Двухтемпературная термо- и гидродинамика при короткоимпульсном лазерном воздействии на металлы

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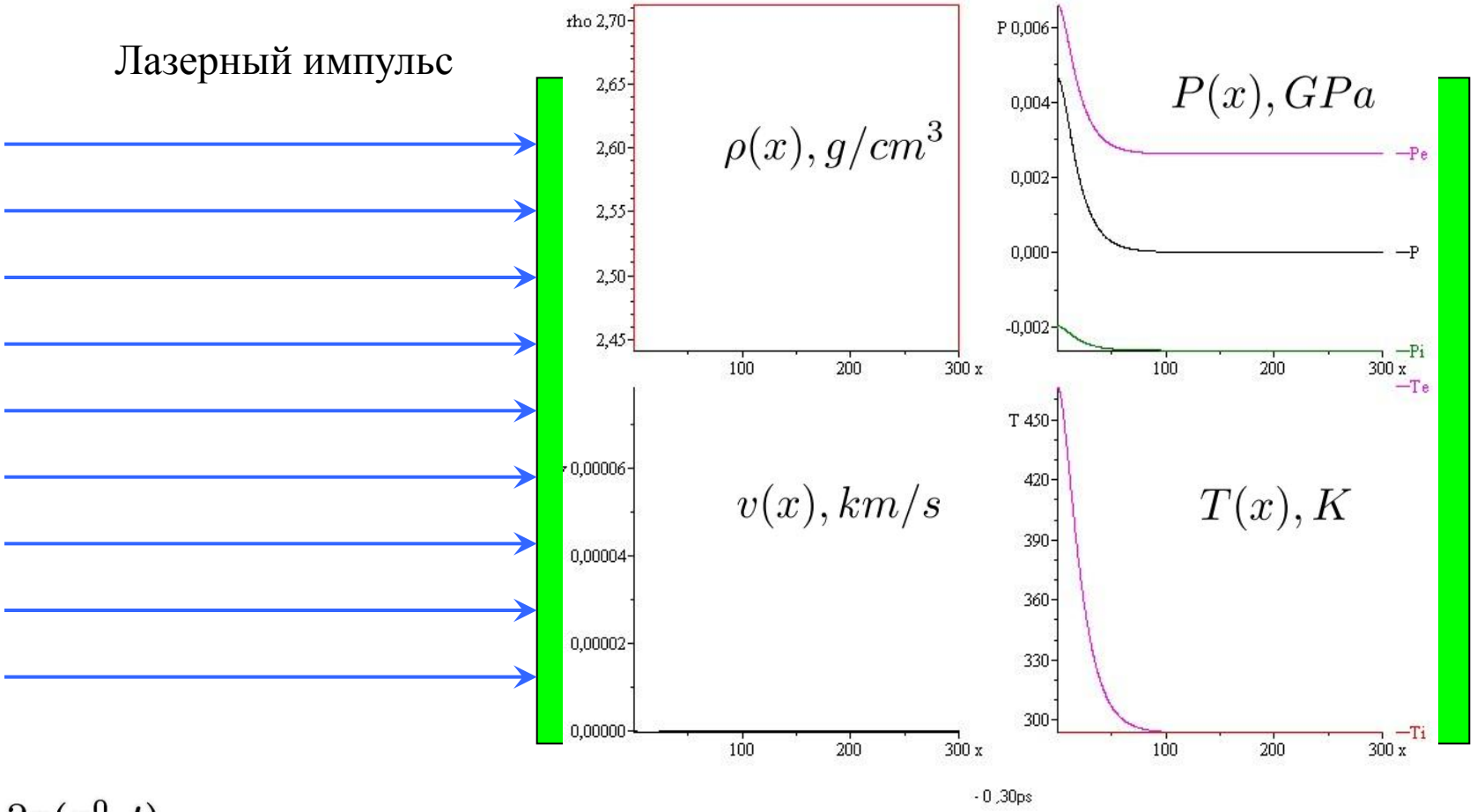
Эксперимент: Агранат, М.Б., Ашитков, С.И. и др., ОИВТ РАН

Лазерный импульс



$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \rho \partial x(x^0,t) = \rho^0 \partial x^0, \quad (1)$$

$$\rho^0 \frac{\partial v}{\partial t} = -\partial p \partial x^0, \quad p = p_e + p_i, \quad (2)$$

$$\rho^0 \frac{\partial (E_e/\rho)}{\partial t} = \frac{\partial}{\partial x^0}\left(\frac{\rho \kappa_e}{\rho^0}\frac{\partial T_e}{\partial x^0}\right) - p_e \frac{\partial v}{\partial x^0} - \bar{\alpha}(T_e - T_i) + \bar{Q}(x^0,t), \quad (3)$$

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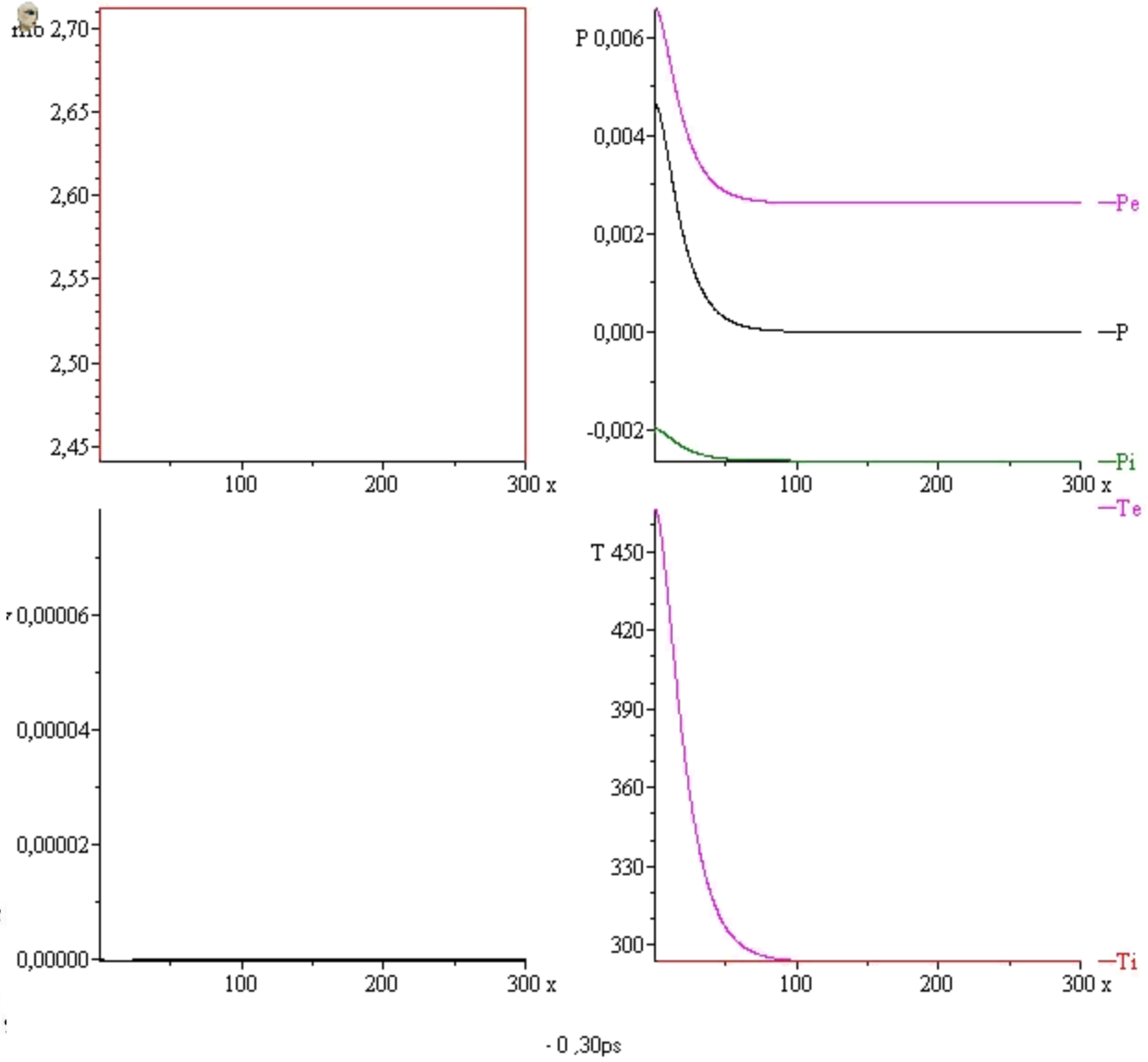
$$p_e = p_e(\rho, T_e), \; p_i = p_i(\rho, T_i), \quad E_e = E_e(\rho, T_e), \; E_i = E_i(\rho, T_i)$$



$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \rho\partial x$$

$$\rho^0\frac{\partial v}{\partial t} = -\partial p\partial x^0,$$

$$\rho^0\frac{\partial(E_e/\rho)}{\partial t} = \frac{\partial}{\partial x^0}\left(\frac{\rho\kappa_e}{\rho^0}\frac{\partial T_e}{\partial x^0}\right) - p_e\frac{\partial v}{\partial x^0} - \bar{\alpha}(T_e - T_i) + \bar{Q}(x^0,t), \quad (3)$$

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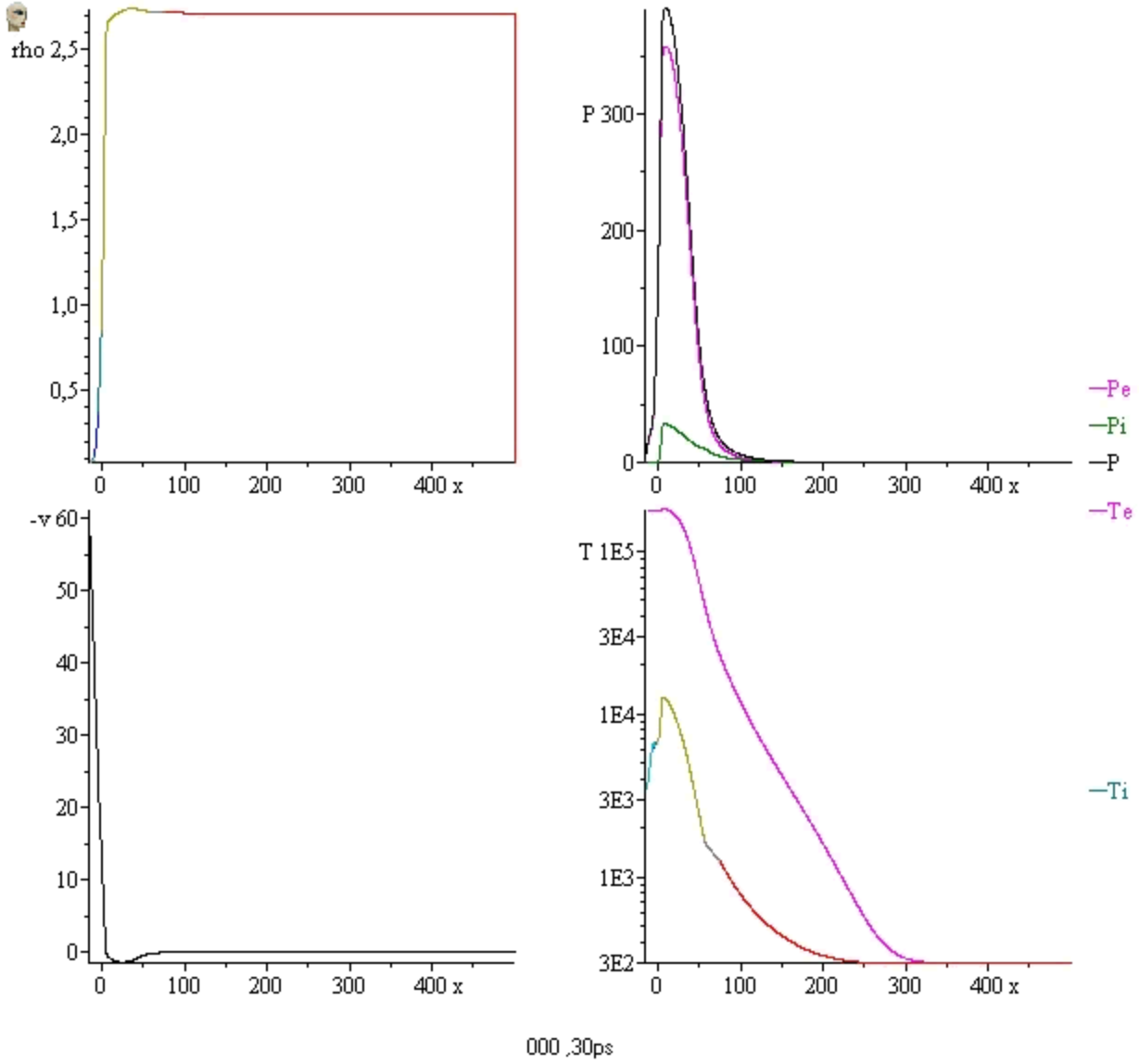

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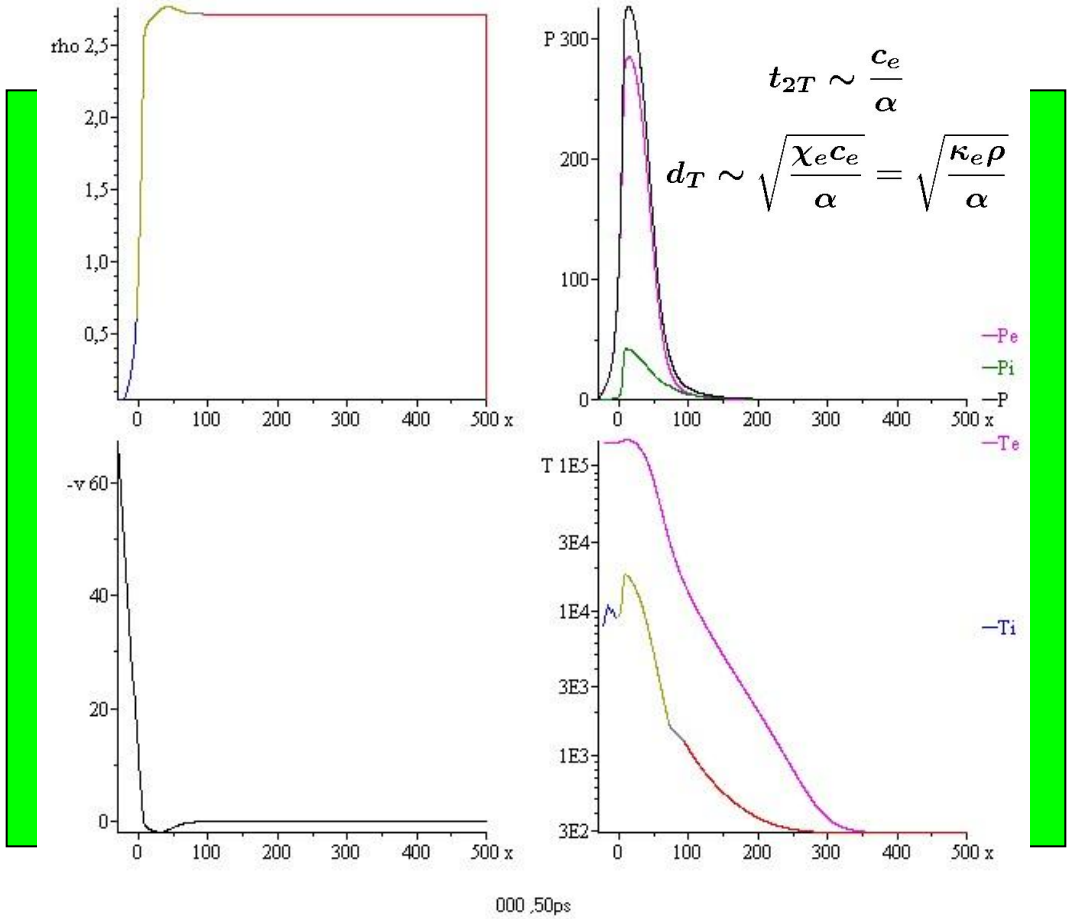

$$t_{2T} \sim \frac{c_e}{\alpha}$$

$$d_T \sim \sqrt{\frac{\chi_e c_e}{\alpha}} = \sqrt{\frac{\kappa_e \rho}{\alpha}}$$

$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \rho \partial x(x^0,t) = \rho^0 \partial x^0, \quad (1)$$

$$\rho^0 \frac{\partial v}{\partial t} = -\partial p \partial x^0, \quad p = p_e + p_i, \quad (2)$$

$$\rho^0 \frac{\partial (E_e/\rho)}{\partial t} = \frac{\partial}{\partial x^0}\left(\frac{\rho \kappa_e}{\rho^0}\frac{\partial T_e}{\partial x^0}\right) - p_e \frac{\partial v}{\partial x^0} - \bar{\alpha}(T_e - T_i) + \bar{Q}(x^0,t), \quad (3)$$

