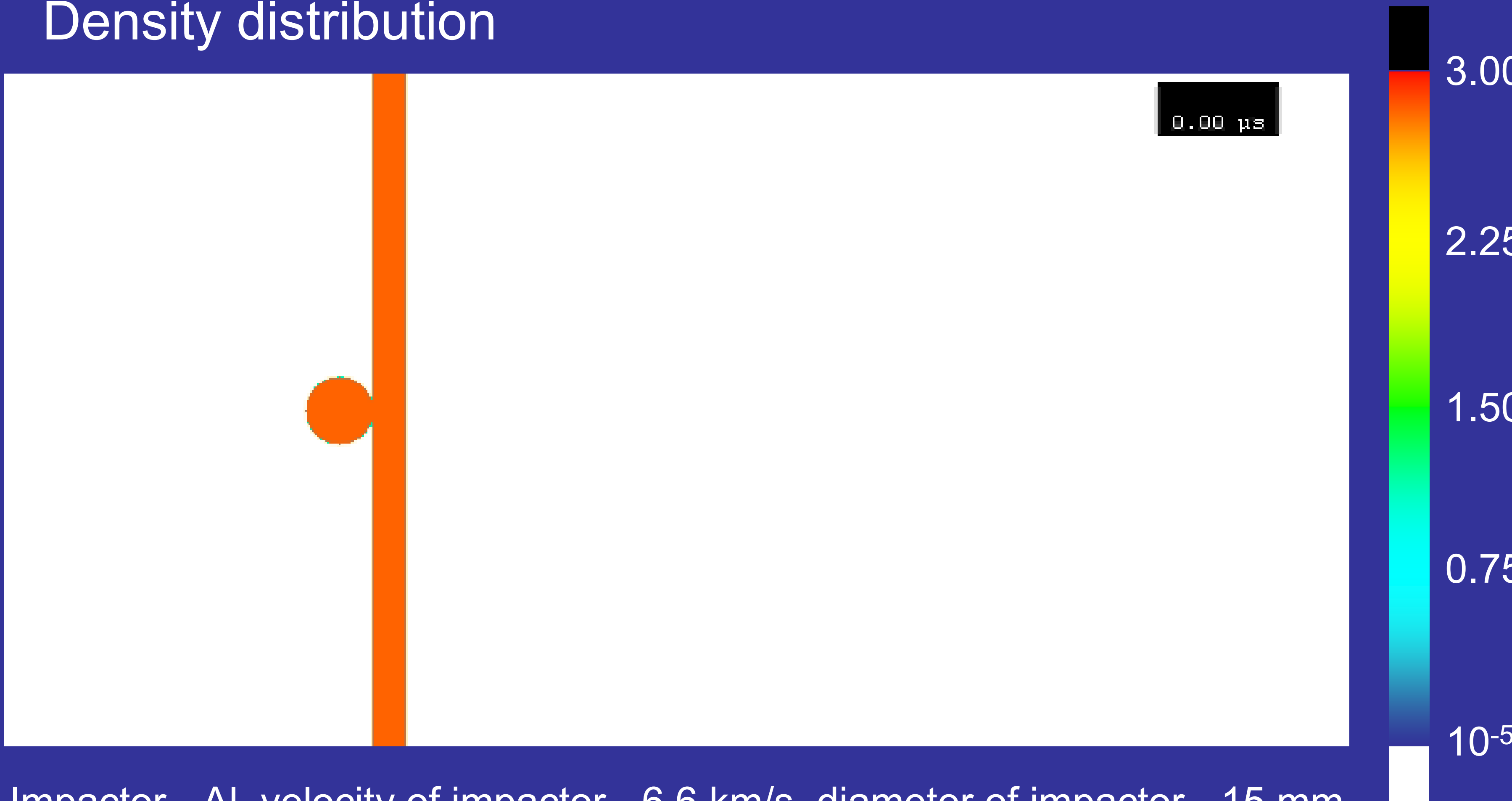
Pressure–Volume–Temperature Surface for Copper



Institute for High Energy Densities RAS, Moscow

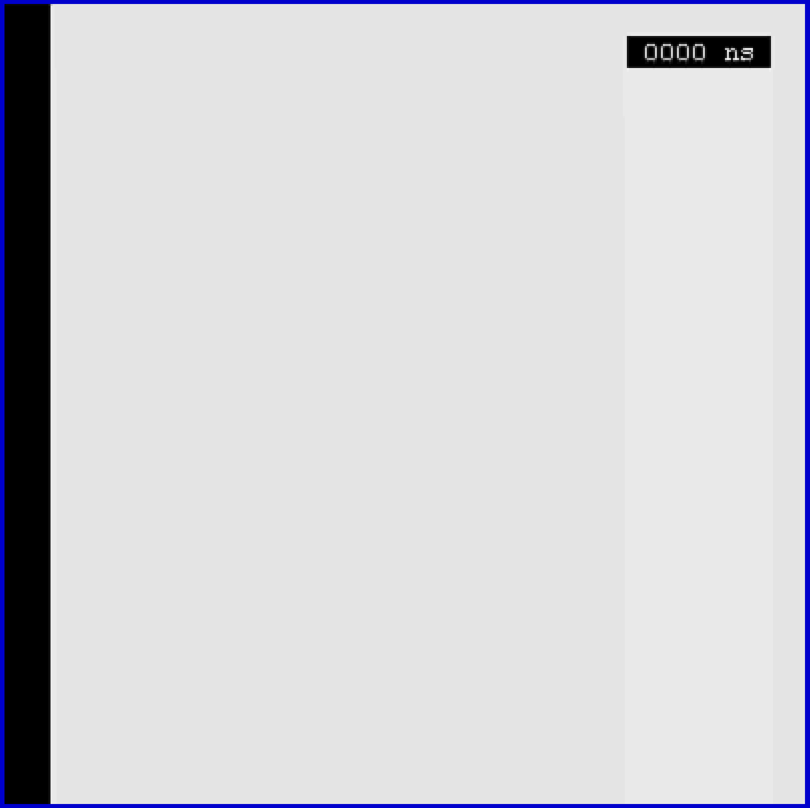
Povarnitsyn M. E., Khishchenko K. V., Levashov P. R. Hypervelocity impact modeling with different equations of state // Int. J. Impact Eng. 2006. V. 33. P. 625–633.

Density distribution



Impactor - Al, velocity of impactor - 6.6 km/s, diameter of impactor - 15 mm
Target - Al, thickness of target - 6.35 mm

Modeling of Laser-Matter Interaction by Mikhail E. Povarnitsyn et al.

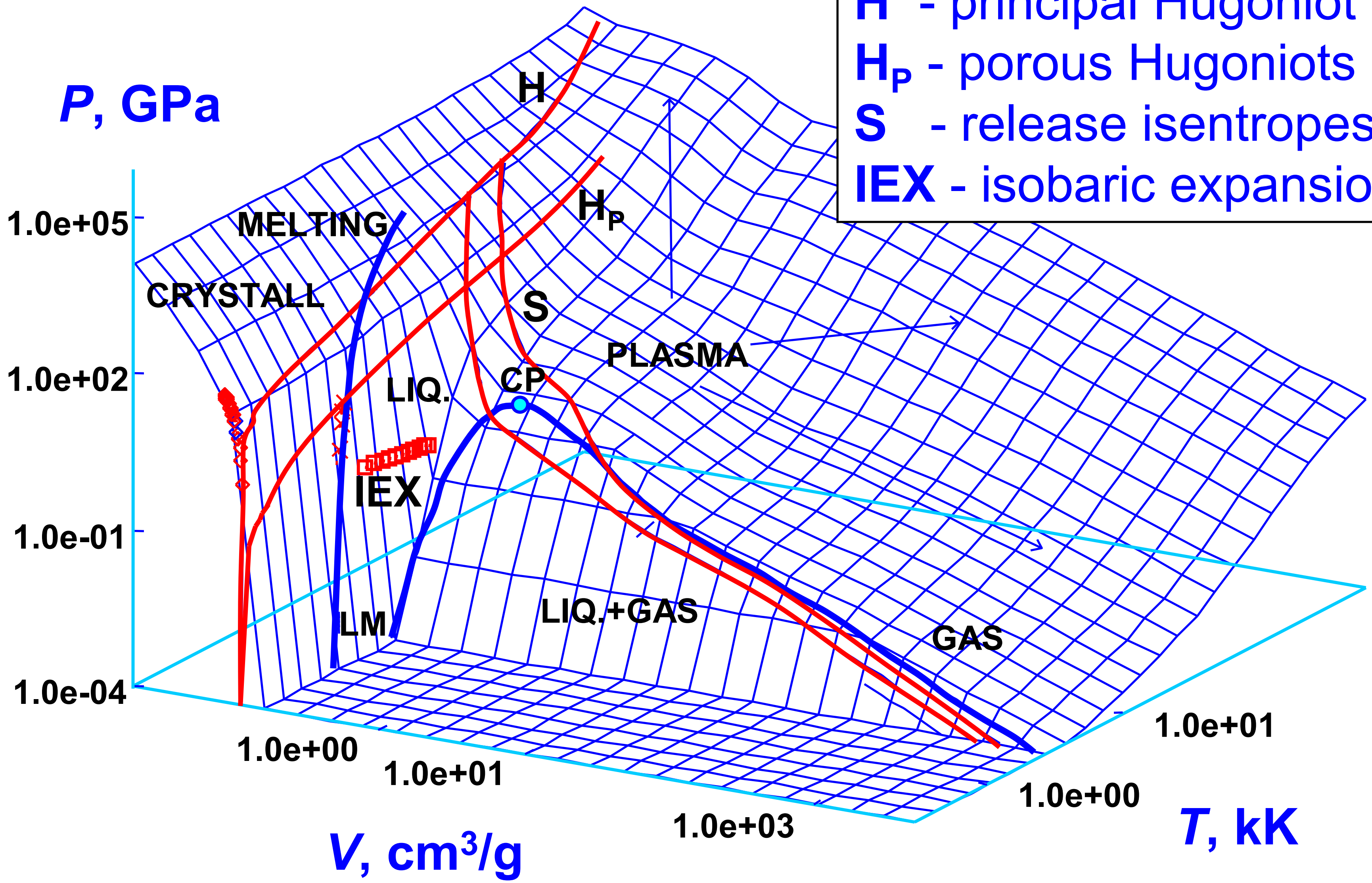


Images of the shockwave in the ambient gas (at normal conditions) and the ejected material after irradiation of the aluminum target with pulse parameters:

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

Pressure–Volume–Temperature Surface for Copper

- **H** - principal Hugoniot
- **H_P** - porous Hugoniots
- **S** - release isentropes
- **IEX** - isobaric expansion



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

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

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

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

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

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

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

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

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

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

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

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).]

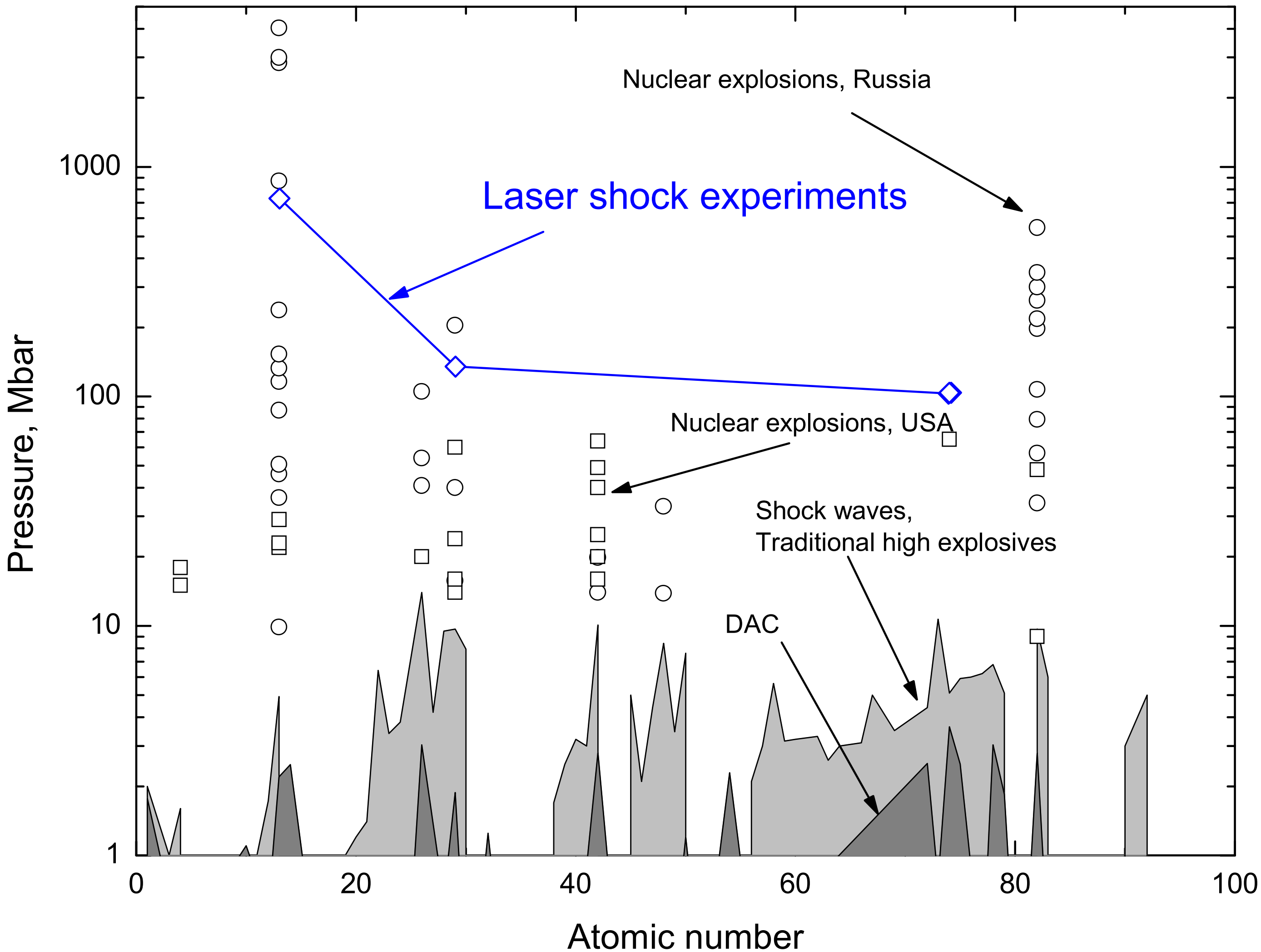
$$F_{\mathrm{e}}(V,T) = -C_{\mathrm{e}}(V,T)T\ln\left\{1 + \frac{B_{\mathrm{e}}(T)T}{2C_{\mathrm{ei}}}\sigma^{-\gamma_{\mathrm{e}}(V,T)}\right\}$$

$$C_{\mathrm{e}}(V,T) = \frac{3R}{2}\left\{Z + \frac{\sigma_{\mathrm{z}}T_{\mathrm{z}}^2(1-Z)}{(\sigma+\sigma_{\mathrm{z}})(T^2+T_{\mathrm{z}}^2)}\right\}\exp(-\tau_{\mathrm{i}}(V)/T) \qquad C_{\mathrm{ei}} = \frac{3RZ}{2}$$