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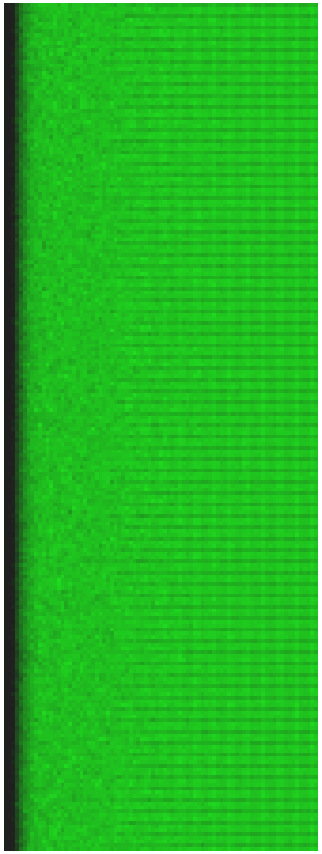
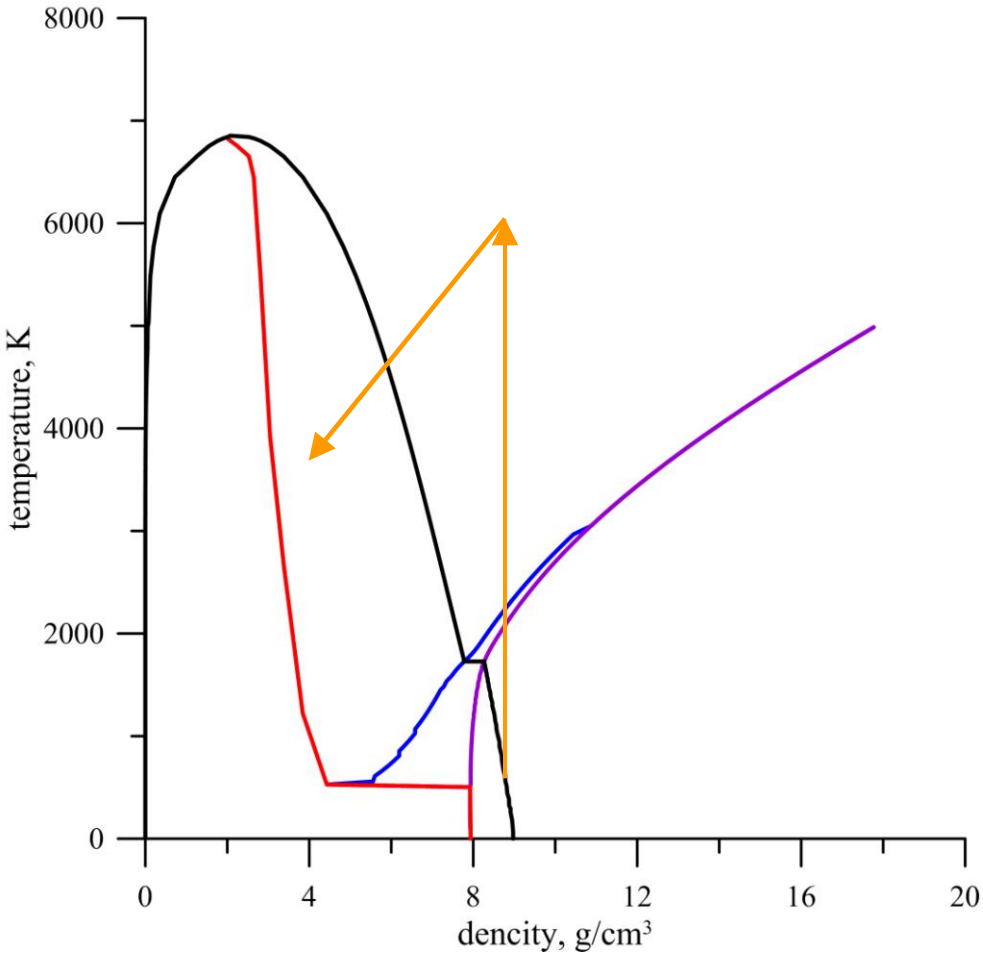
$$p_e = p_e(\rho, T_e), \; p_i = p_i(\rho, T_i), \quad E_e = E_e(\rho, T_e), \; E_i = E_i(\rho, T_i)$$



Фазовая диаграмма (Ni)



Динамический критерий разрыва

$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \rho \partial x(x^0,t) = \rho^0 \partial x^0, \quad (1)$$

$$\rho^0 \frac{\partial v}{\partial t} = -\partial p \partial x^0, \quad p = p_e + p_i, \quad (2)$$

$$\rho^0 \frac{\partial (E_e/\rho)}{\partial t} = \frac{\partial}{\partial x^0}\left(\frac{\rho \kappa_e}{\rho^0}\frac{\partial T_e}{\partial x^0}\right) - p_e \frac{\partial v}{\partial x^0} - \bar{\alpha}(T_e - T_i) + \bar{Q}(x^0,t), \quad (3)$$

$$\rho^0 \frac{\partial (E_i/\rho)}{\partial t} = \frac{\partial}{\partial x^0}\left(\frac{\rho \kappa_i}{\rho^0}\frac{\partial T_e}{\partial x^0}\right) - p_i \frac{\partial v}{\partial x^0} + \bar{\alpha}(T_e - T_i). \quad (4)$$

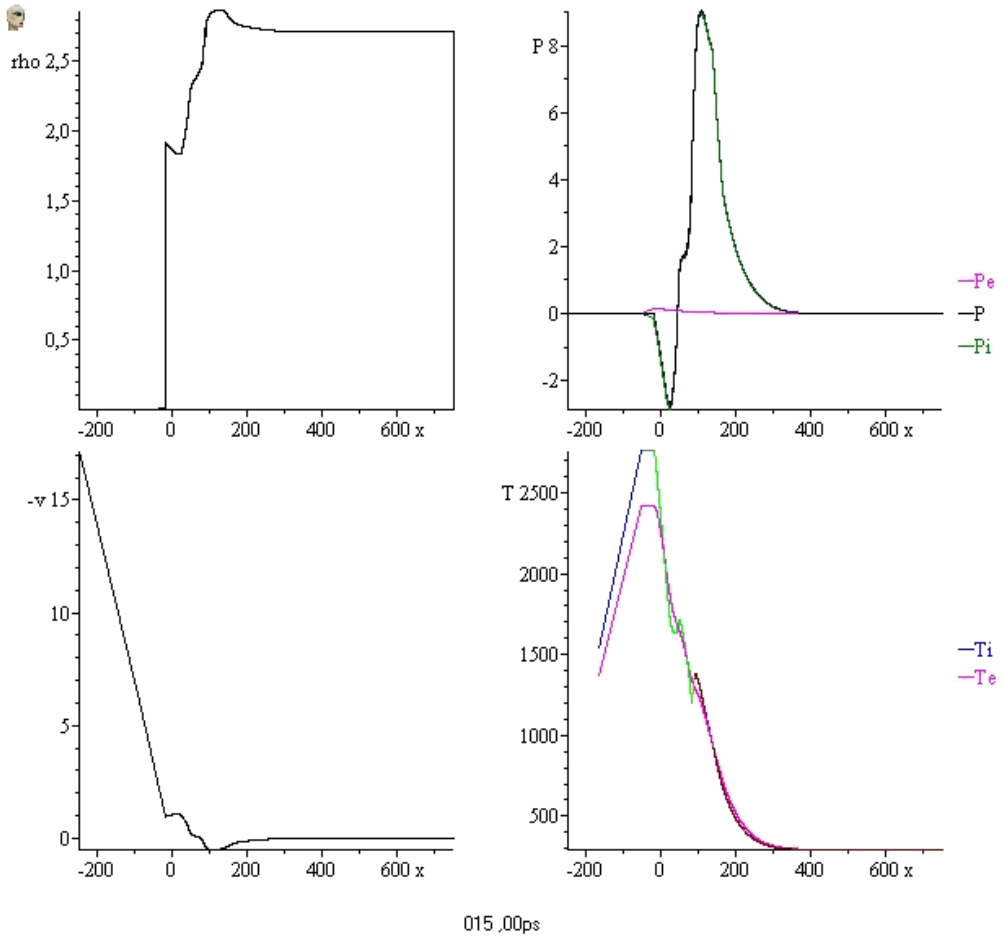
$$p_e = p_e(\rho, T_e), \; p_i = p_i(\rho, T_i), \quad E_e = E_e(\rho, T_e), \; E_i = E_i(\rho, T_i)$$

$$t_{str} \geq \tau_{nucl}, \quad t_{str} = \min\left(\frac{\rho}{d\rho/dt}, t - t_{s0}\right),$$

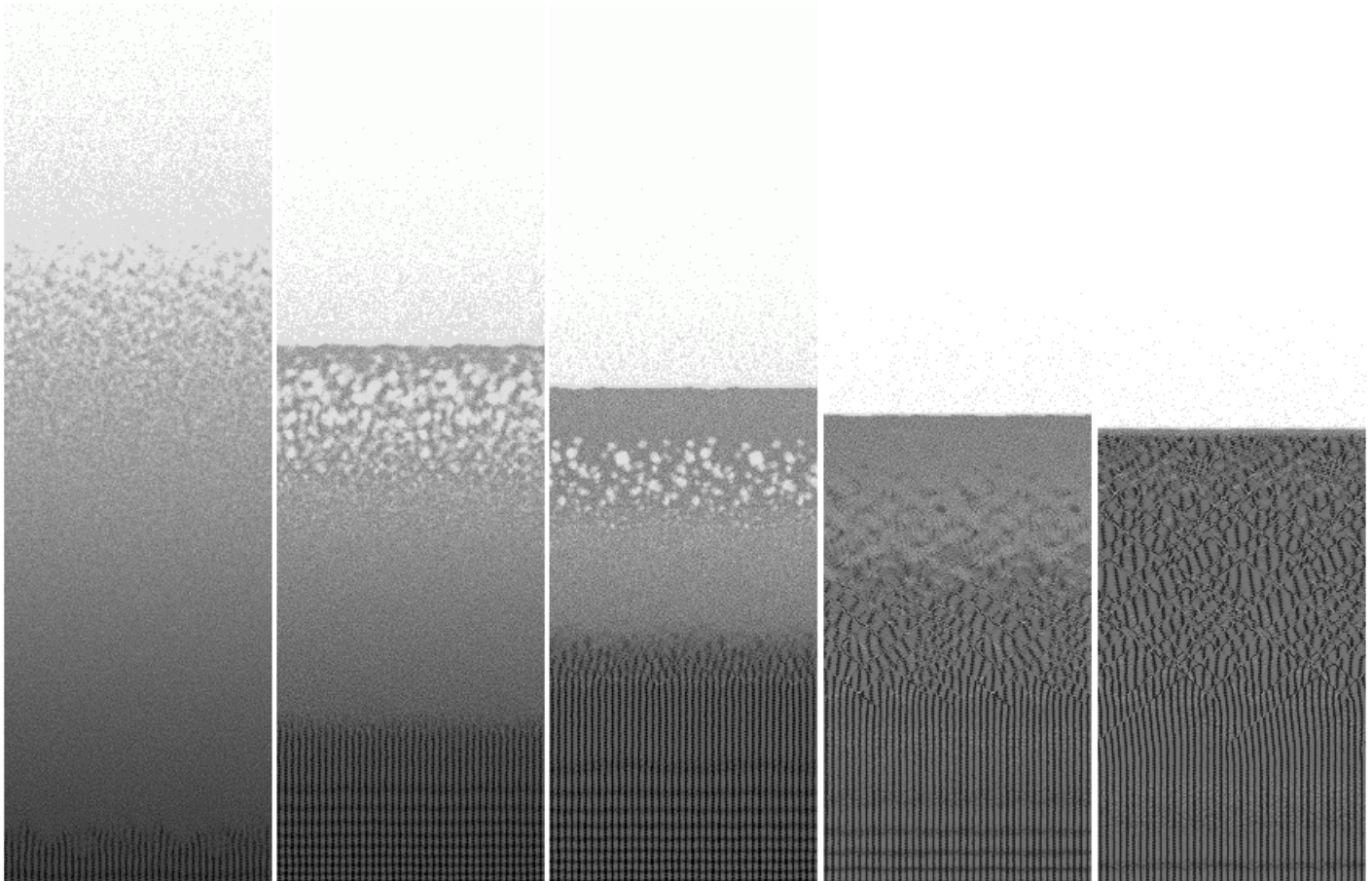
$$\tau_{nucl} = \frac{-p\eta}{V n_{at}^2 \sigma(T_i)^{3/2} (k_B T_i)^{1/2}} \exp\left(\frac{W}{k_B T_i}\right), W = \frac{16\pi}{3}\frac{\sigma(T_i)^3}{p^2}$$

$$V = \frac{4\pi}{3}(c_s t_{str})^3$$

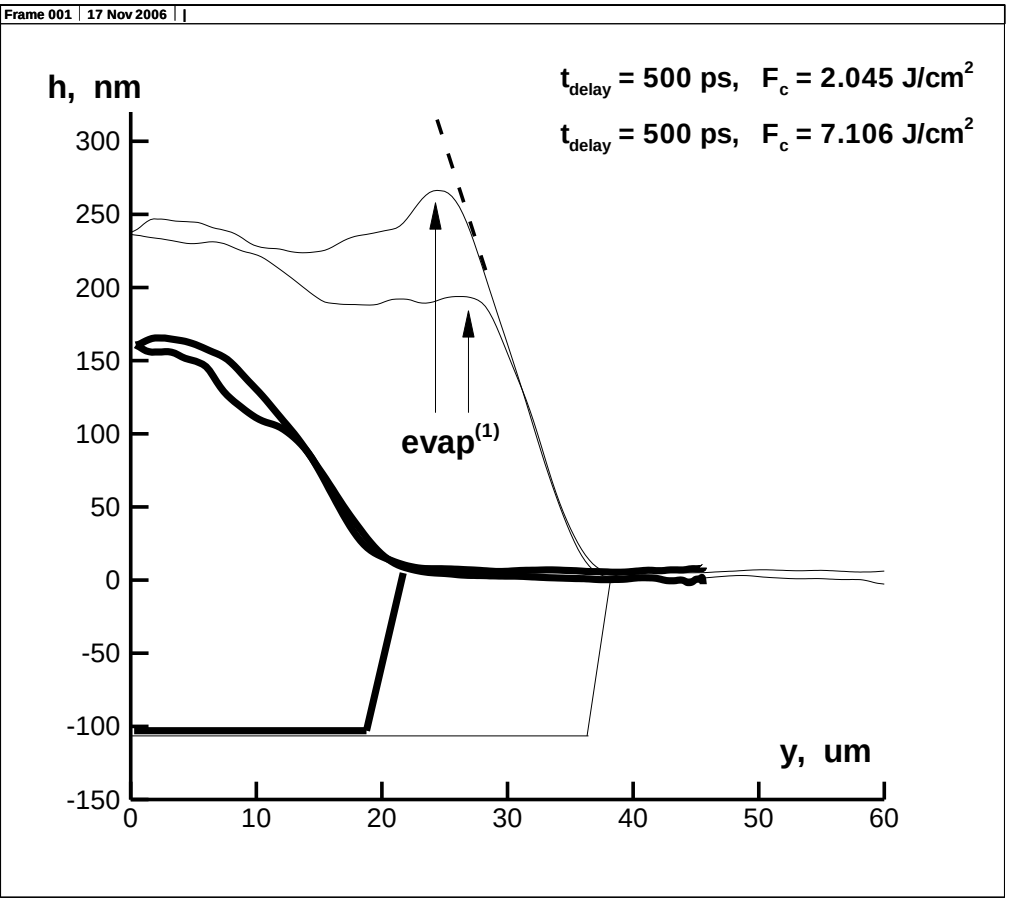
Отрыв приповерхностного слоя

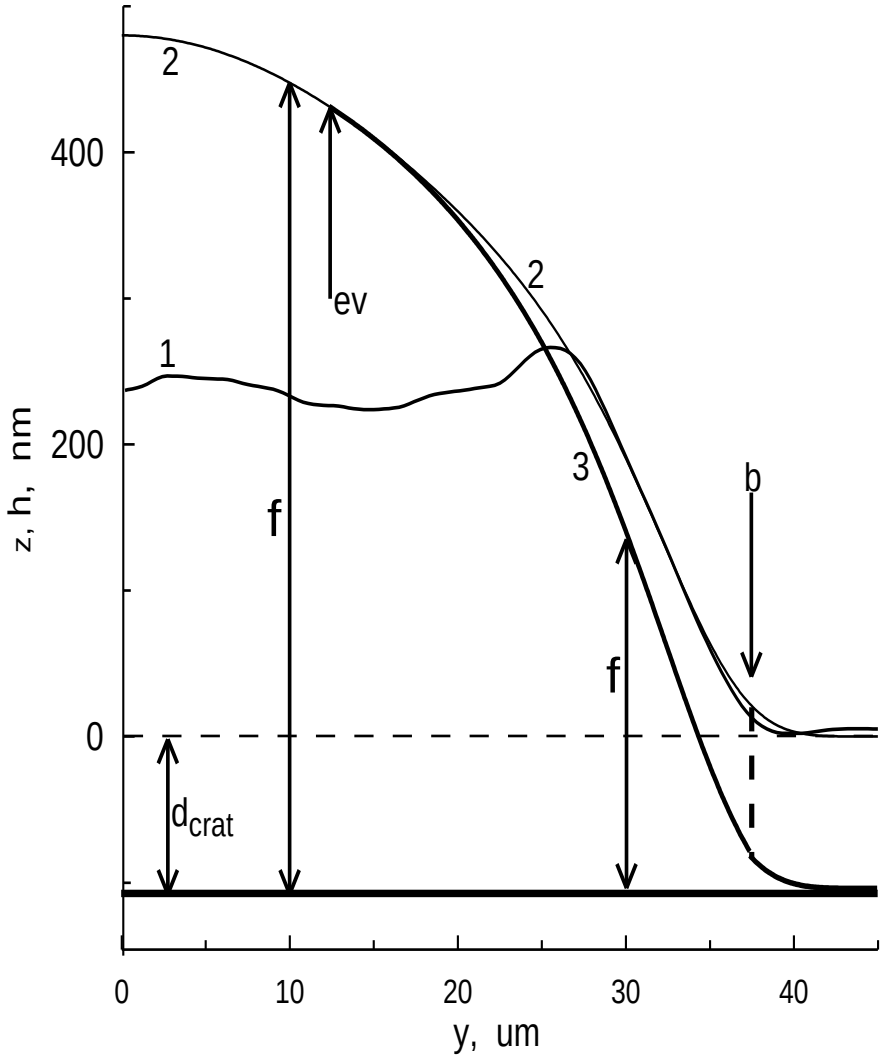


Формирование отлетающего купола и кратера

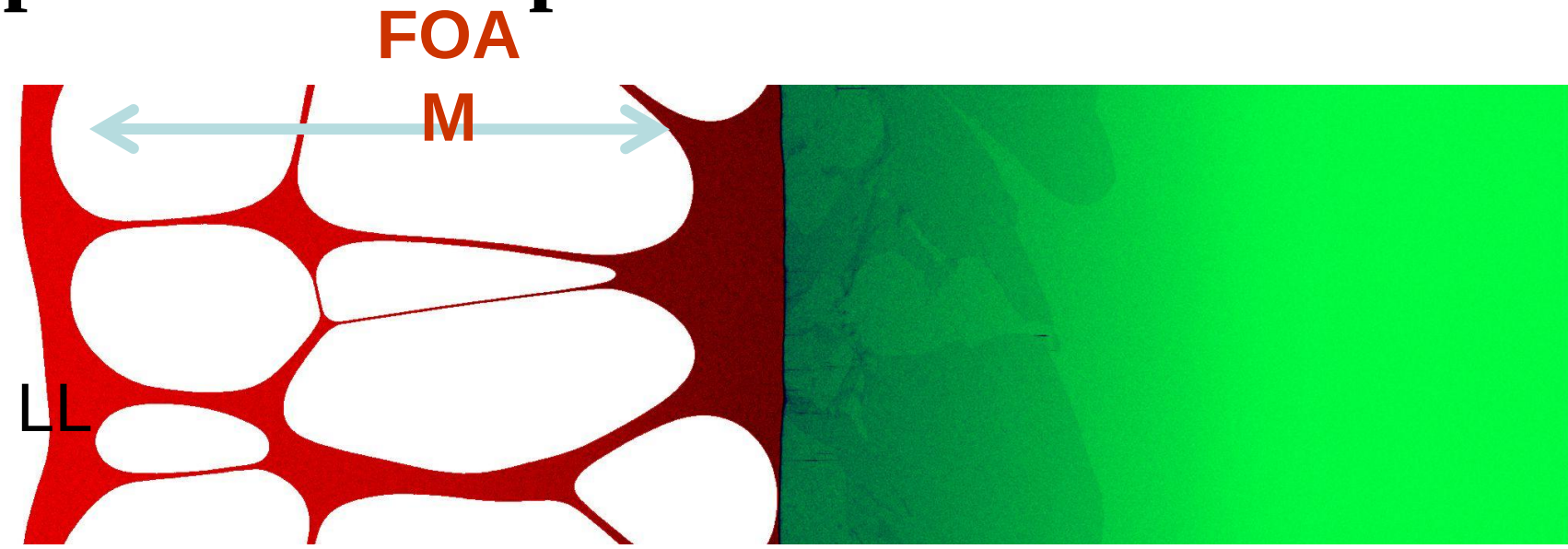


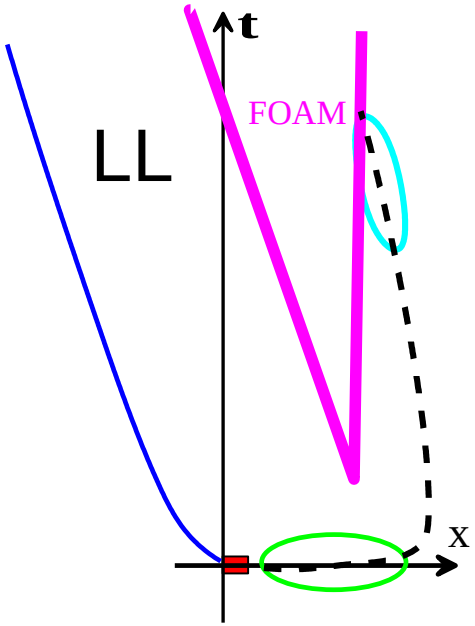
Формирование отлетающего купола и кратера





Dynamics of FOAM expansion and freezing process – competition between them





Red – liquid, **Green** – solid,

Al simulated by Zhakhovsky 2009 EAM

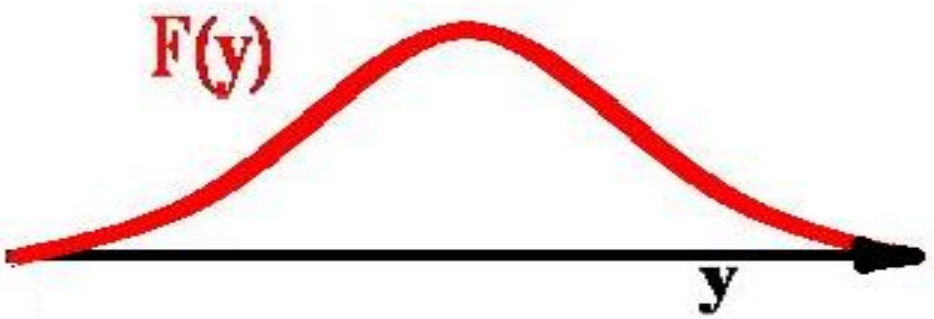
F_{abs} = 120 mJ/cm^2, τ_L = 100 fs - duration

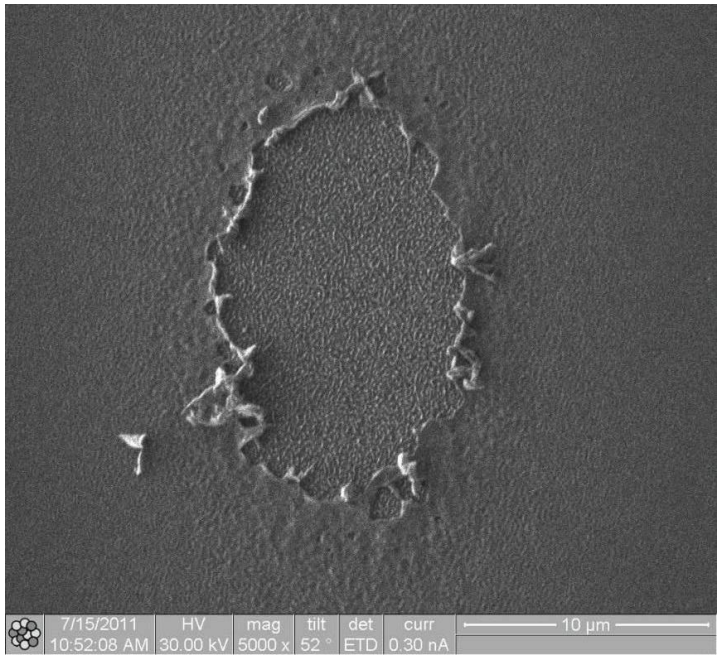
time instant = 512 ps

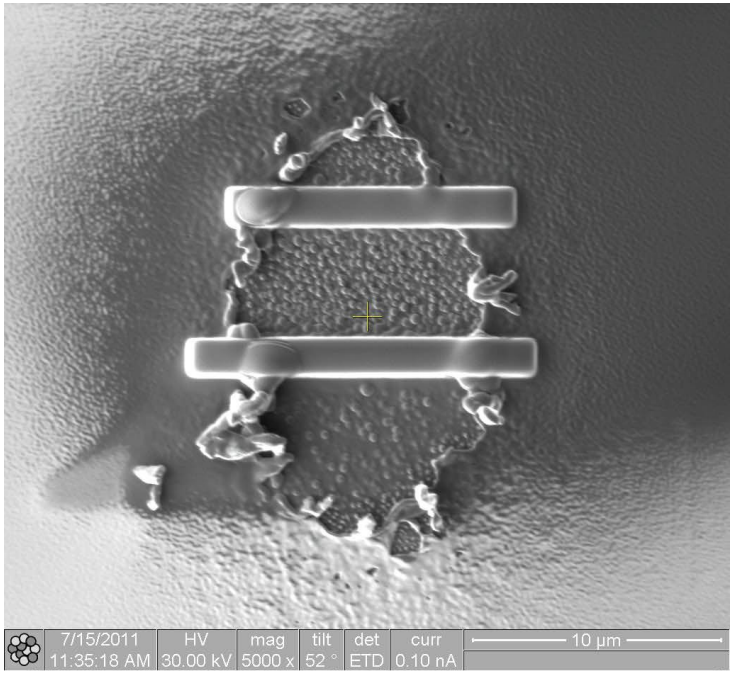
Huge MD sim.: lateral distance = 240 nm.

Crystallization front interacts with bottom of foam

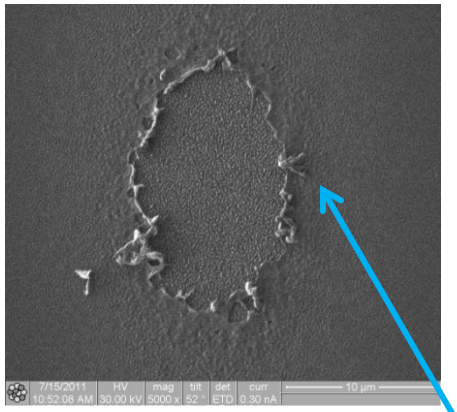
Laser beam profile and crater profile

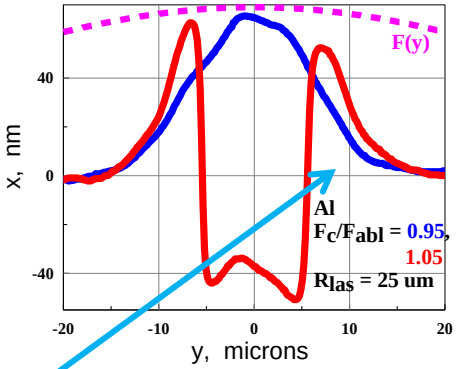


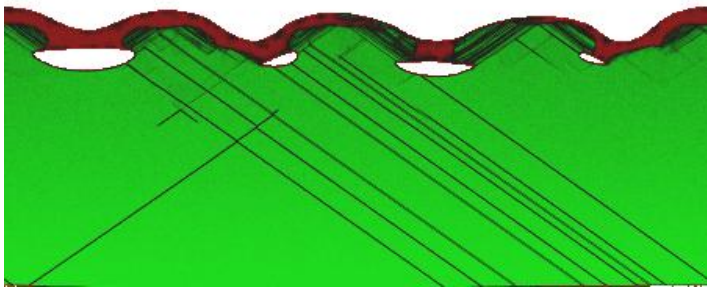


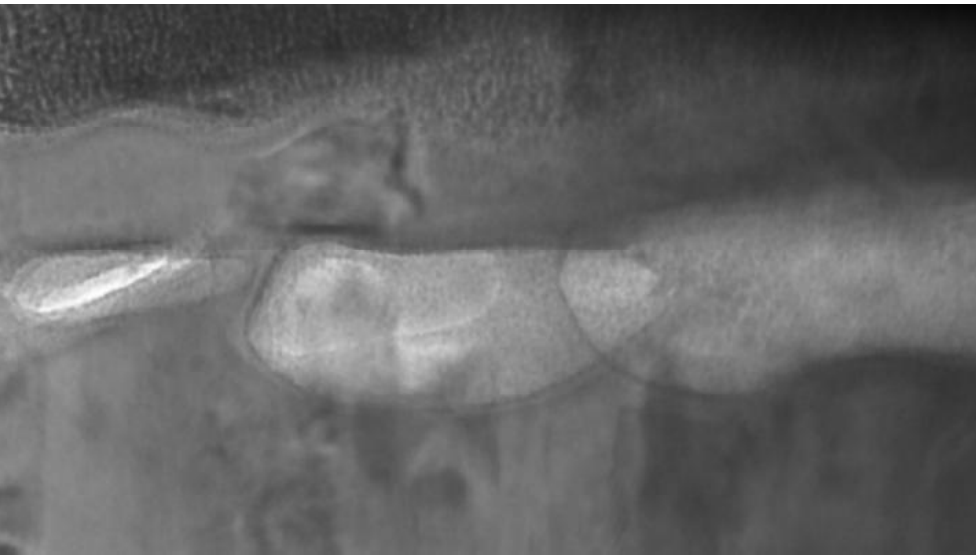


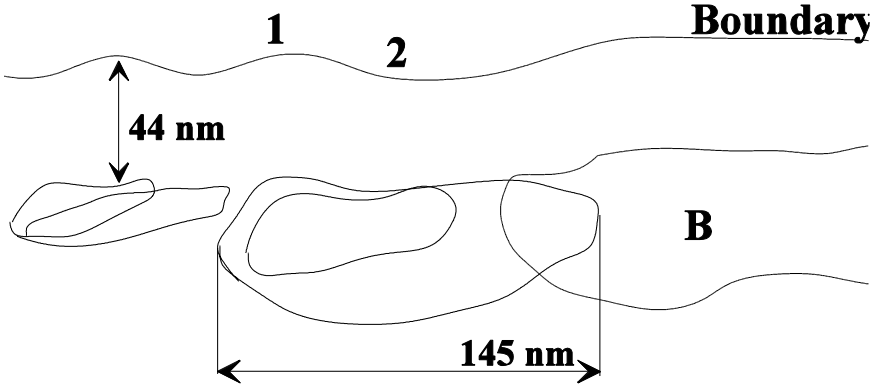
Huge residual deformations (swellings) and frozen nano-bubbles seen in exp & sim











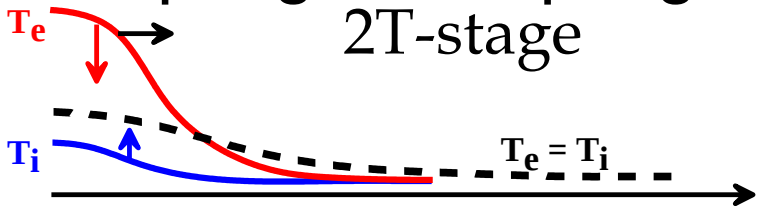
Diagnostics: Lamella FIB/TEM (Ashitkov et al., JETP Lett., 2012)

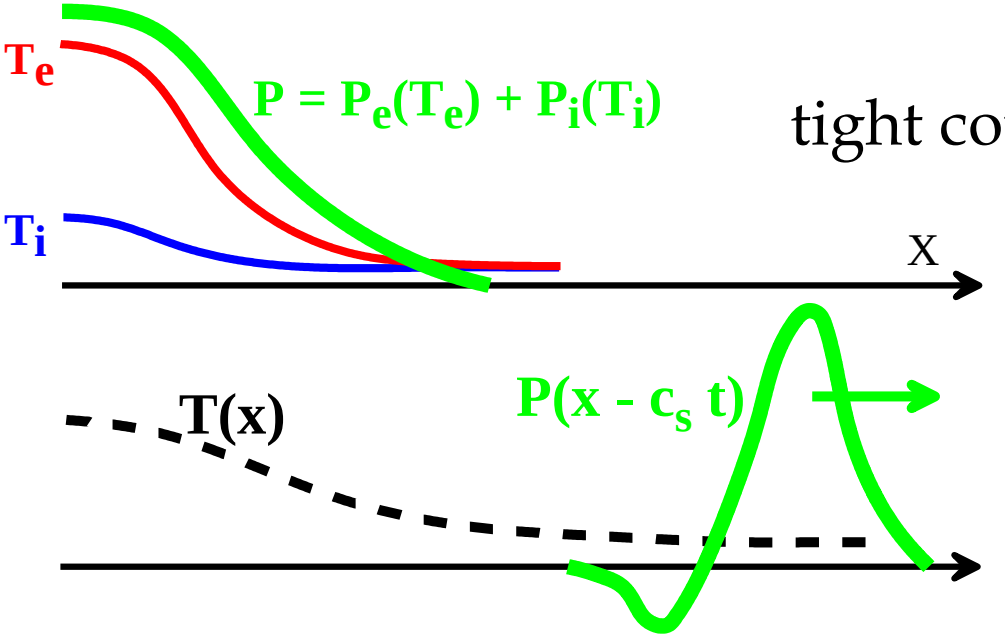
Large scale very long time MD sims. Spatial scales, depth under surface,shape of nano-bubbles, and shape of surface above them

Disk type (oblate spheroids) nano-bubbles, bubbles and surface above are in anti-phase → surface above bubble is not convex, it is concave !

Exps and Sims

Thermal and dynamical phenomena - coupling/decoupling

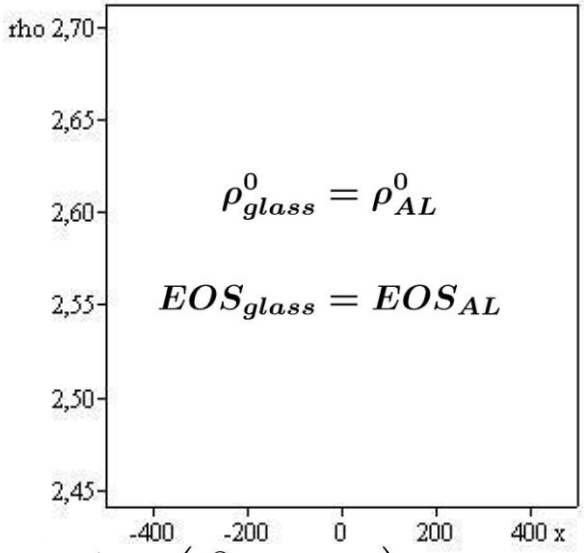


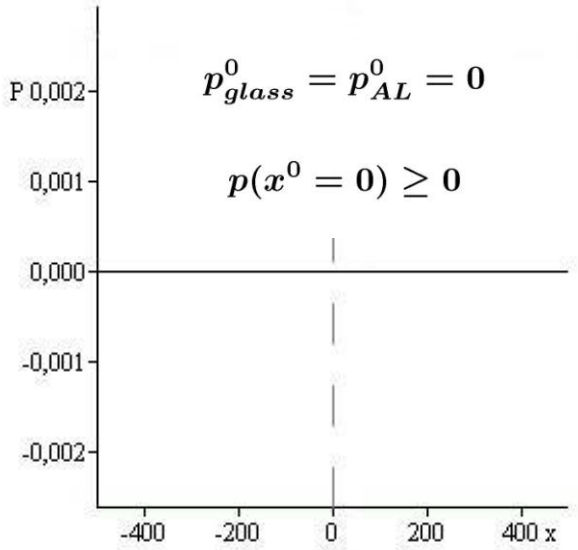


tight coupling of T and P-profiles

T – P decoupling

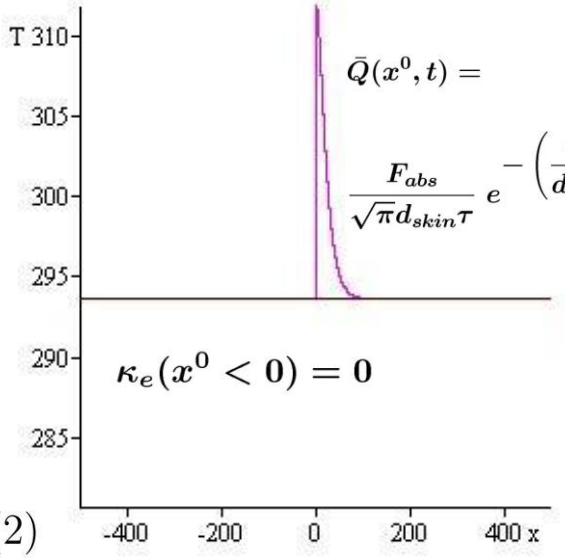
- At the two-temperature state, pressure "immediately" follows T_e and T_i – tight coupling of P-profile to local internal energy
- While after relaxation T-profile remains "frozen" near surface but P-profile runs away with speed of sound (total decoupling)





$$S_{xx} = F_{Sol} S_1, \quad S_1 = \frac{4}{3} G \left(\frac{\partial x}{\partial x^0} - R_{rc} \right)$$

$$\bar{E}_S = \frac{S_{xx}}{2\rho^0} \left(\frac{\partial x}{\partial x^0} - R_{rc} \right)$$



$$\rho^0 \frac{\partial v}{\partial t} = \frac{4}{3} G \frac{\partial}{\partial x^0} \frac{\partial x}{\partial t \partial x^0} = S_{xx} \frac{\partial v}{\partial x^0}$$