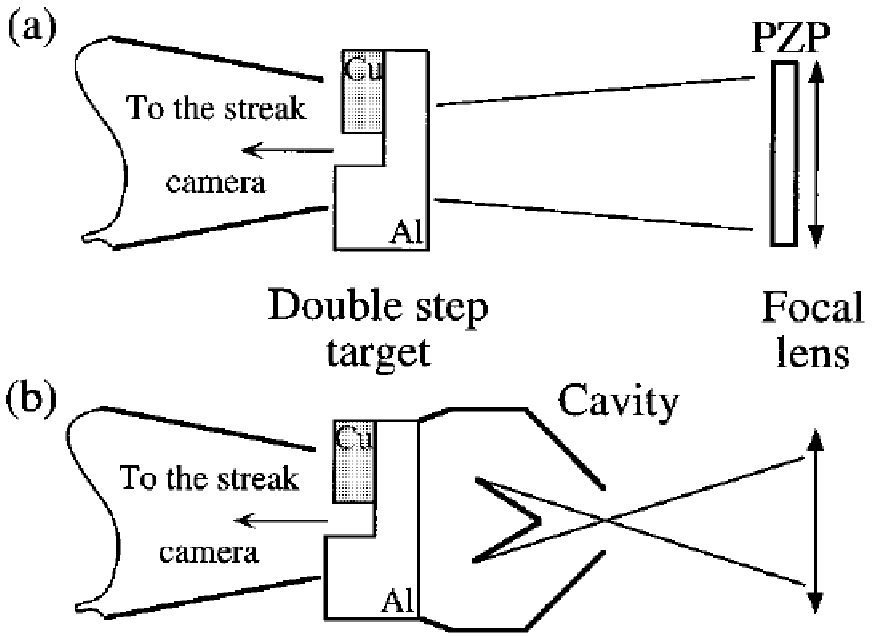
$$B_{\mathrm{e}}(T) = \frac{2}{T^2}\int_0^T\!\!\int \beta(\tau)\,d\tau\,dT \qquad \beta(T) = \beta_{\mathrm{i}} + (\beta_0 - \beta_{\mathrm{i}} + \beta_{\mathrm{m}}T/T_{\mathrm{b}})\exp(-T/T_{\mathrm{b}})$$

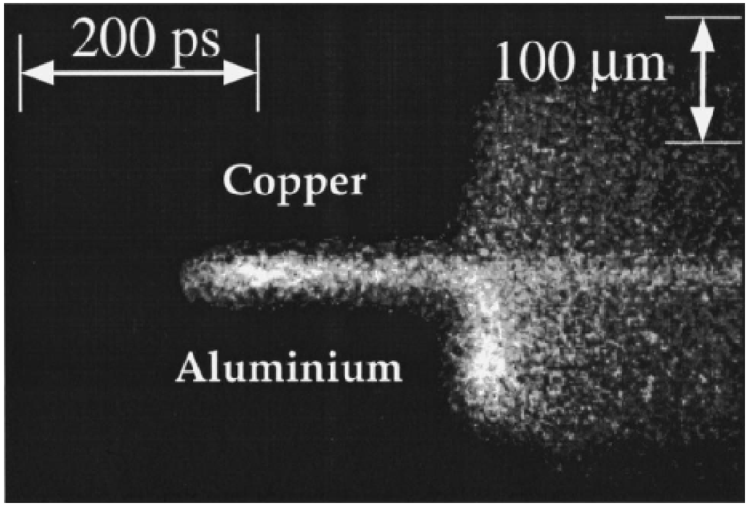
$$\tau_{\mathrm{i}}(V) = T_{\mathrm{i}}\exp(-\sigma_{\mathrm{i}}/\sigma) \qquad \gamma_{\mathrm{e}}(V,T) = \gamma_{\mathrm{ei}} + (\gamma_{\mathrm{e0}} - \gamma_{\mathrm{ei}} + \gamma_{\mathrm{m}}T/T_{\mathrm{g}})\exp(-T/T_{\mathrm{g}})$$

Shock-Wave Pressure in Experiments with Different Driving Systems



Direct (a) and Indirect (b) Laser Driven Shock Wave Setups





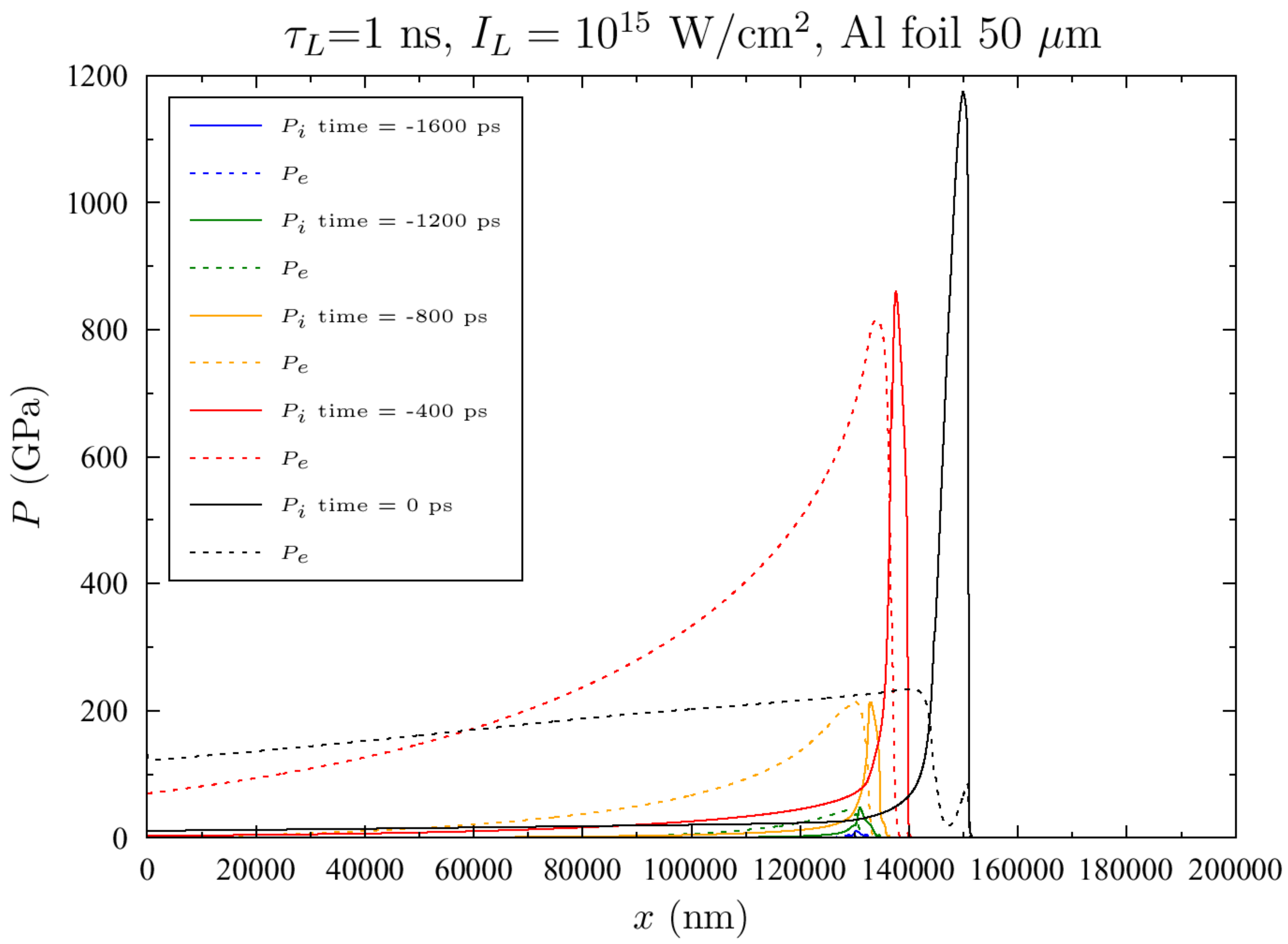
Alessandra Benuzzi et al., Phys. Rev. E 54 (1996) 2162