$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \frac{\partial x(x^0,t)}{\partial x^0} = \frac{\rho^0}{\rho}, \qquad (1)$$

$$\rho^0 \frac{\partial v}{\partial t} = -\frac{\partial P_{xx}}{\partial x^0}, \; P_{xx} = P_h - S_{xx}, \; P_h = P_e + P_i, \qquad (2)$$

$$\rho^0 \frac{\partial \bar{E}_e}{\partial t} = \frac{\partial}{\partial x^0} \left(\frac{\rho \kappa_e}{\rho^0} \frac{\partial T_e}{\partial x^0} \right) - P_e \frac{\partial v}{\partial x^0} - \bar{\alpha}(T_e - T_i) + \bar{Q}(x^0, t), \qquad (3)$$

$$\rho^0 \frac{\partial (\bar{E}_i + \bar{E}_S)}{\partial t} = \frac{\partial}{\partial x^0} \left(\frac{\rho \kappa_i}{\rho^0} \frac{\partial T_i}{\partial x^0} \right) - (P_i - S_{xx}) \frac{\partial v}{\partial x^0} + \bar{\alpha}(T_e - T_i) \qquad (4)$$

$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \frac{\partial x(x^0,t)}{\partial x^0} = \frac{\rho^0}{\rho}, \qquad (1)$$

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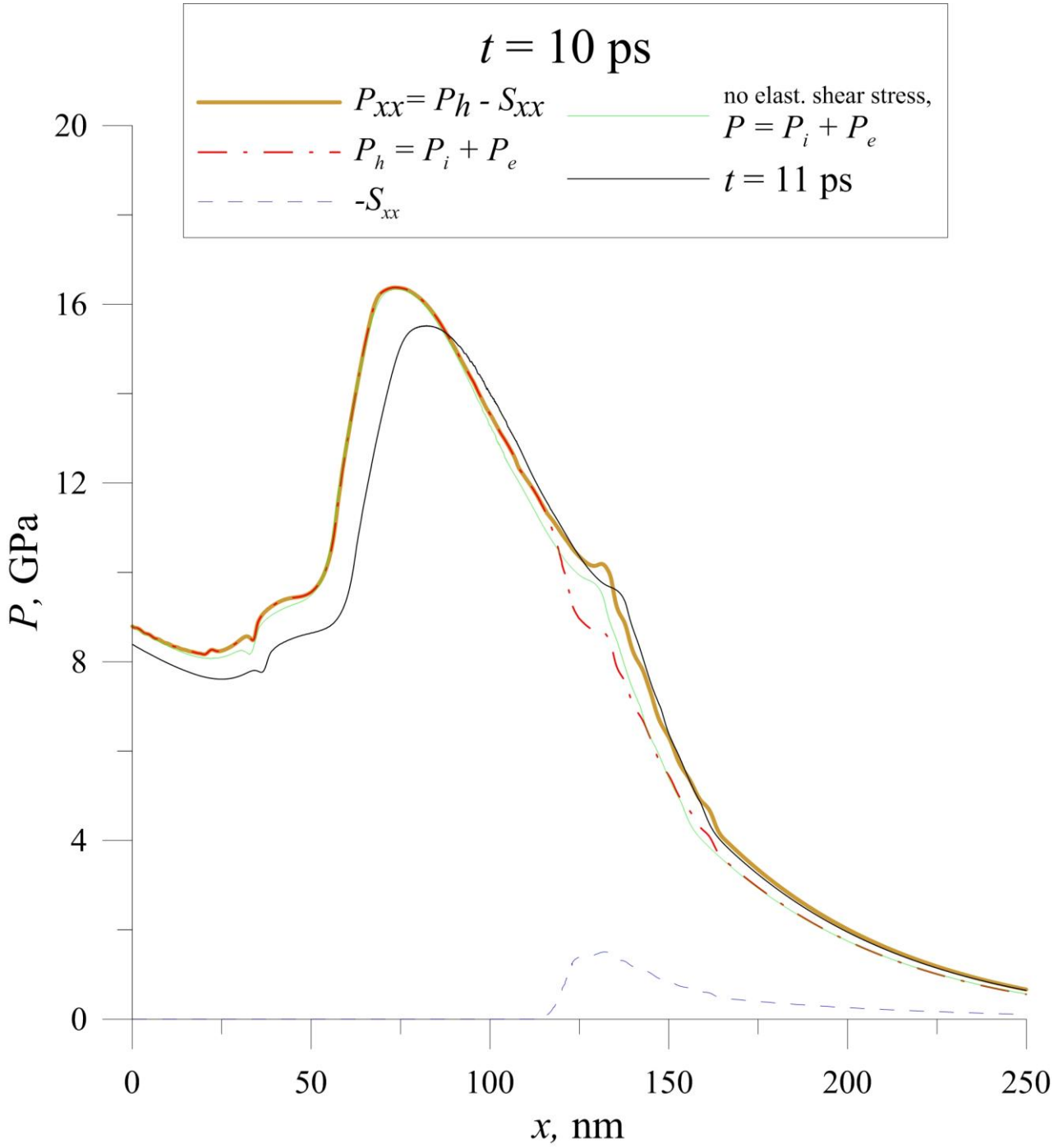
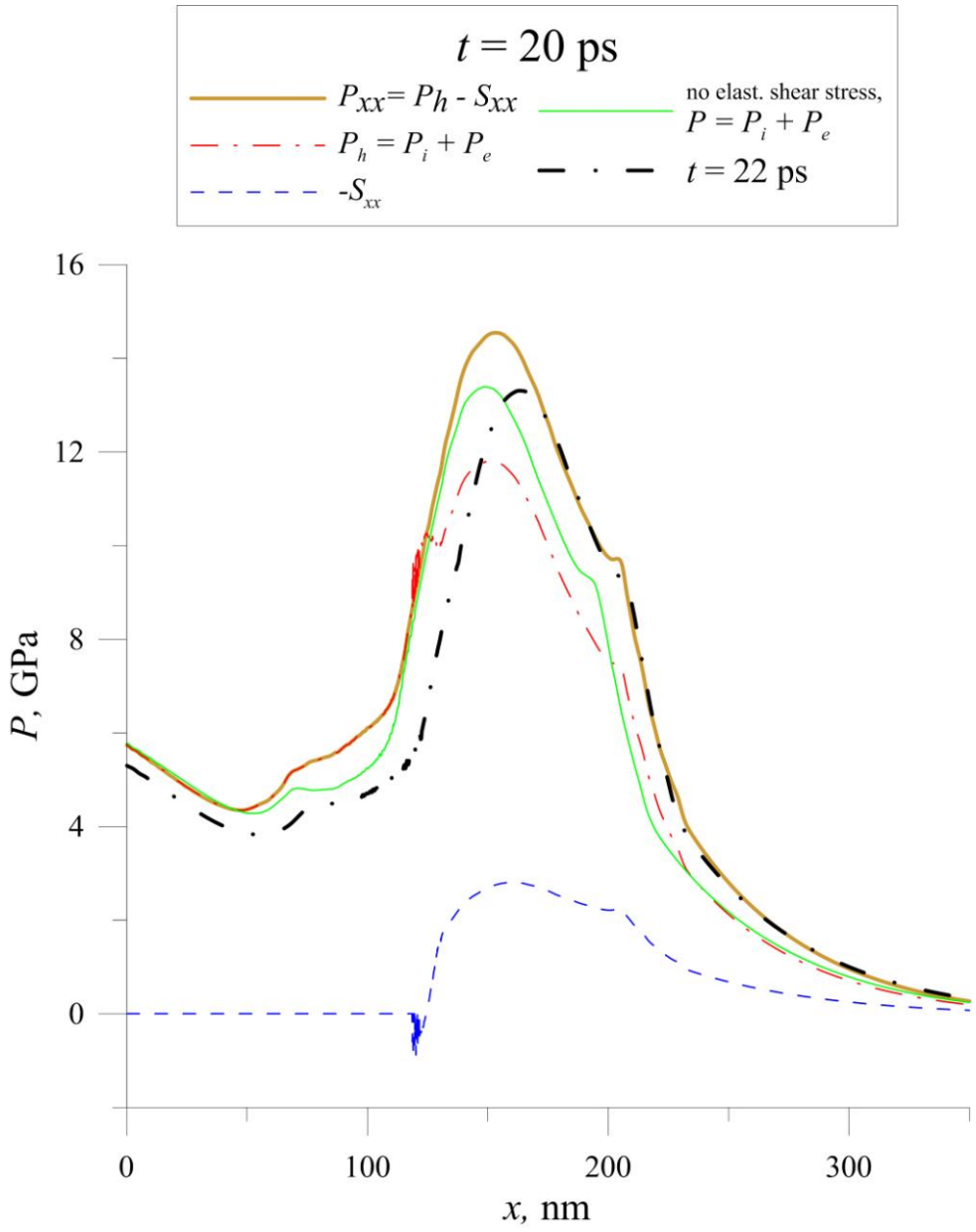
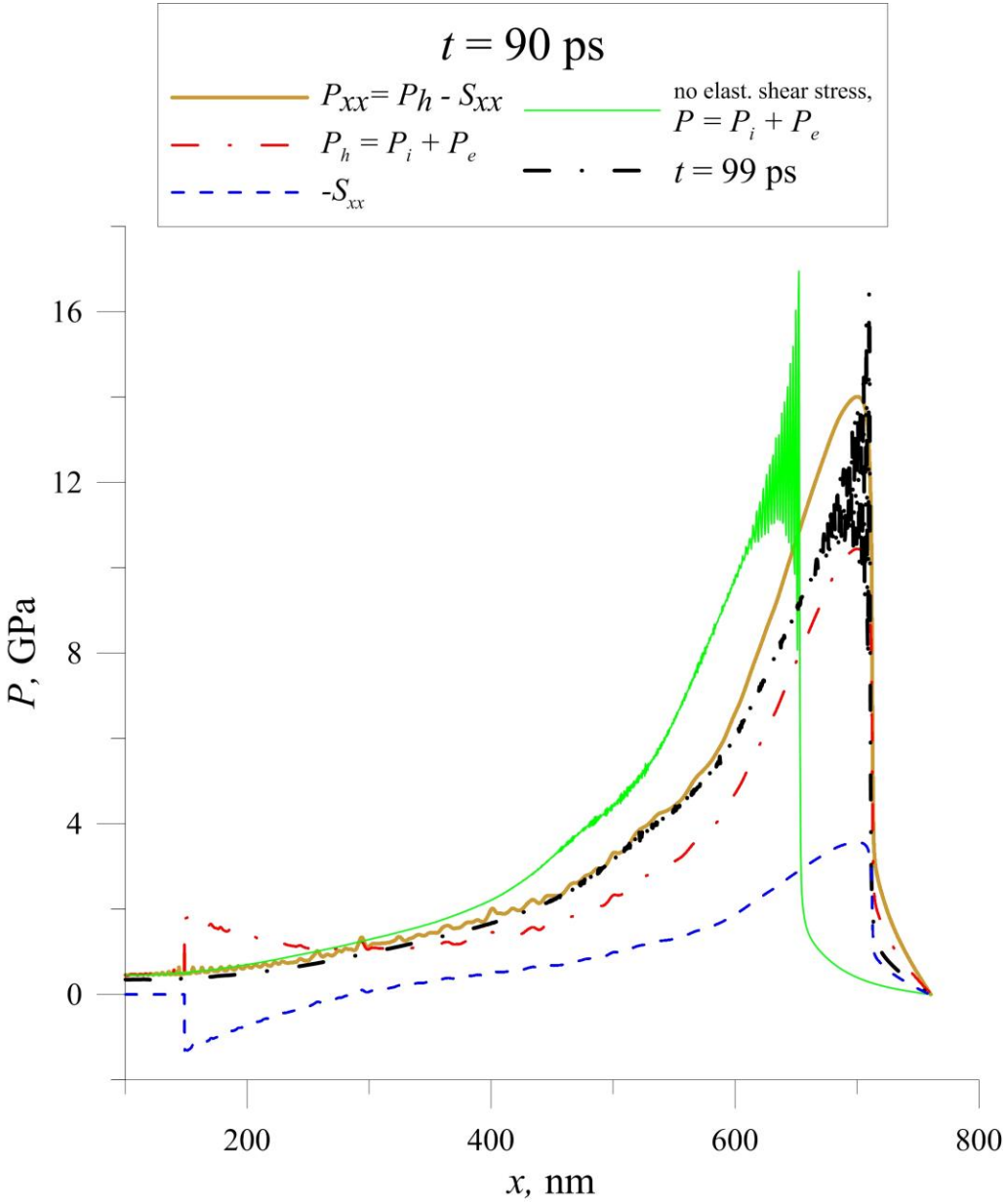
$$E = E_h + E_S, \quad E_h = E_e + E_i$$

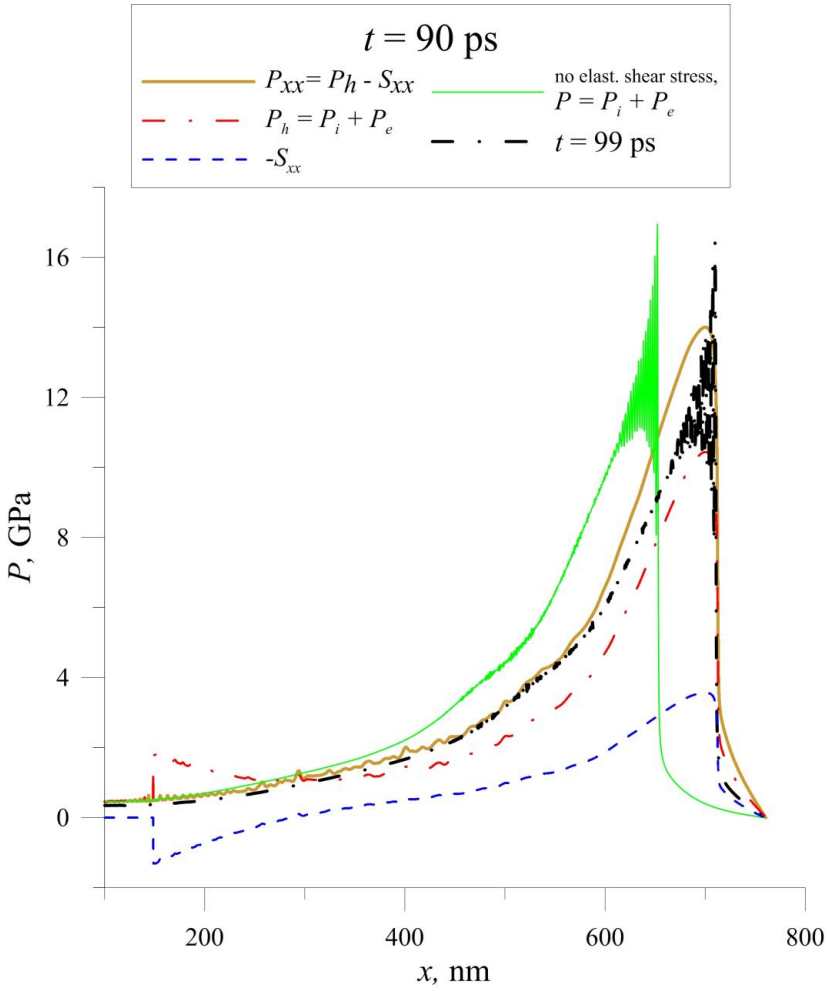
P_h, E_h К.В. Хищенко и др. http://teos.ficp.ac.ru/rusbank/

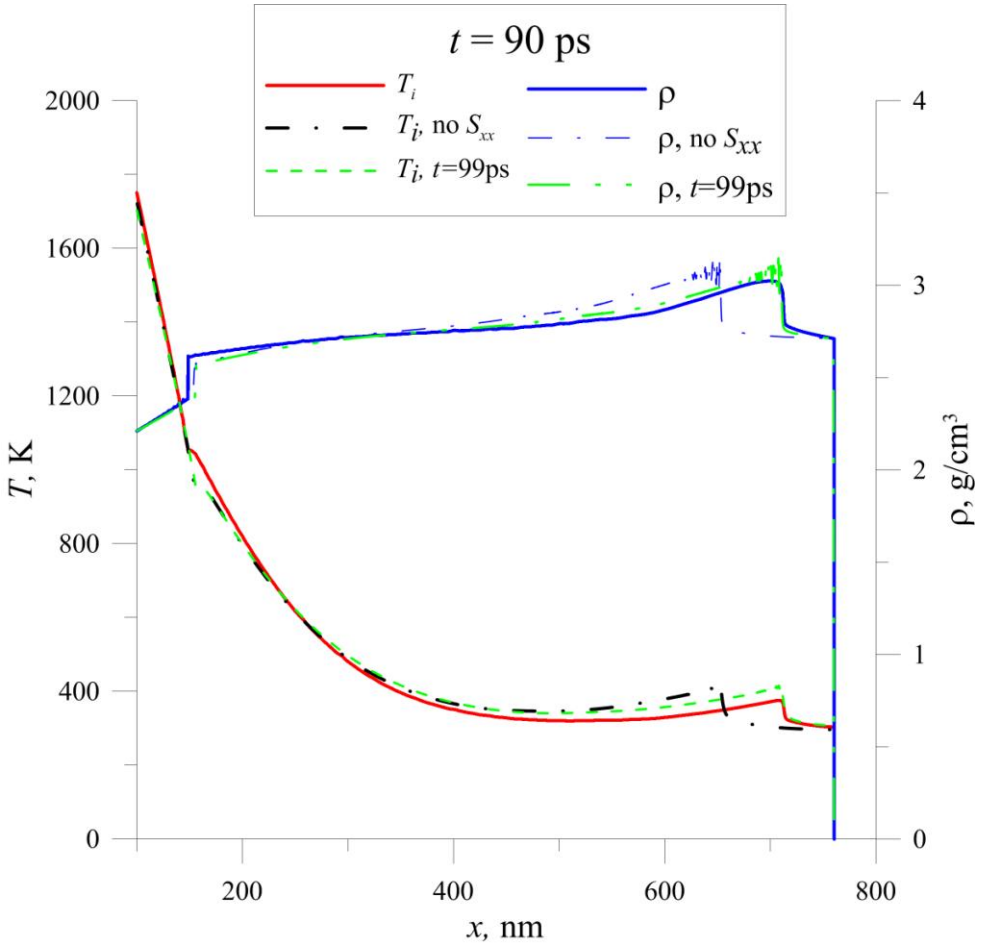
κ_e Н.А. Иногамов, Ю.В. Петров, Эльбрус-2010, ЖЭТФ, т. 137(3), 505-529