Experimental Area

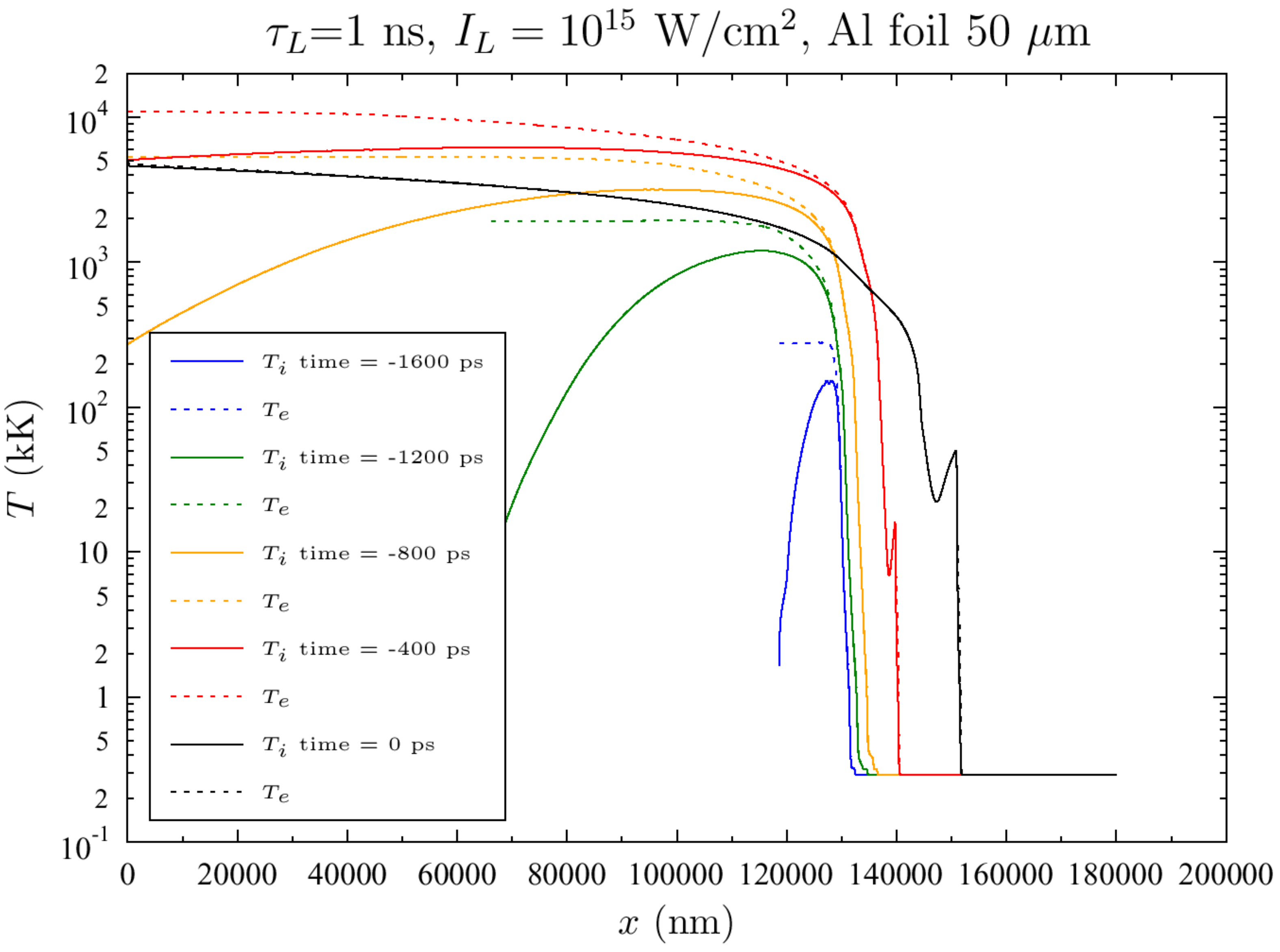
PHELIX – Laser at Z6:
τ_L=1–10 ns; E_L<= 300 J, focal spot 150 mkm, I_L<=10^{15} W/cm^2

Sample – foil of 10–40 μm
of Al, Graphite,…

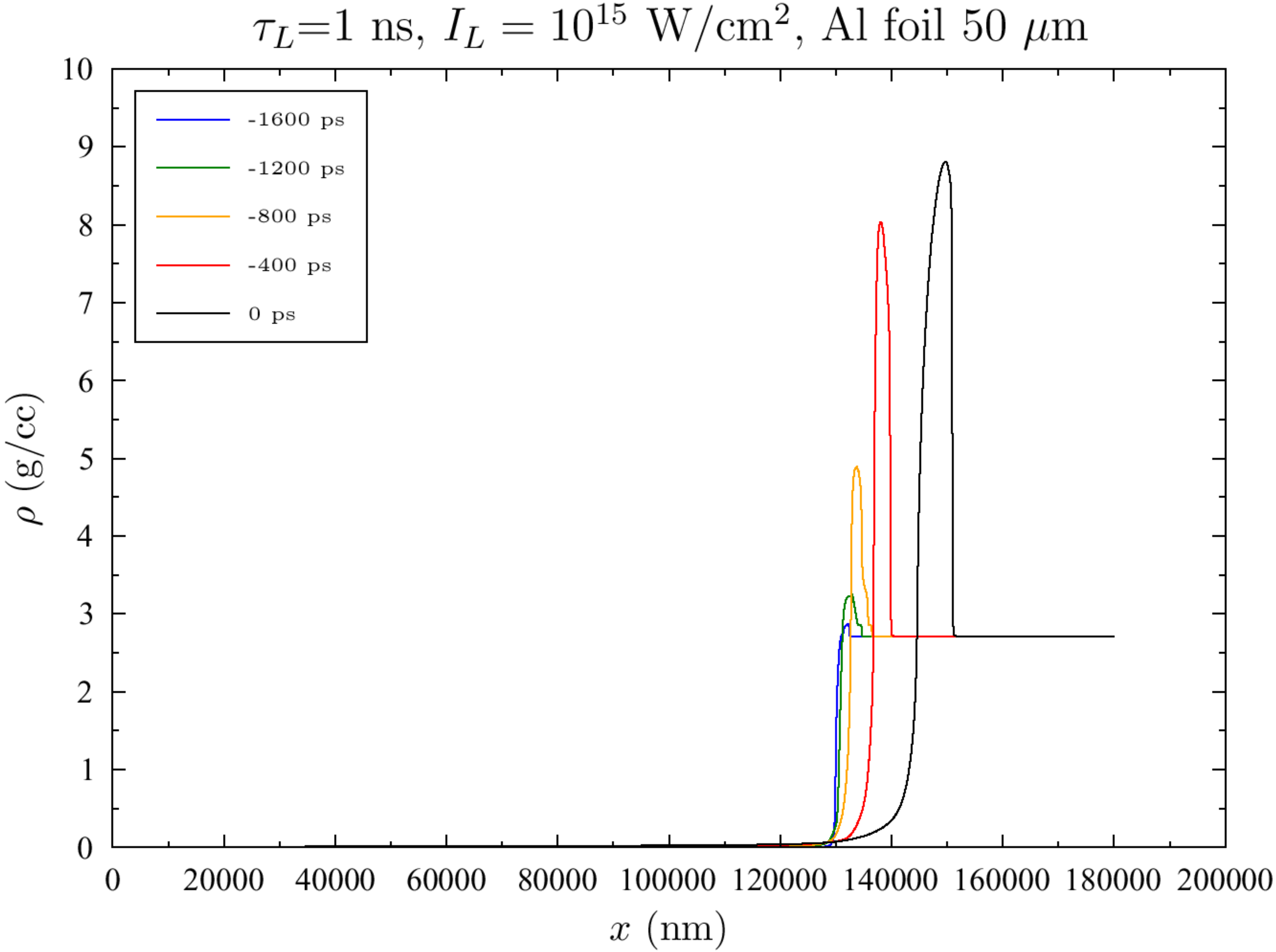
Pressure in Al Target



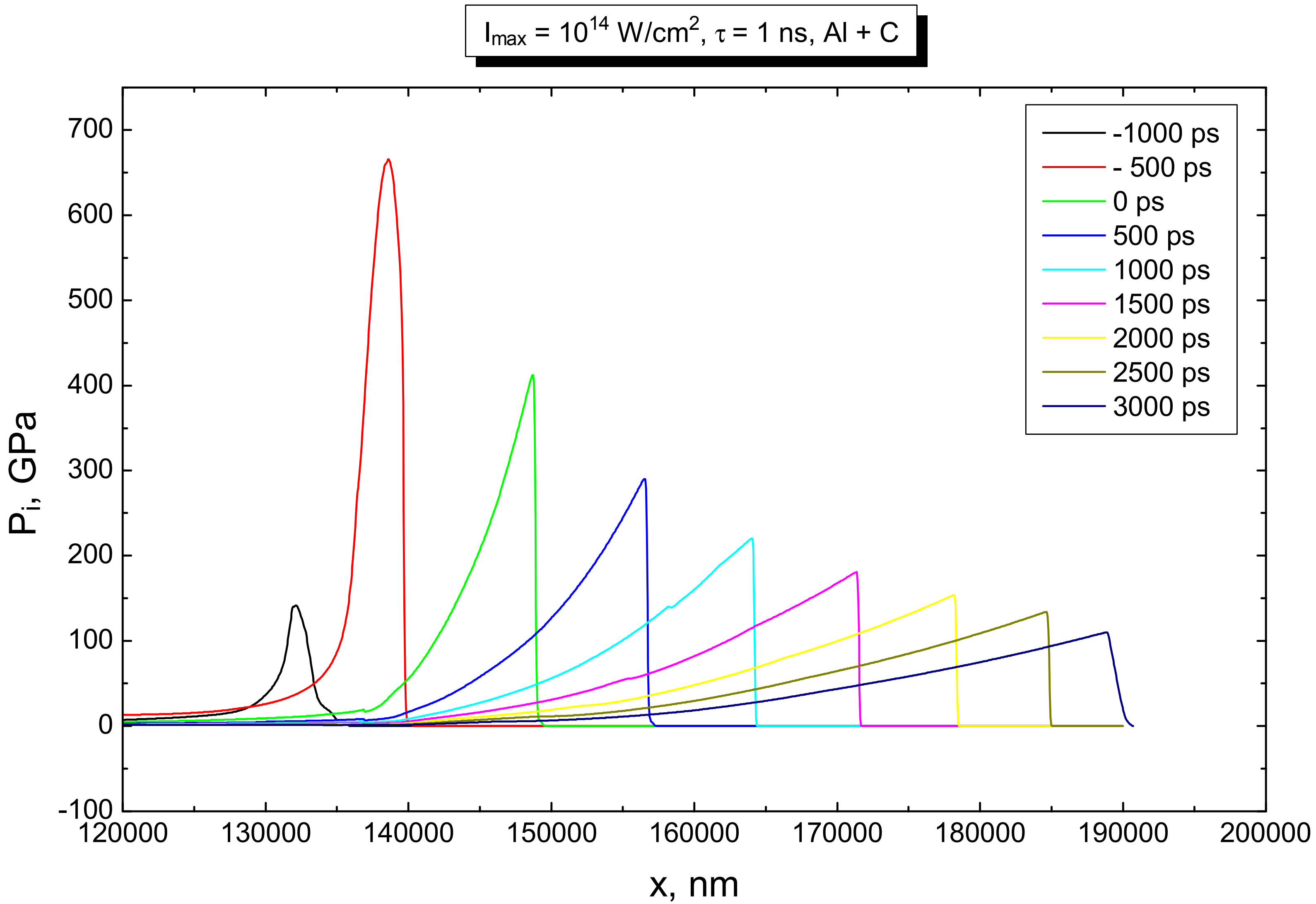
Temperature in Al Target



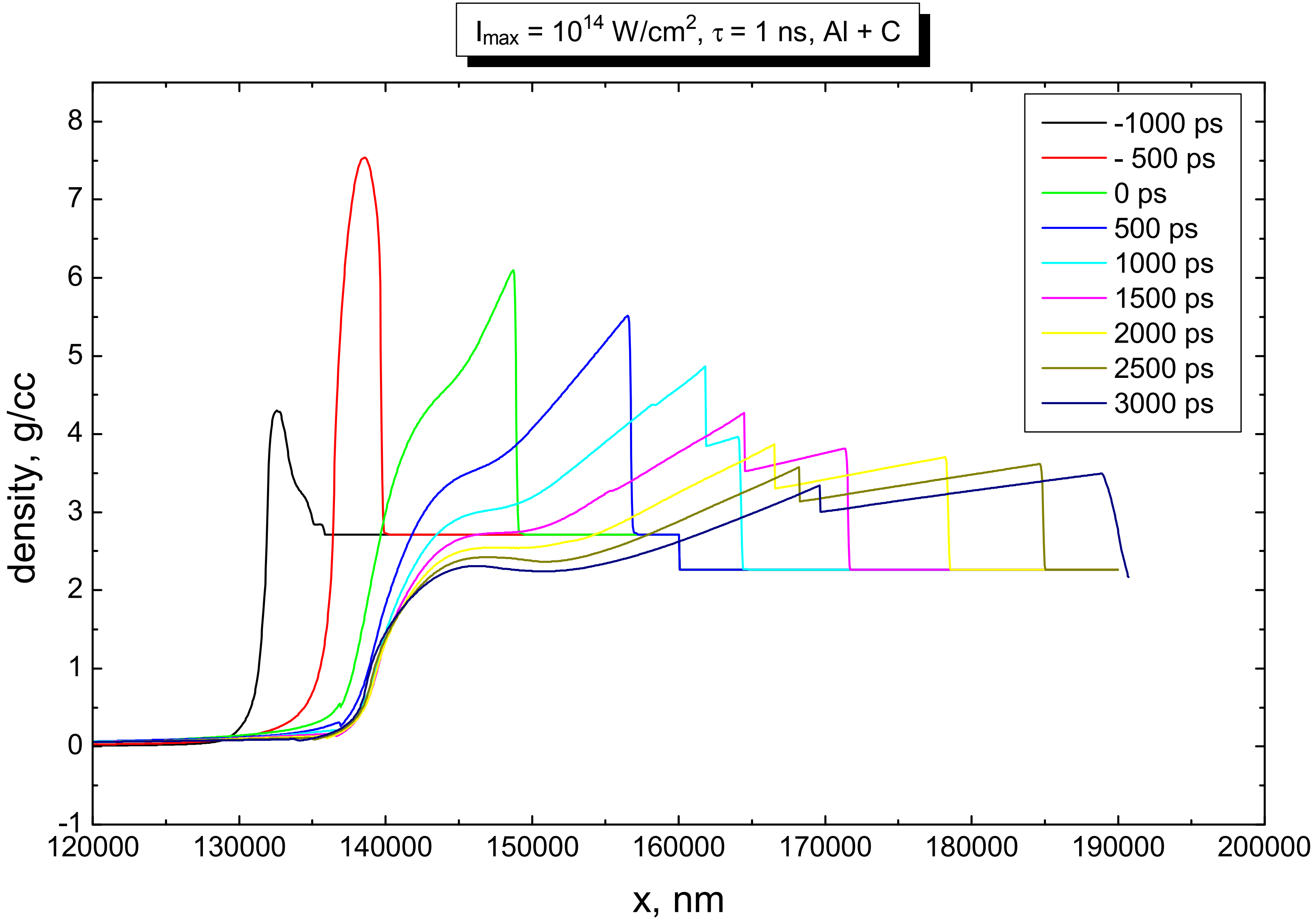
Density in Al Target