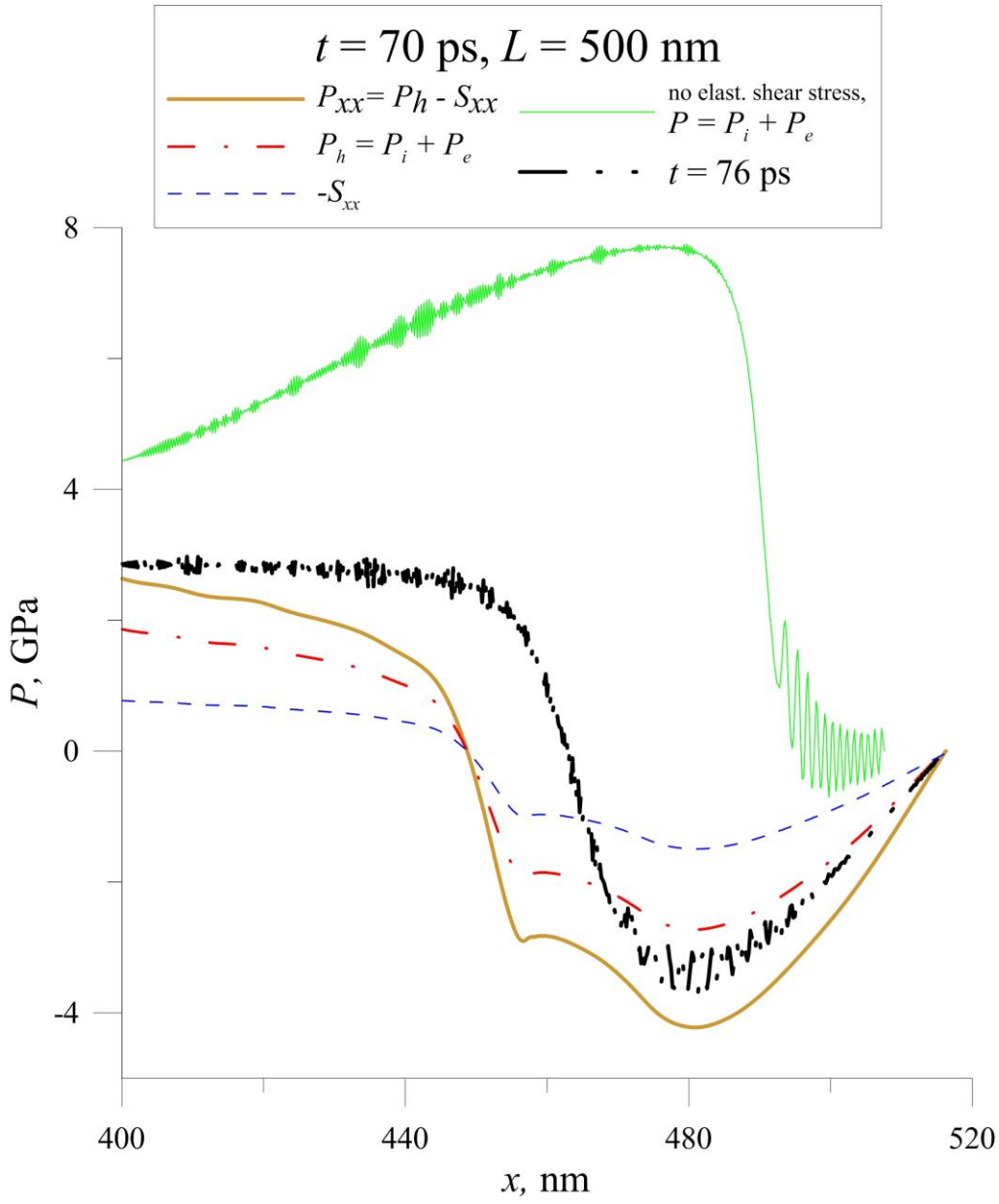

t = 10 ps
Pxx= Ph - Sxx
Ph = Pi + Pe
-Sxx
no elast. shear stress,
P = Pi + Pe
t = 11 ps
P, GPa
x, nm
0
4
8
12
16
20
0
50
100
150
200
250

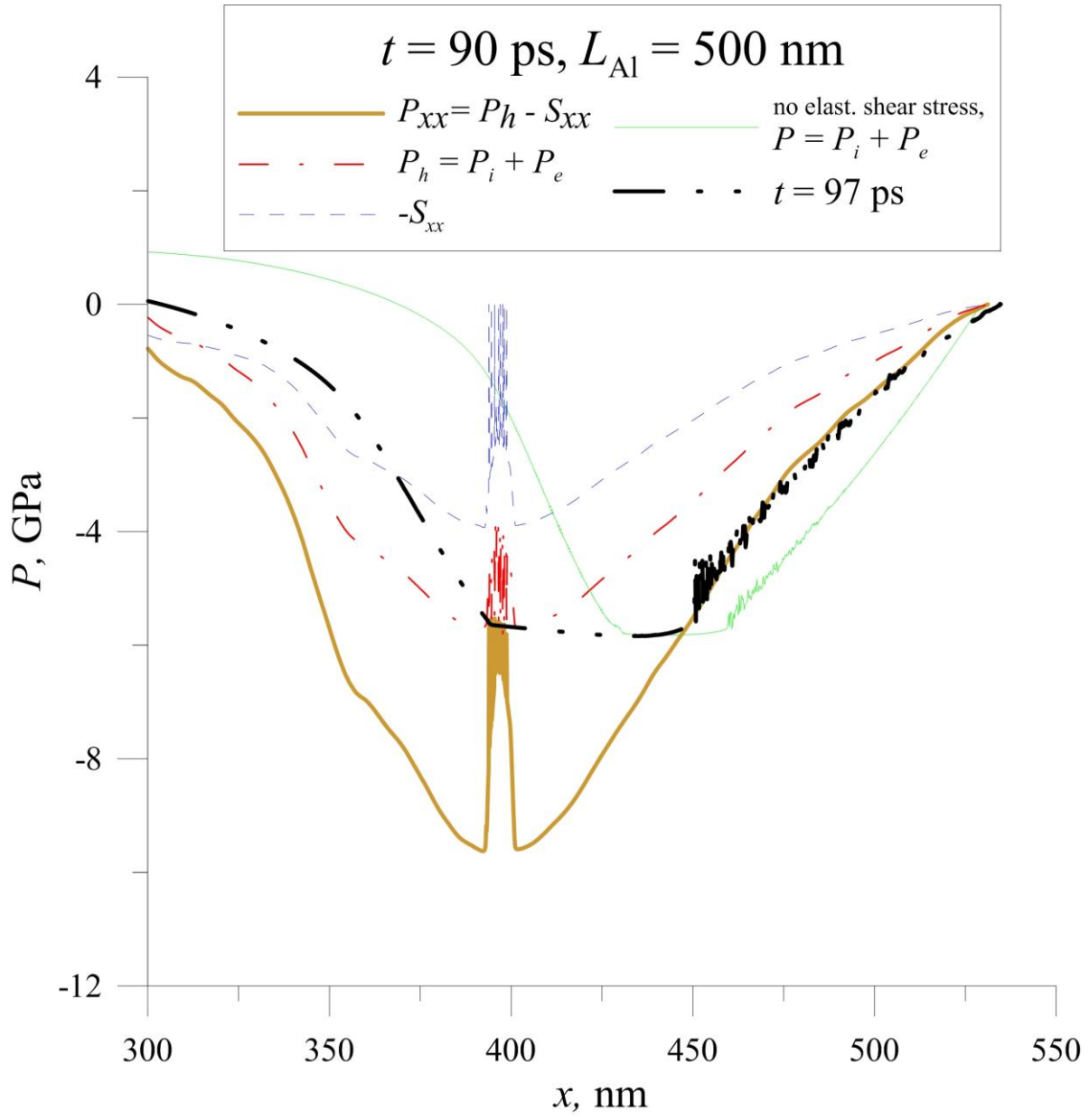

t = 20 ps
Pxx= Ph - Sxx
Ph = Pi + Pe
-Sxx
no elast. shear stress,
P = Pi + Pe
t = 22 ps
16
12
8
4
0
P, GPa
0
100
200
300
x, nm

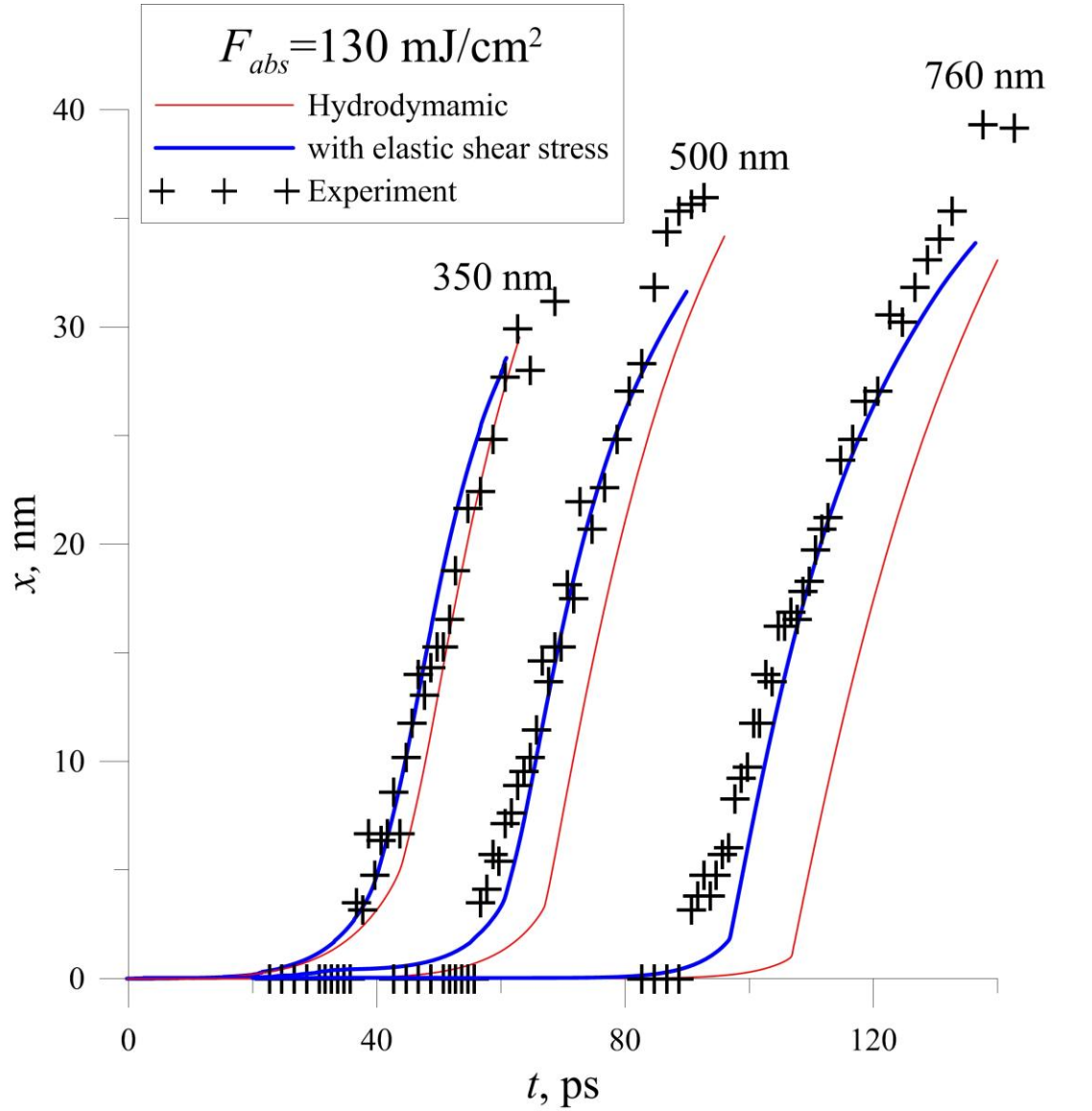

t = 90 ps
Pxx= Ph - Sxx
Ph = Pi + Pe
-Sxx
no elast. shear stress,
P = Pi + Pe
t = 99 ps
P, GPa
0
4
8
12
16
200
400
600
800
x, nm


t = 90 ps
Pxx= Ph - Sxx
Ph = Pi + Pe
-Sxx
no elast. shear stress,
P = Pi + Pe
t = 99 ps
P, GPa
x, nm
0
4
8
12
16
200
400
600
800


t = 90 ps
Ti
Ti, no Sxx
Ti, t=99ps
ρ
ρ, no Sxx
ρ, t=99ps
T, K
ρ, g/cm3
x, nm
0
400
800
1200
1600
2000
0
1
2
3
4
200
400
600
800


t = 70 ps, L = 500 nm
Pxx= Ph - Sxx
Ph = Pi + Pe
-Sxx
no elast. shear stress,
P = Pi + Pe
t = 76 ps
8
4
0
-4
P, GPa
400
440
480
520
x, nm

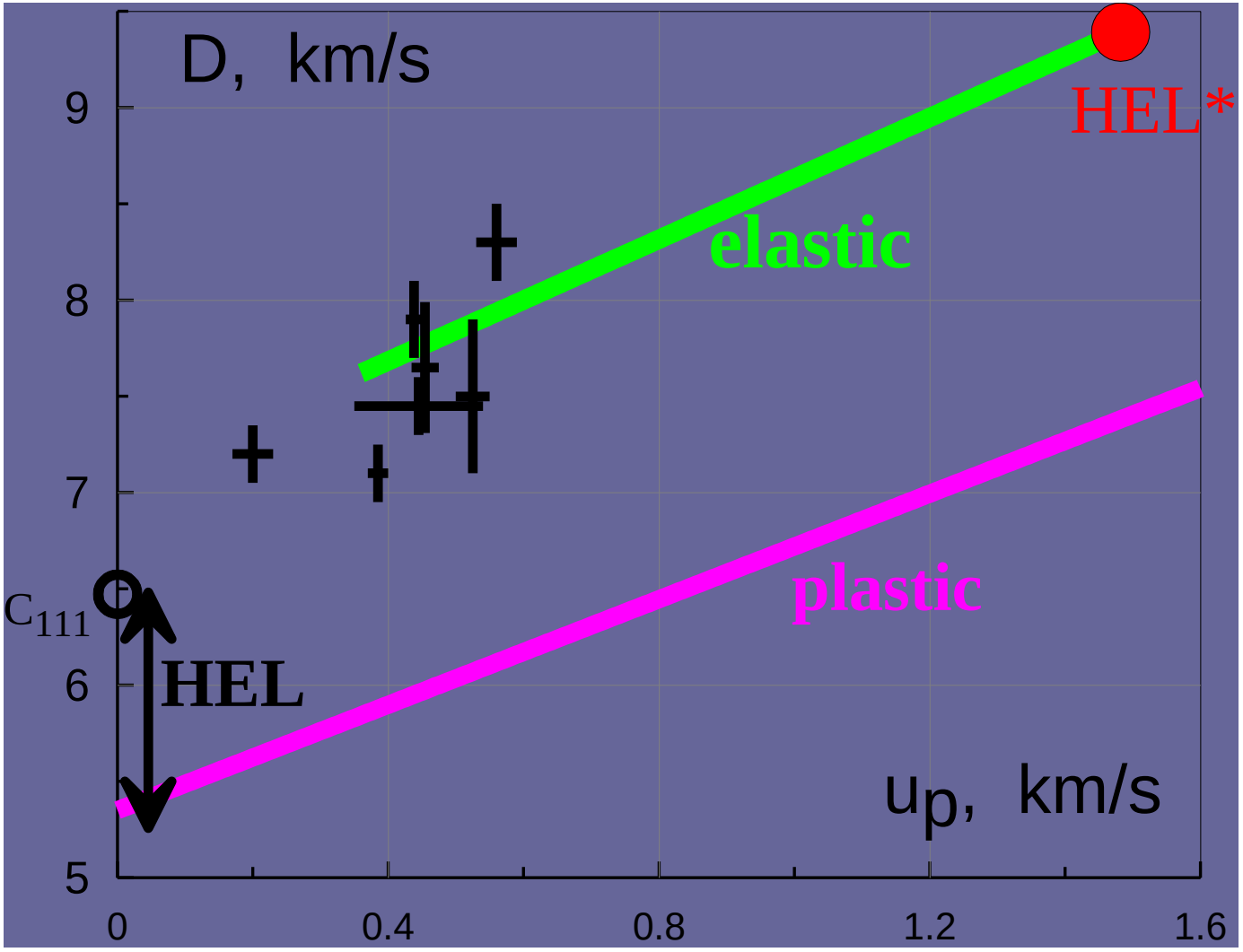

$t = 90$ ps, $L_{Al} = 500$ nm
$P_{xx} = P_h - S_{xx}$
$P_h = P_i + P_e$
$-S_{xx}$
no elast. shear stress, $P = P_i + P_e$
$t = 97$ ps
4
0
-4
-8
-12
P, GPa
300
350
400
450
500
550
x, nm


F_{abs}=130 mJ/cm^2
Hydrodymamic
with elastic shear stress
Experiment
350 nm
500 nm
760 nm
40
30
20
10
0
x, nm
0
40
80
120
t, ps