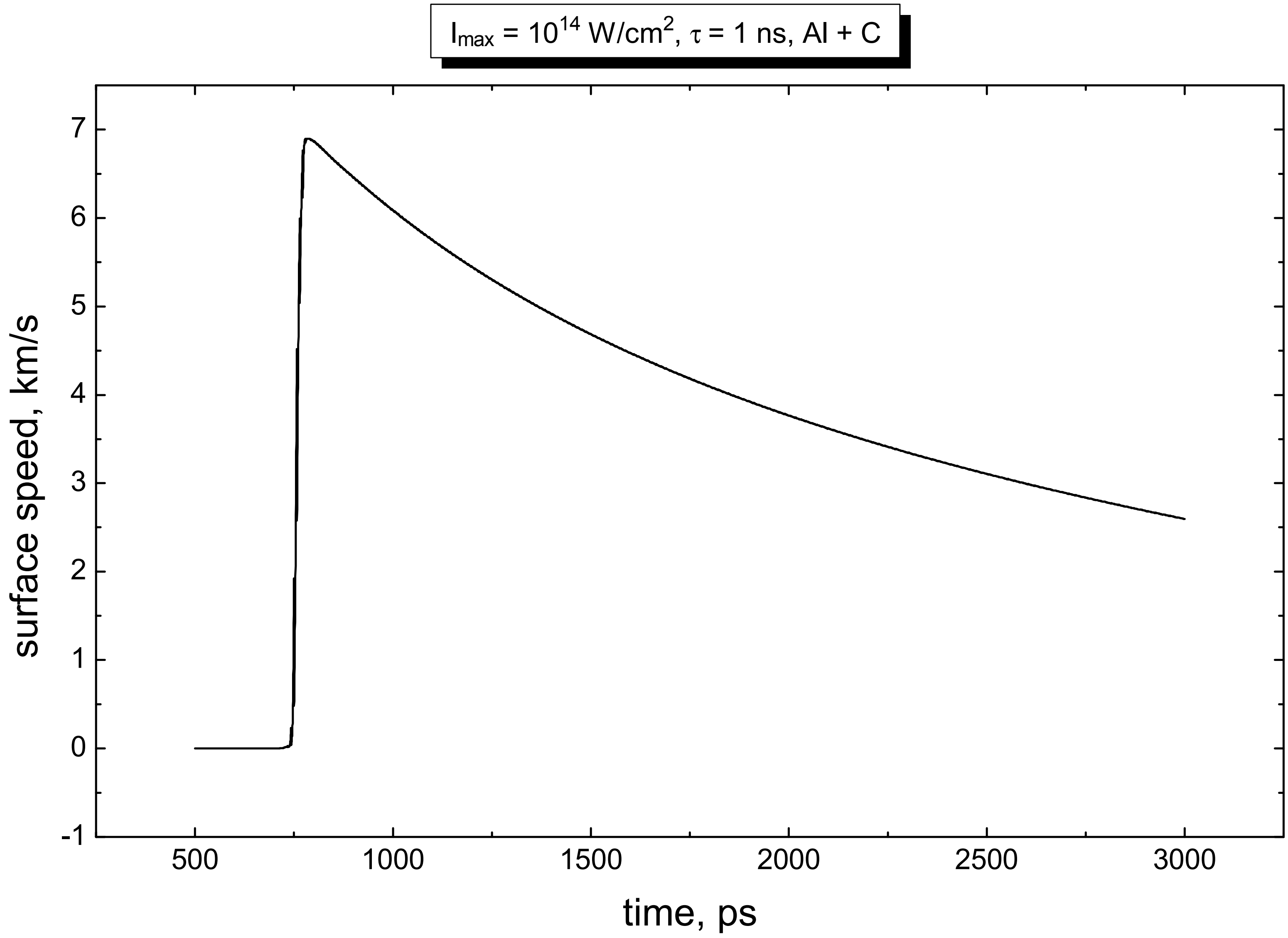
Pressure in Al + C Target



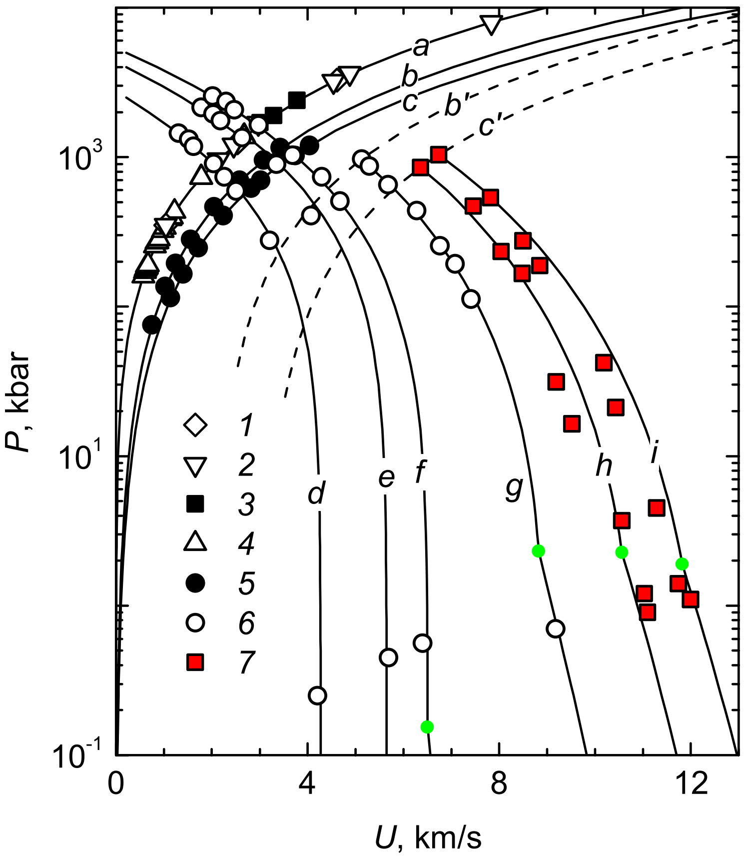
Density in Al + C Target

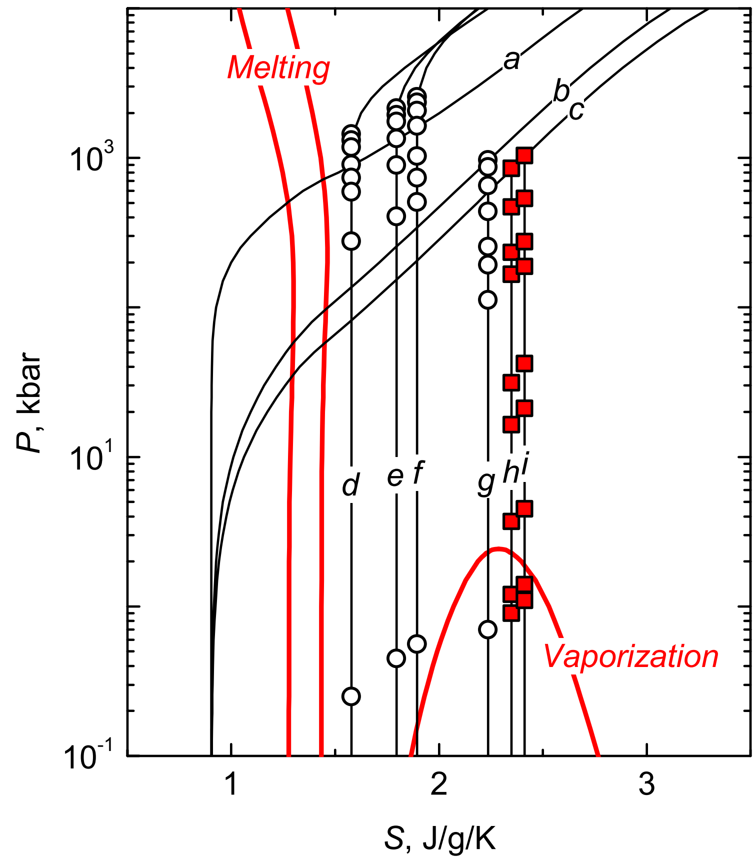


Velocity of Surface Al – C (VISAR profile)