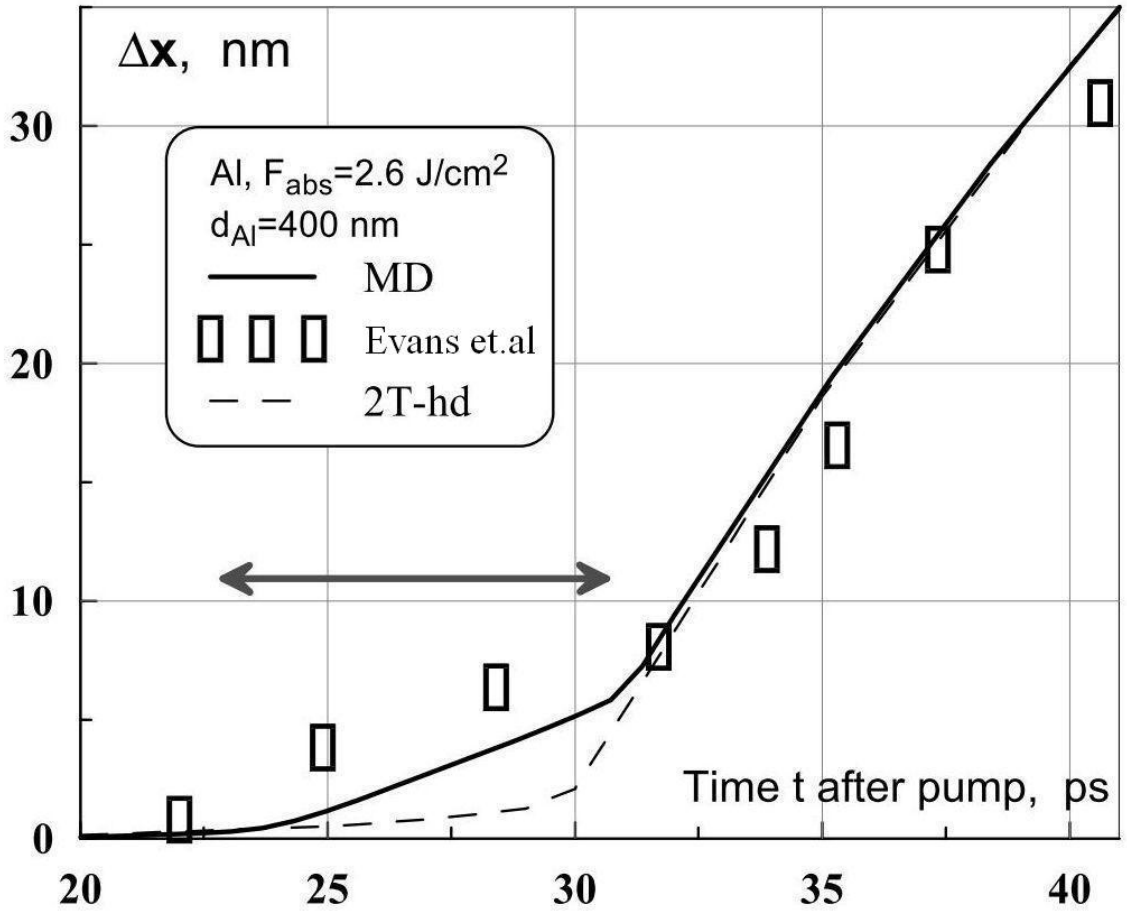
0 40 80 120

Comparison of elastic and plastic Hugoniot with experiment

[M.B. Agranat, S.I. Anisimov, S.I. Ashitkov et.al, JETP Letters, 91 (2010) 471, S.I. Ashitkov, M.B. Agranat, G.I. Kanel' et. al, JETP Letters, 92 (2010) 516] (crosses).



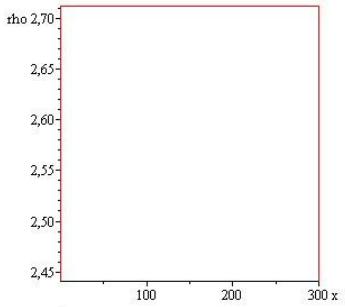
Displacement of the boundary with the glass Δx at passage of compression wave through the border.
Experiment [R. Evans, A.D. Badger, F. Fallies et. al., Phys. Rev. Lett., 77 (1996) 3359] and MD.
Horizontal arrow indicates elastic precursor.



2T-thermo-gydrodynamics

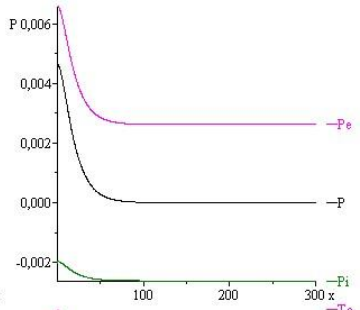
Density

$\rho,\ g/cm^3$



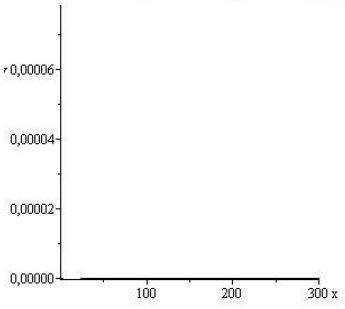
Pressure

$p,\ GPa$



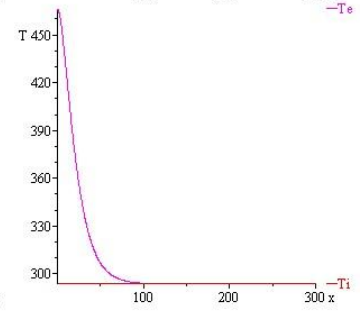
Velocity

$v,\ km/s$



Temp.

$T,\ K$



- 0 ,30ps

$$\frac{\partial x(x^0,t)}{\partial t} = v, \quad \frac{\partial x(x^0,t)}{\partial x^0} = \frac{\rho^0}{\rho}, \qquad (1)$$

$$\rho^0 \frac{\partial v}{\partial t} = -\frac{\partial P_{xx}}{\partial x^0},\ P_{xx} = P_h - S_{xx},\ P_h = P_e + P_i, \qquad (2) \qquad S_{xx} = F_{Sol} S_1, \quad S_1 = \frac{4}{3} G \left(\frac{\partial x}{\partial x^0} - R_{rc} \right)$$

$$\rho^0 \frac{\partial \bar{E}_e}{\partial t} = \frac{\partial}{\partial x^0} \left(\frac{\rho \kappa_e}{\rho^0} \frac{\partial T_e}{\partial x^0} \right) - P_e \frac{\partial v}{\partial x^0} - \bar{\alpha}(T_e - T_i) + \bar{Q}(x^0,t), \qquad (3)$$

$$\rho^0 \frac{\partial \bar{E}_i}{\partial t} = \frac{\partial}{\partial x^0} \left(\frac{\rho \kappa_i}{\rho^0} \frac{\partial T_i}{\partial x^0} \right) - P_i \frac{\partial v}{\partial x^0} + \bar{\alpha}(T_e - T_i) \qquad (4)$$

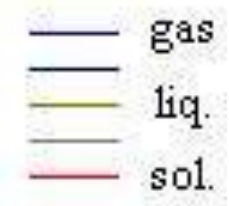
$$\rho^0 \frac{\partial (\bar{E}_i + \bar{E}_S)}{\partial t} = \frac{\partial}{\partial x^0} \left(\frac{\rho \kappa_i}{\rho^0} \frac{\partial T_i}{\partial x^0} \right) - (P_i - S_{xx}) \frac{\partial v}{\partial x^0} + \bar{\alpha}(T_e - T_i)$$, solid+liquid

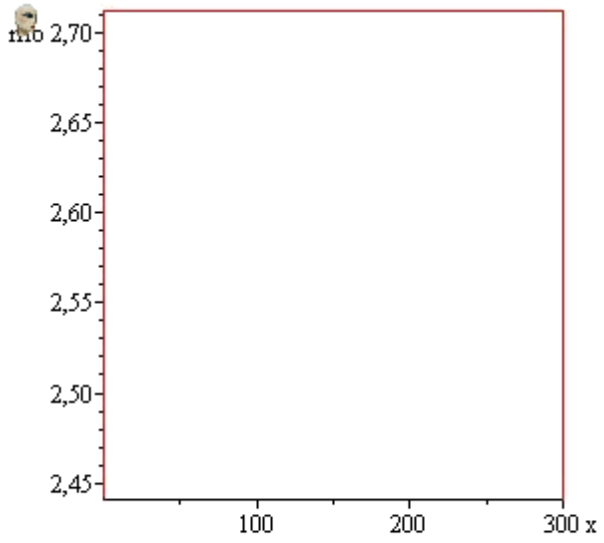
$$E = E_h + E_S, \quad E_h = E_e + E_i \qquad \bar{E}_S = \frac{S_{xx}}{2\rho^0} \left(\frac{\partial x}{\partial x^0} - R_{rc} \right)$$

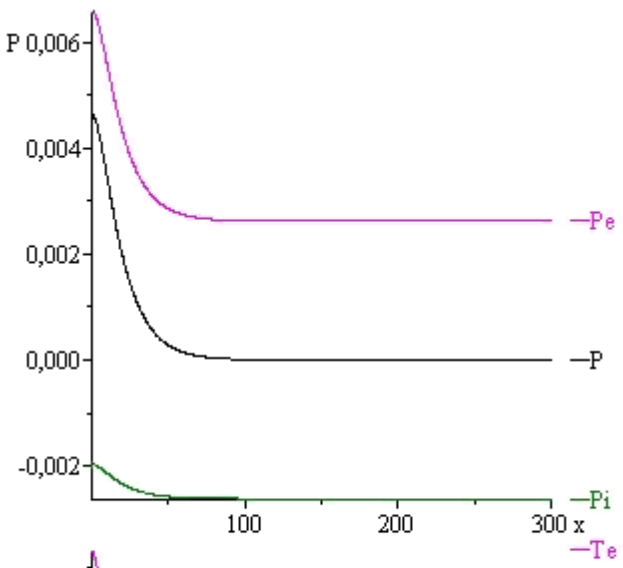
Electrons heating by laser pulse. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$







Pressure

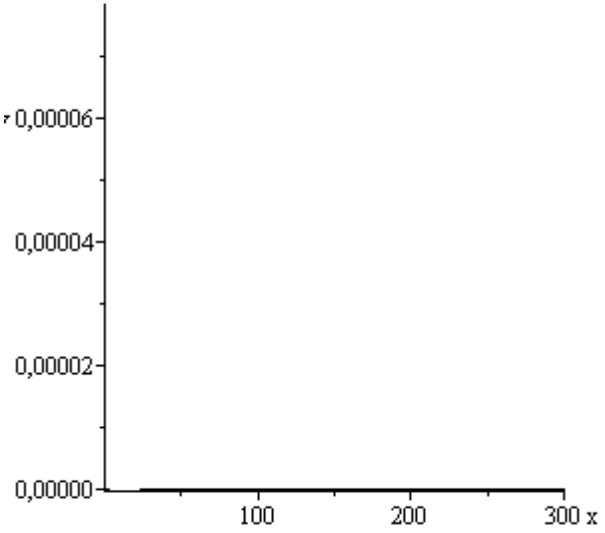
$p,\ GPa$

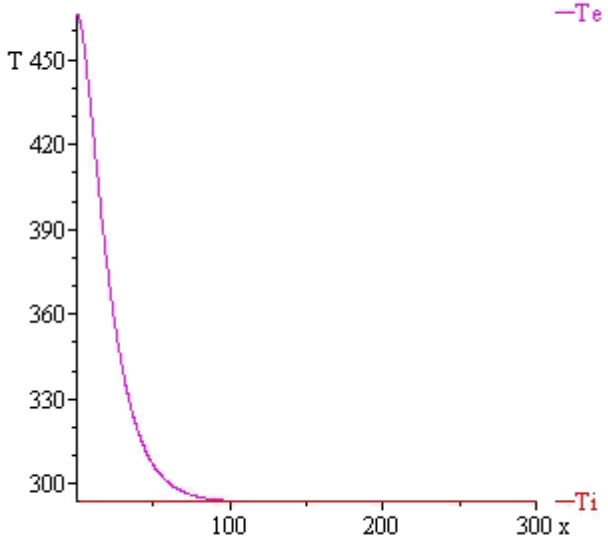
Pe

Pi

Velocity

$v,\ km/s$

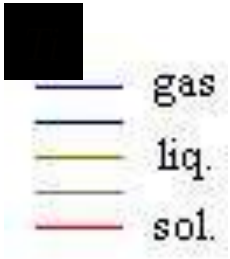




Temperature

$T,\ K$

Te

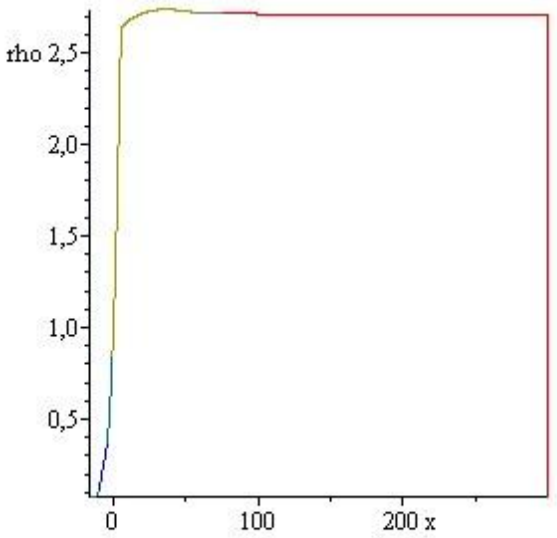


- 0 ,30ps

Electrons heating by laser pulse. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$



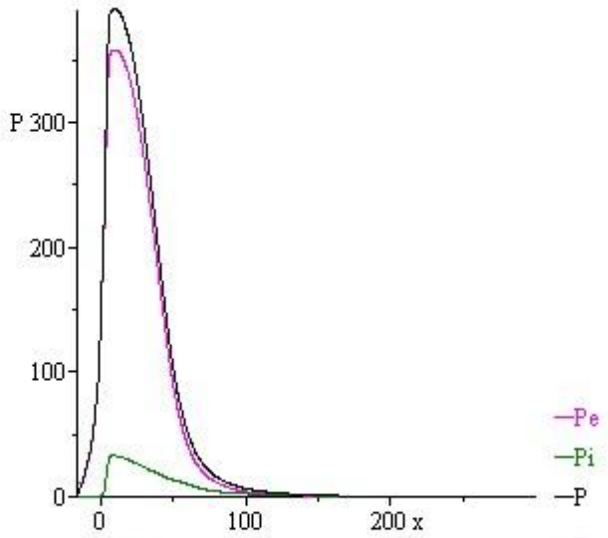
gas
liq.
sol.

Pressure

$p,\ GPa$

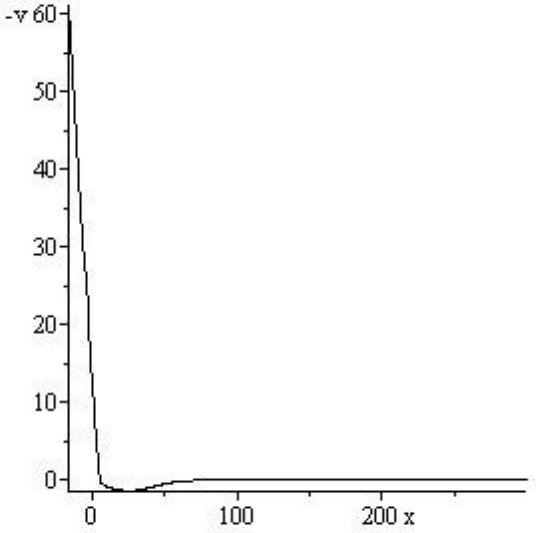
Pe

Pi



Velocity

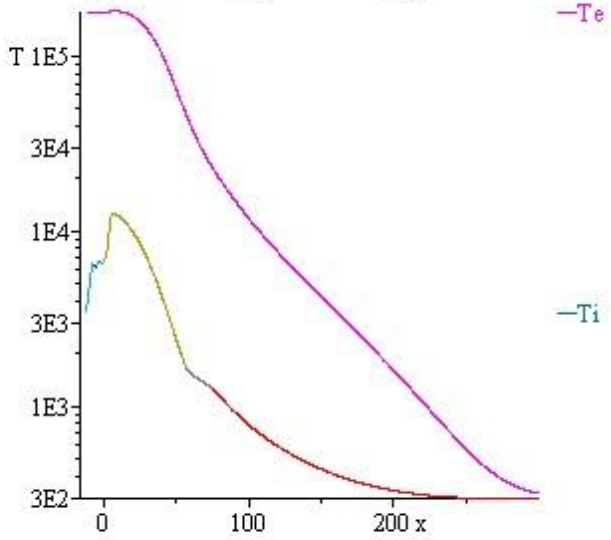
$v,\ km/s$



Temperature

$T,\ K$

Te



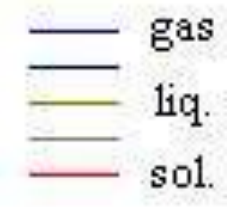
gas
liq.
sol.

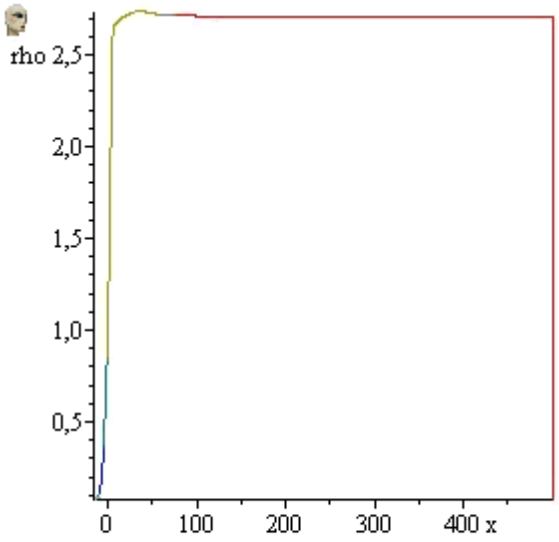
000 ,30ps

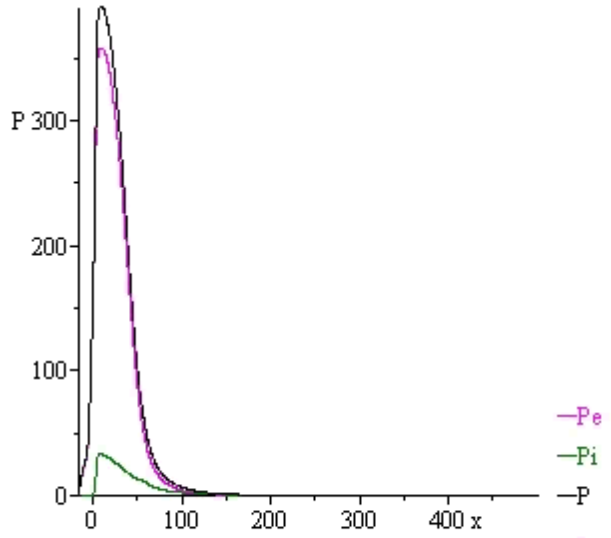
Thermodiffusion and e-i relaxation . (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$







Pressure

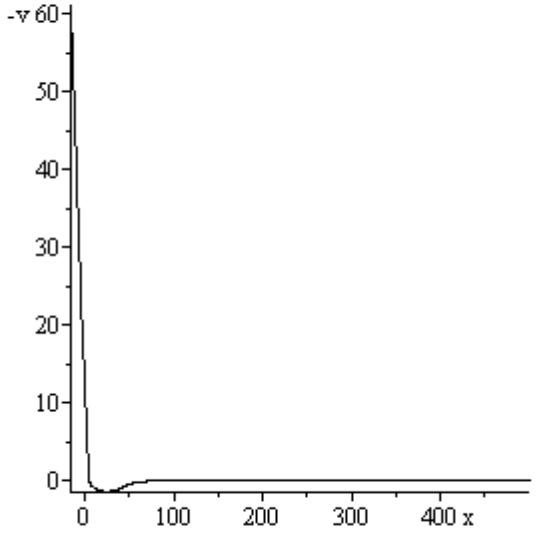
$p,\ GPa$

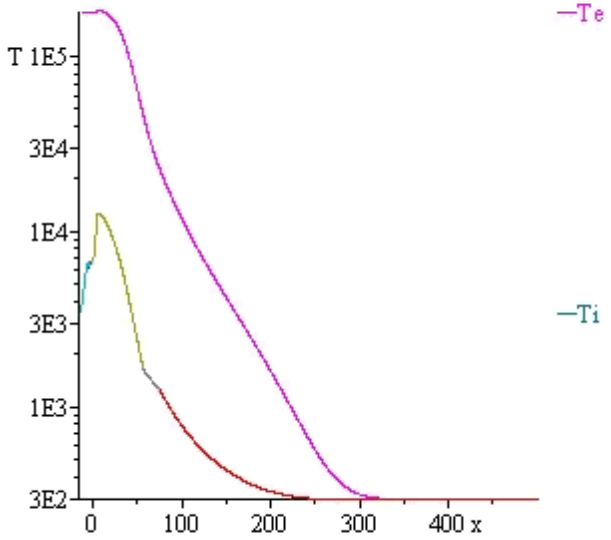
Pe

Pi

Velocity

$v,\ km/s$

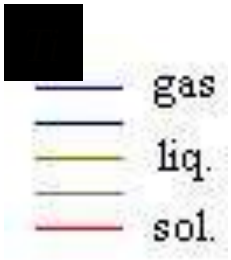




Temperature

$T,\ K$

Te

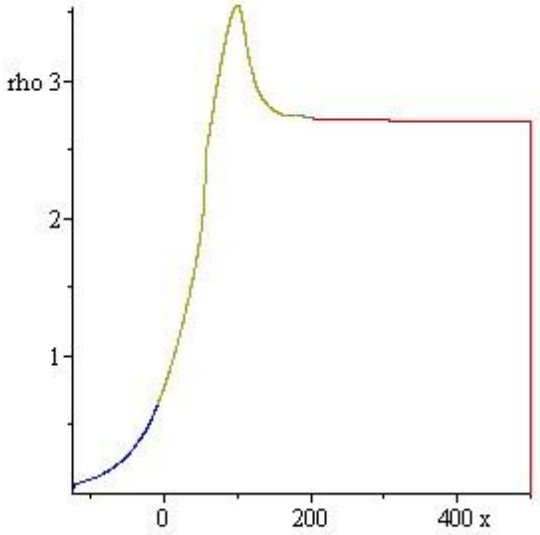


000 ,30ps

Thermodiffusion and e-i relaxation . (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$



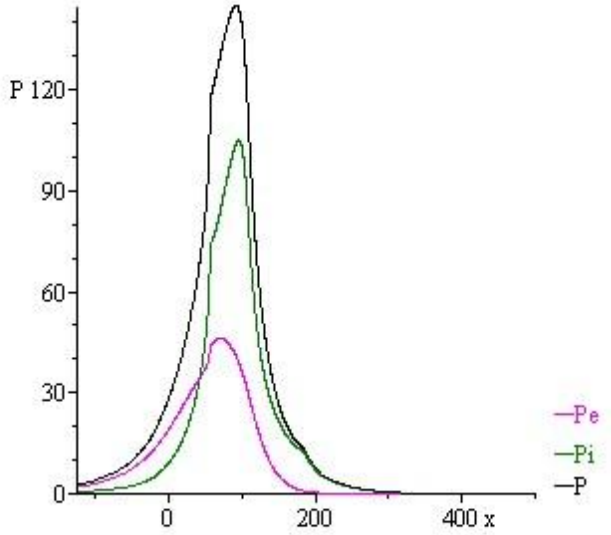
gas
liq.
sol.

Pressure

$p,\ GPa$

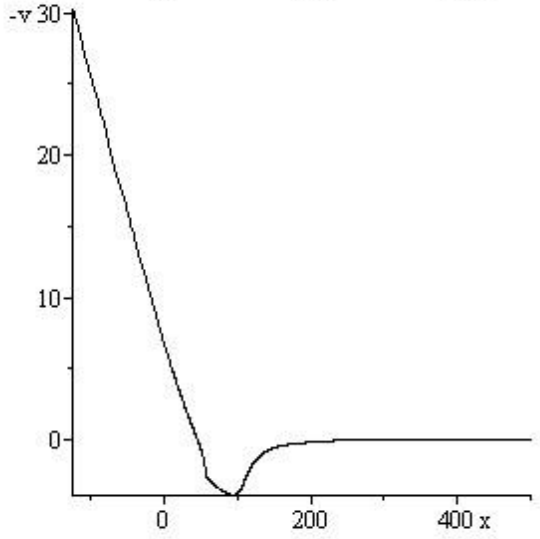
Pe

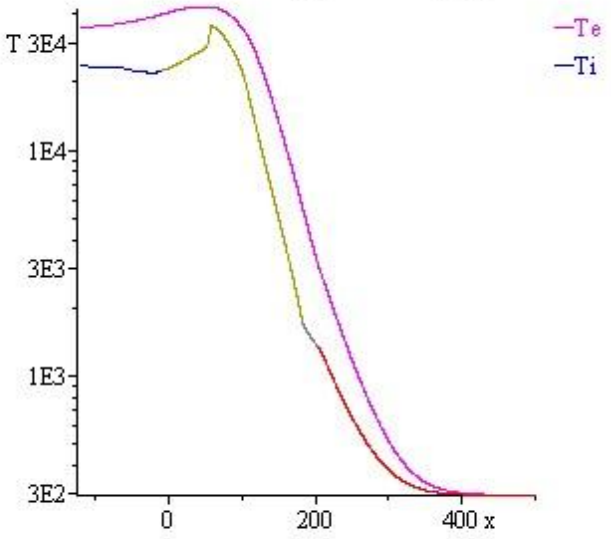
Pi



Velocity

$v,\ km/s$





Temperature

$T,\ K$

Te

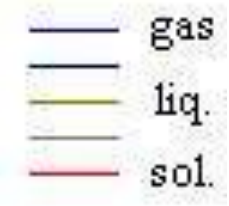
gas
liq.
sol.

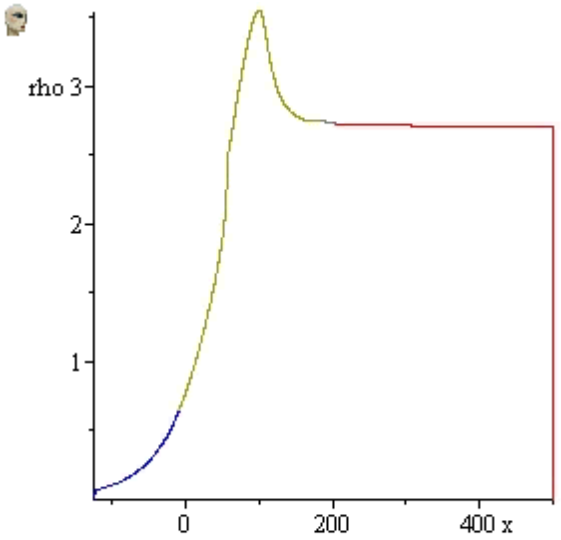
005 ,00ps

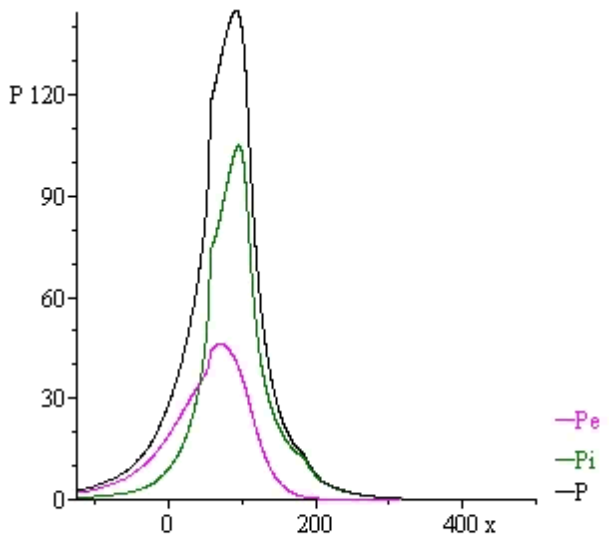
Formation of shock waves. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$







Pressure

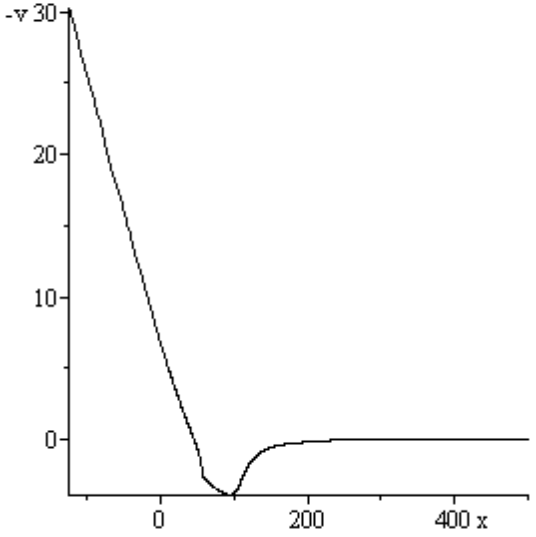
$p,\ GPa$

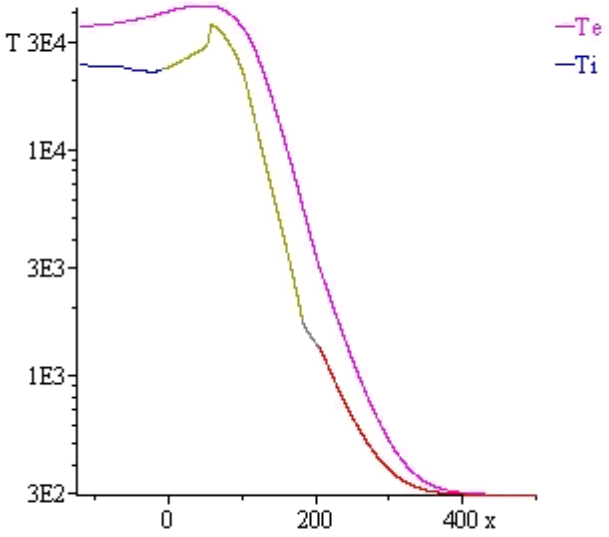
Pe

Pi

Velocity

$v,\ km/s$

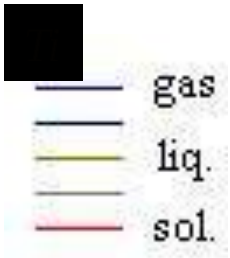




Temperature

$T,\ K$

Te

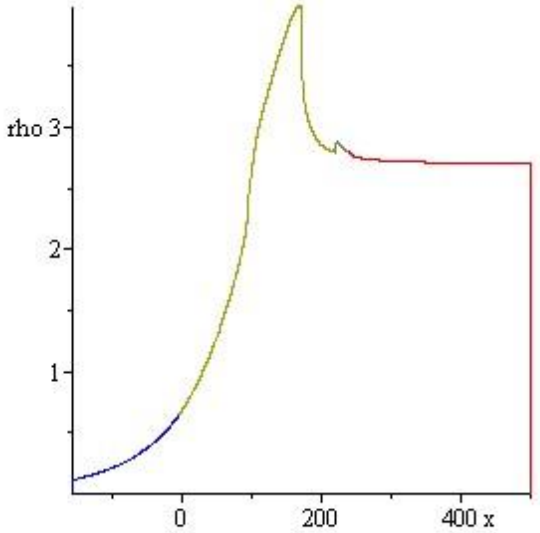


005 ,00ps

Formation of shock waves. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$



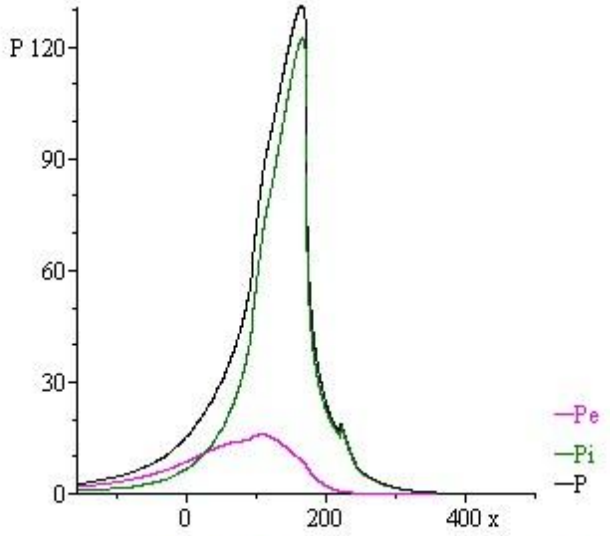
gas
liq.
sol.

Pressure

$p,\ GPa$

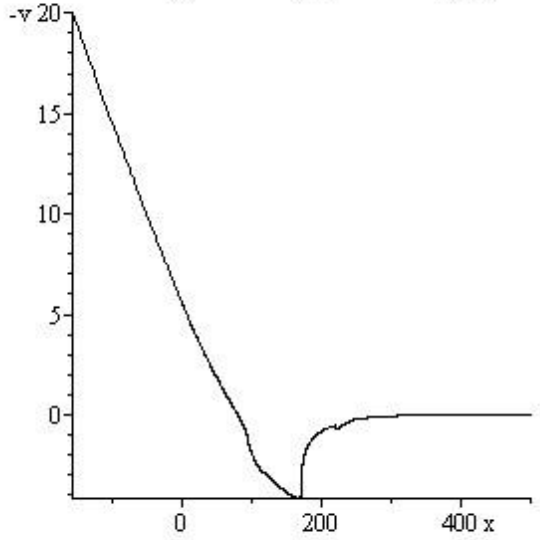
Pe

Pi



Velocity

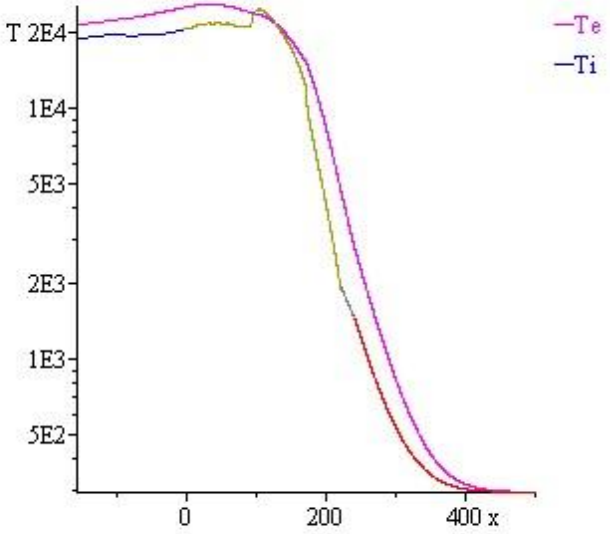
$v,\ km/s$



Temperature

$T,\ K$

Te



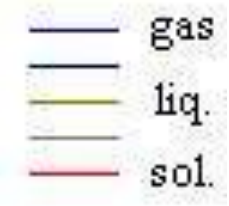
gas
liq.
sol.