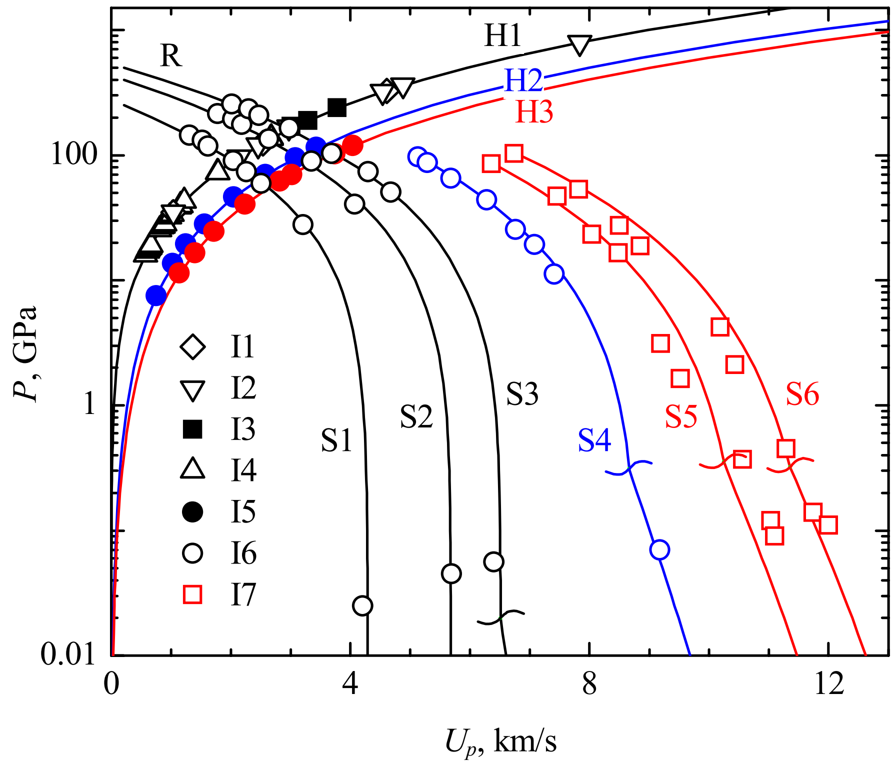
Shock Hugoniots & Release Isentropes

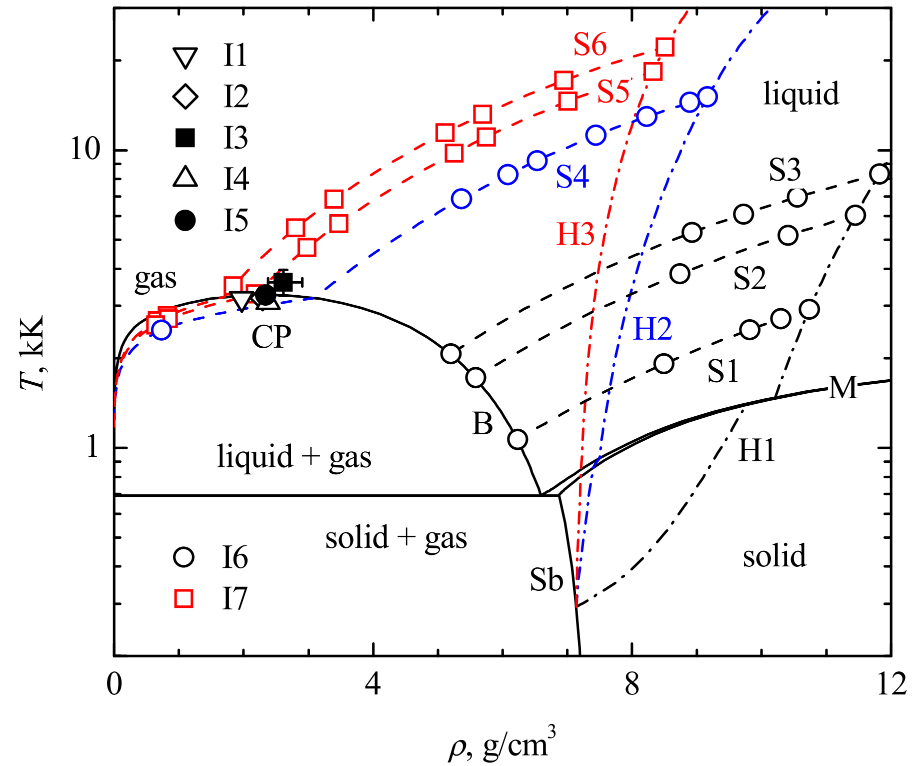




Khishchenko K. V., Zhernokletov M. V., Fortov V. E. , Kirshanov S. I., Kovalev A. E., Lomonosov I. V., Mochalov M. A., Shuikin A. N. // High Temp.–High Press. 2008. V. 37. Issue 4. P. 291–298.

Equation of State for Zinc in Shock and Release Waves





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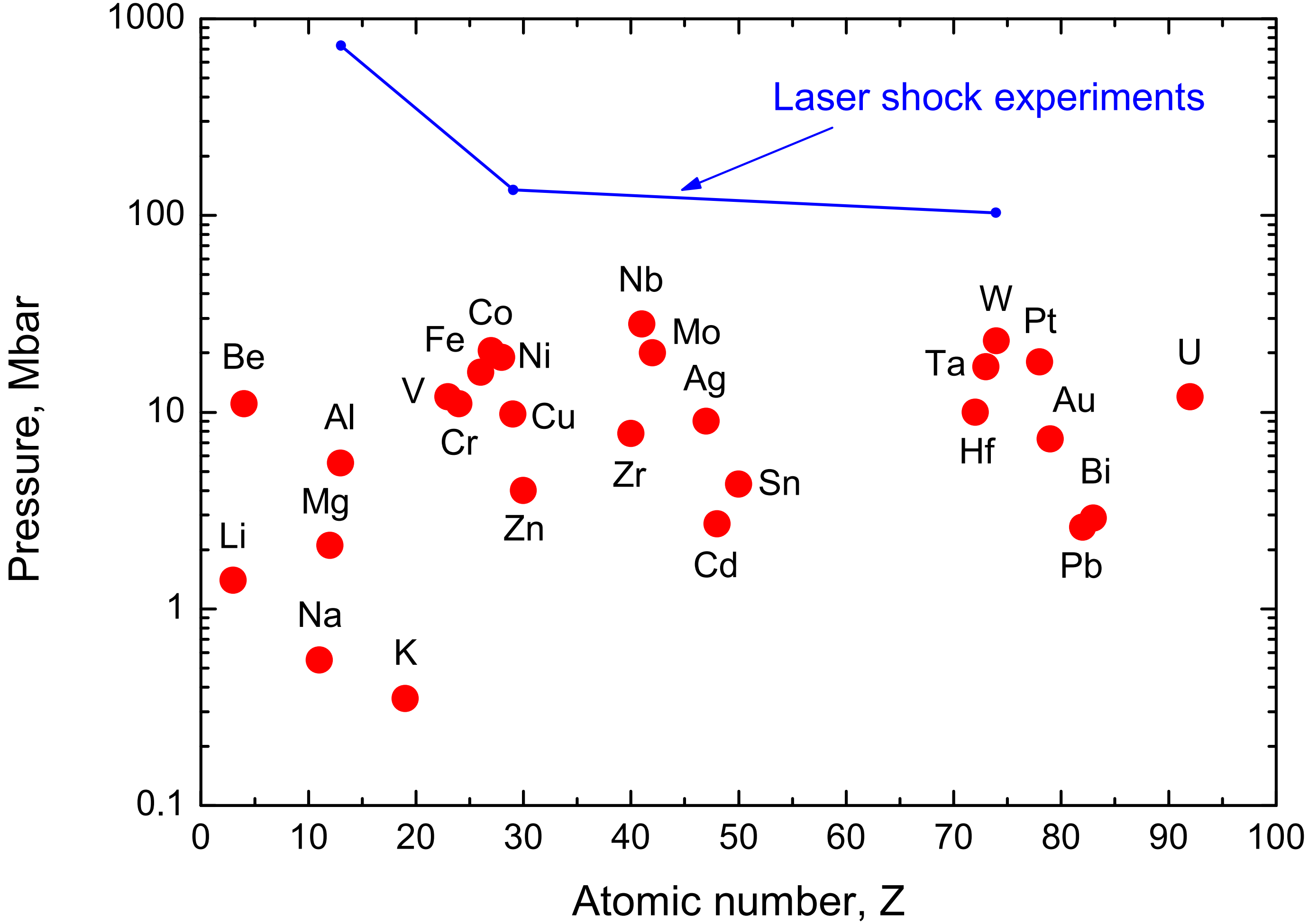
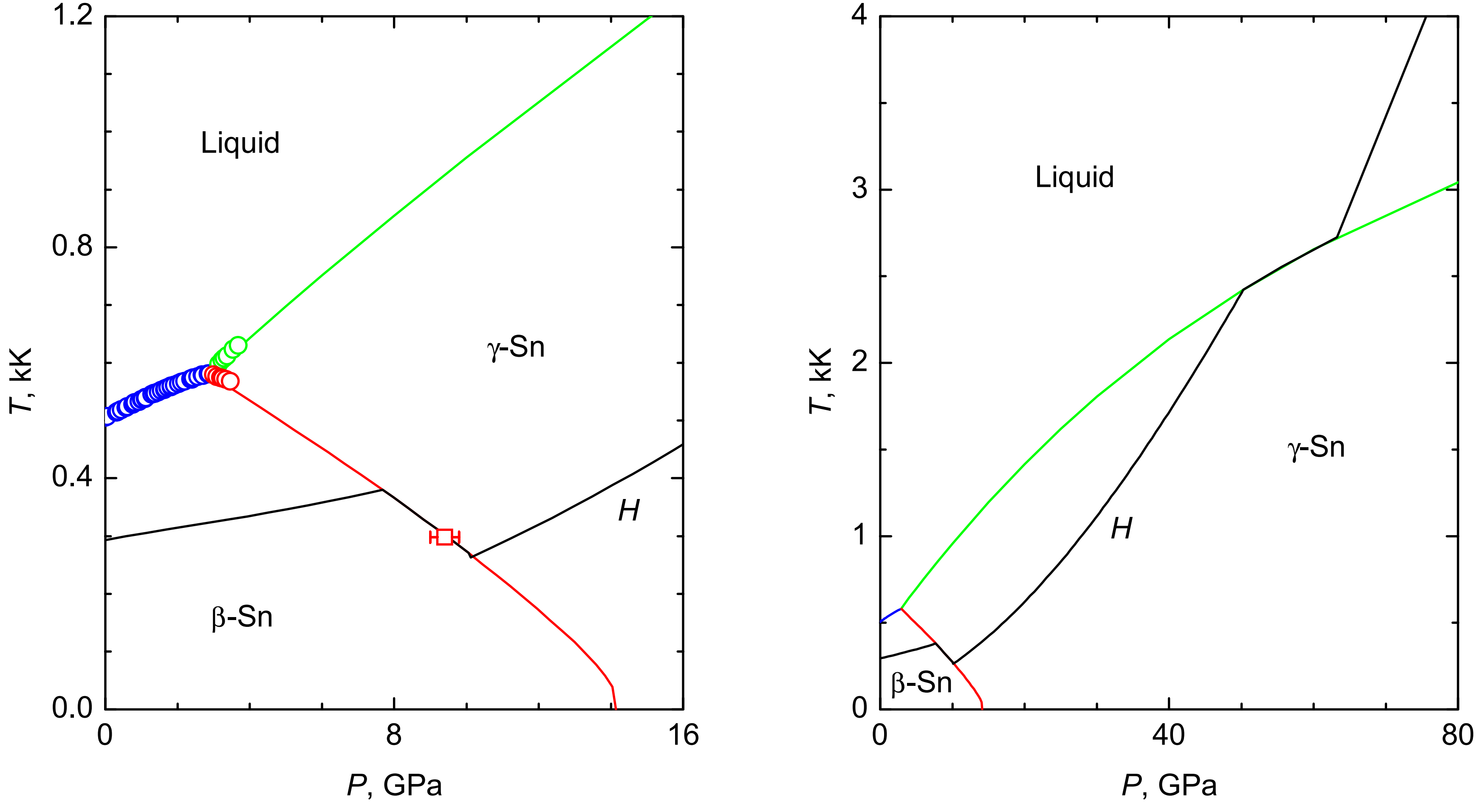
Pressure of Shock Compression of a Sample to Be Achieved for Critical Point Investigation in Isentropic Release Waves

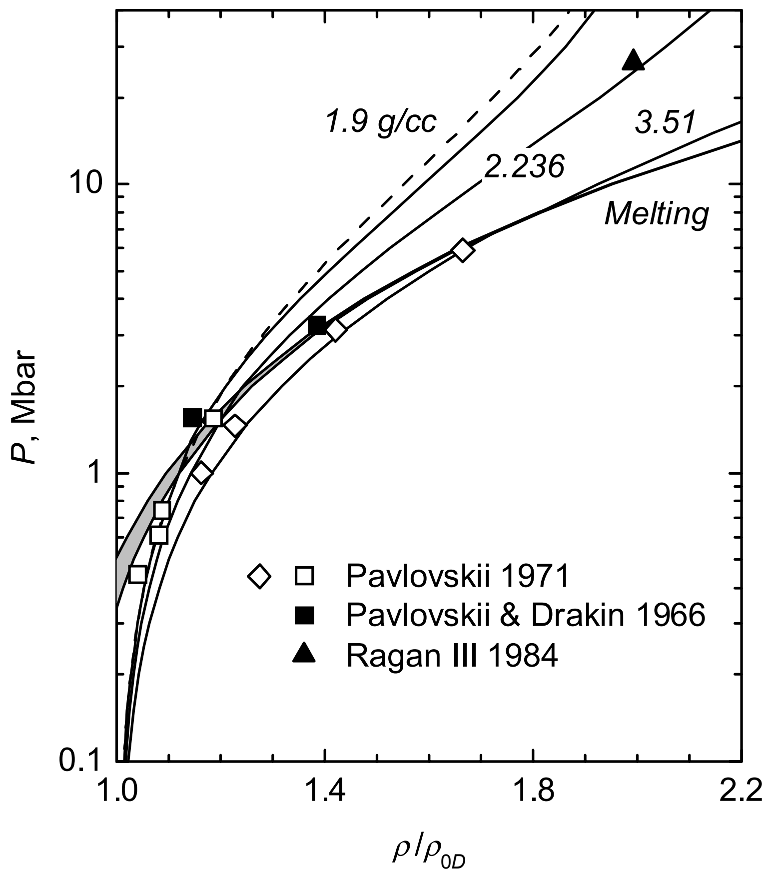


Phase Diagram of Tin

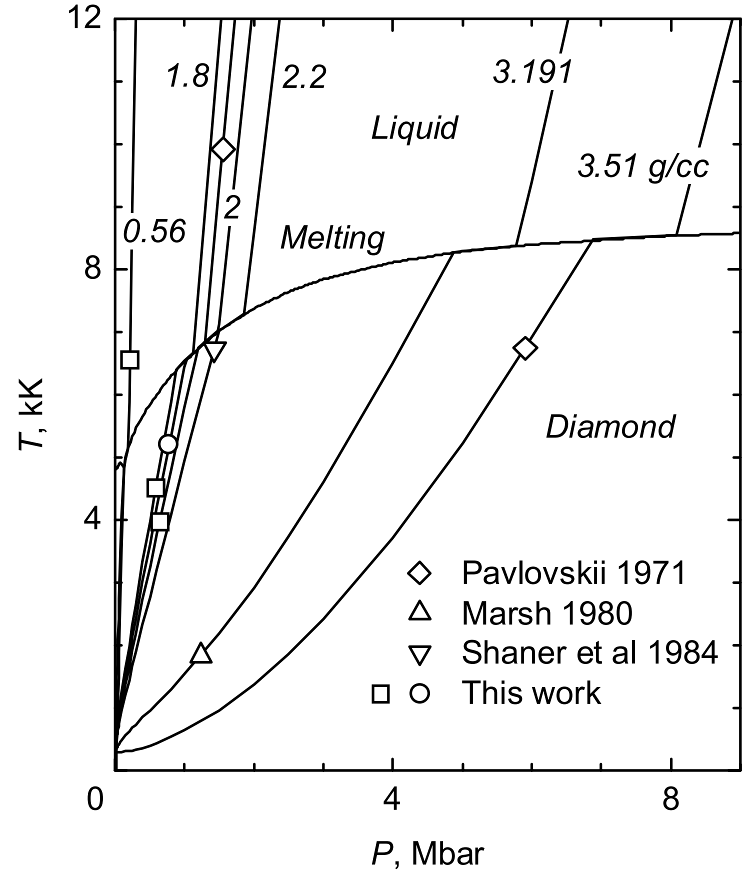


Equation of State for Carbon

Shock Hugoniots of Diamond



Carbon Phase Diagram



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Thank You