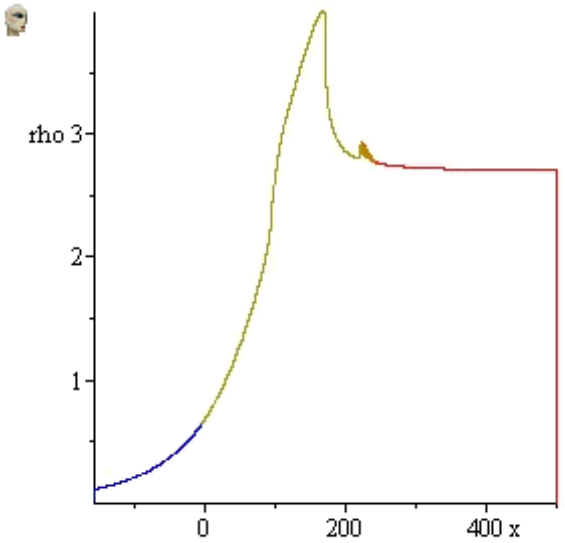
010 ,00ps

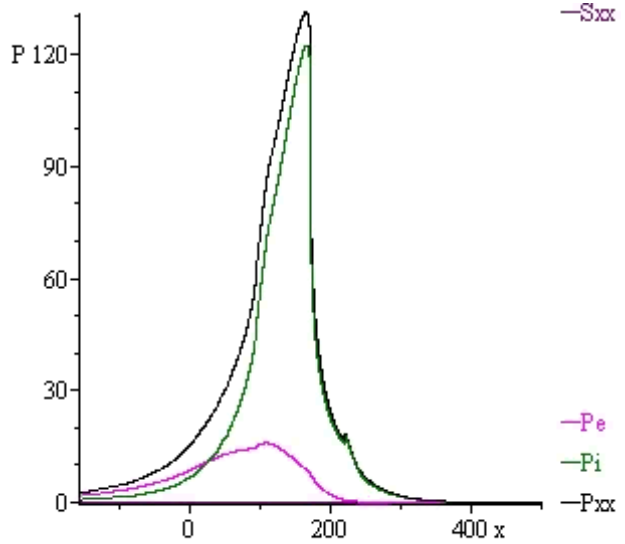
Absorption of precursor. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$







Pressure

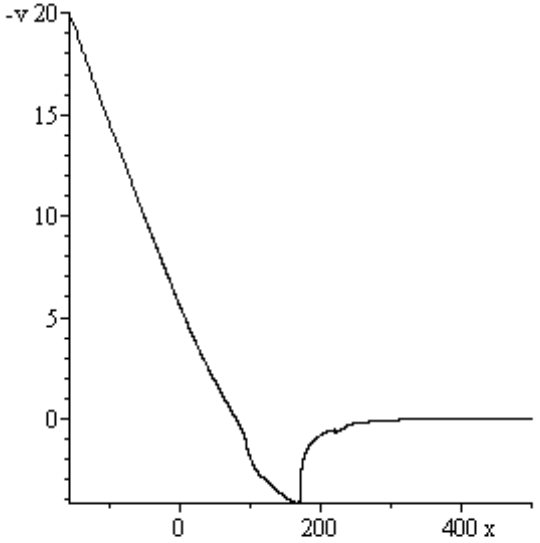
$p,\ GPa$

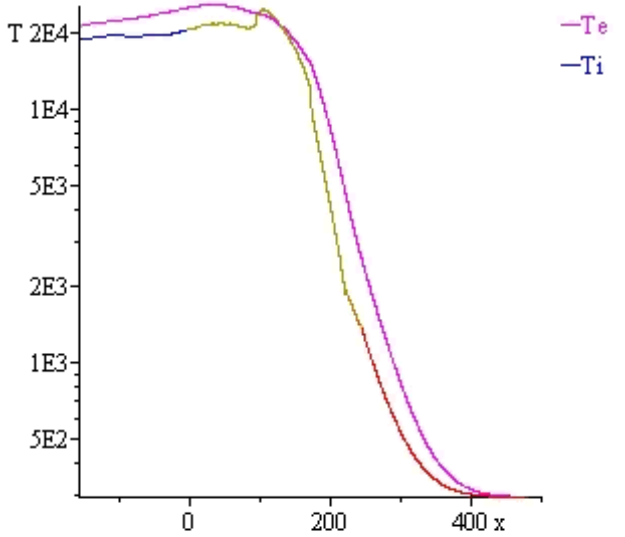
Pe

Pi

Velocity

$v,\ km/s$

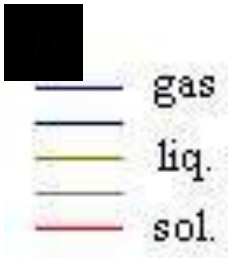




Temperature

$T,\ K$

Te

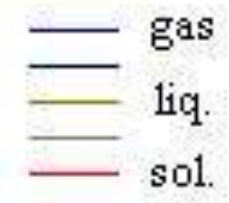


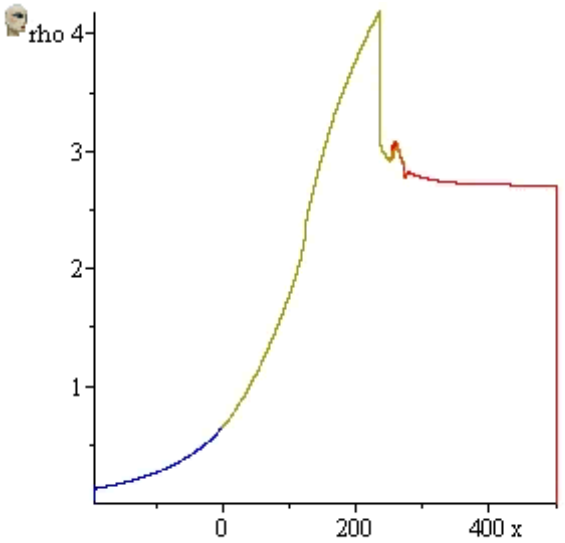
010 ,00ps

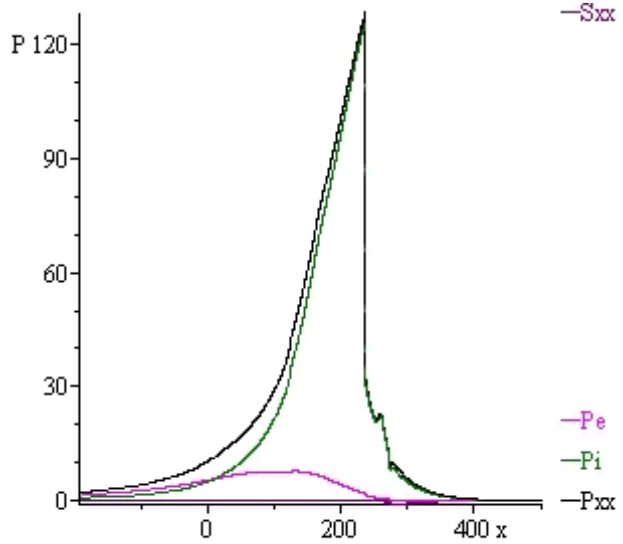
Absorption of precursor. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$







Pressure

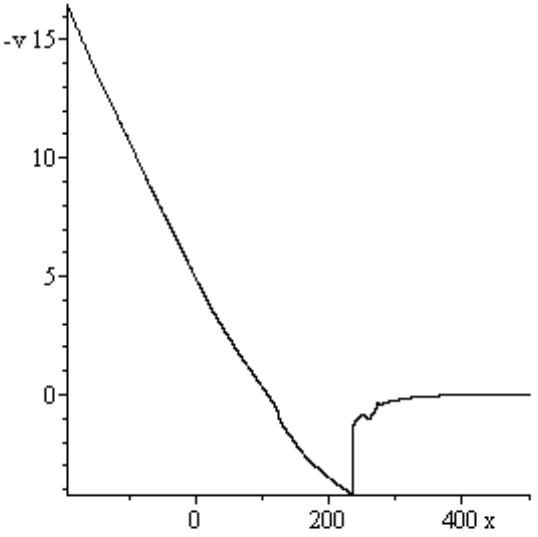
$p,\ GPa$

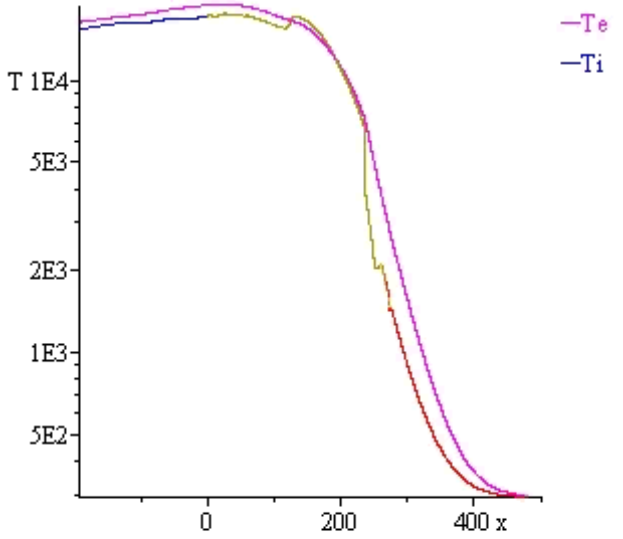
Pe

Pi

Velocity

$v,\ km/s$

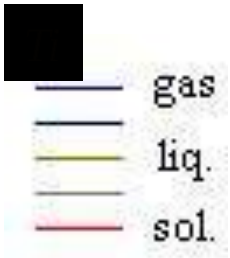




Temperature

$T,\ K$

Te

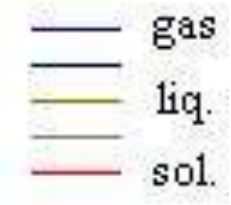


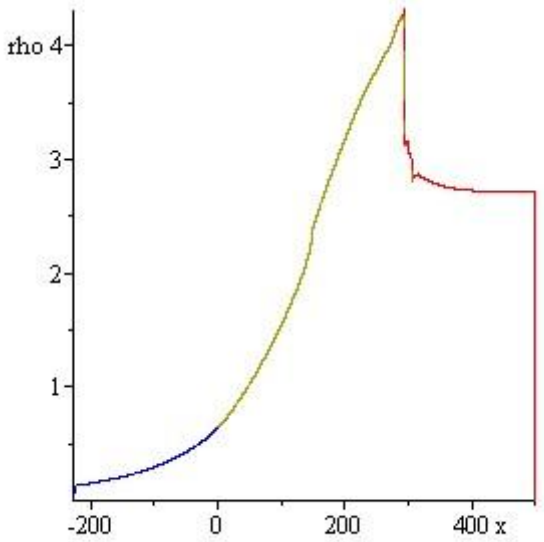
015 ,10ps

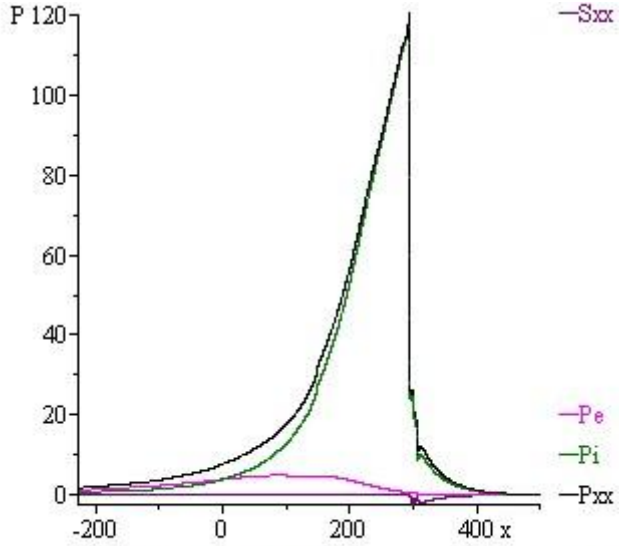
Absorption of precursor. (2T-thermo-hydrodynamic calculations)

Density

$\rho,\ g/cm^3$







Pressure

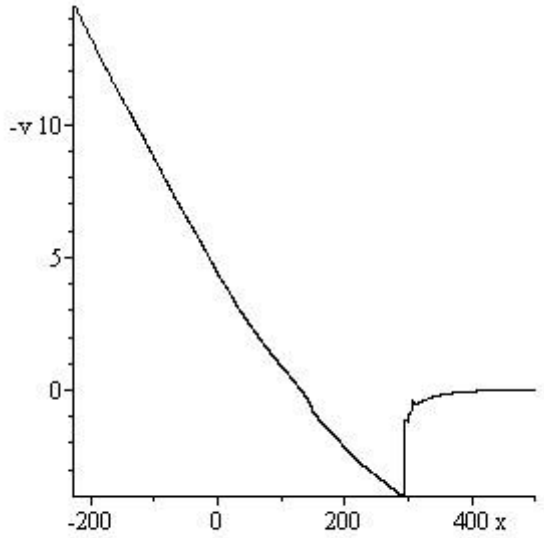
$p,\ GPa$

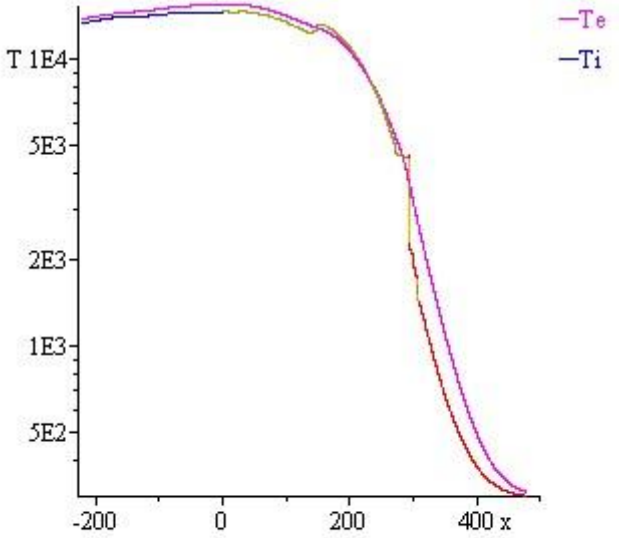
Pe

Pi

Velocity

$v,\ km/s$

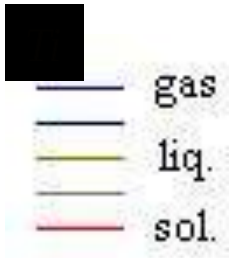




Temperature

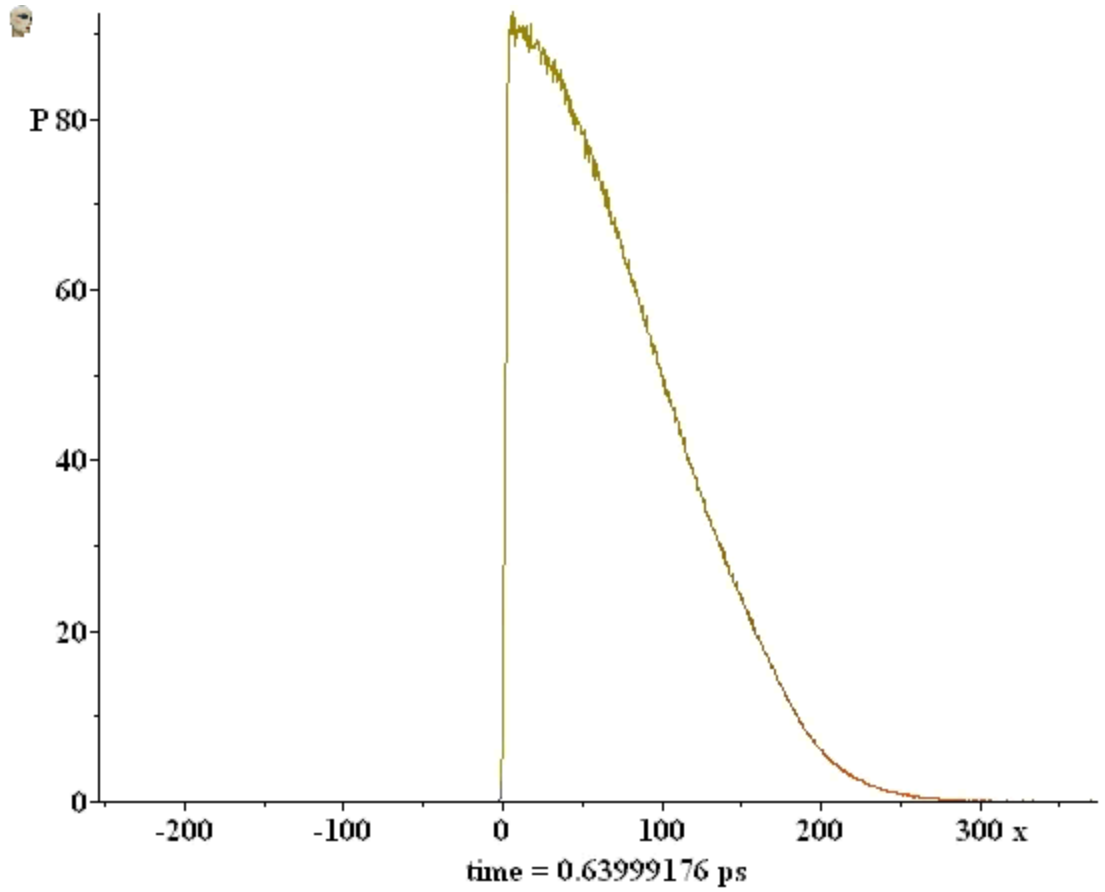
$T,\ K$

Te

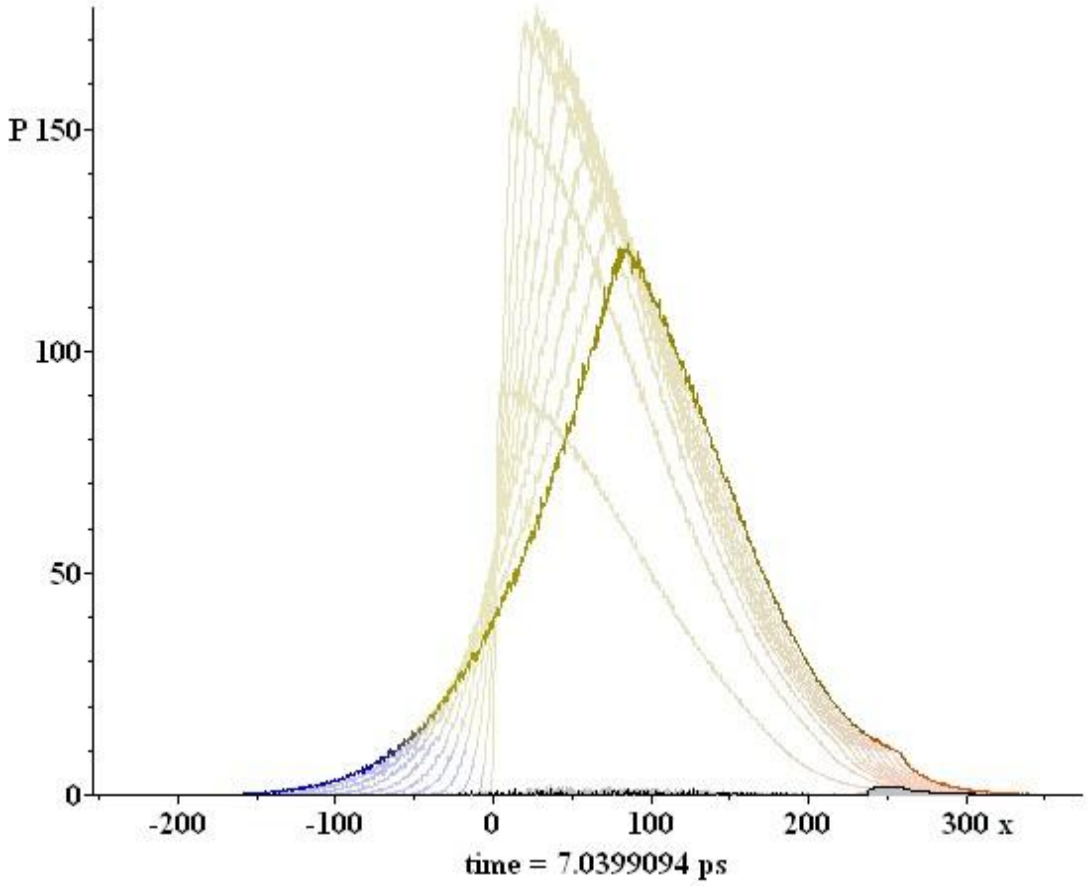


020 ,00ps

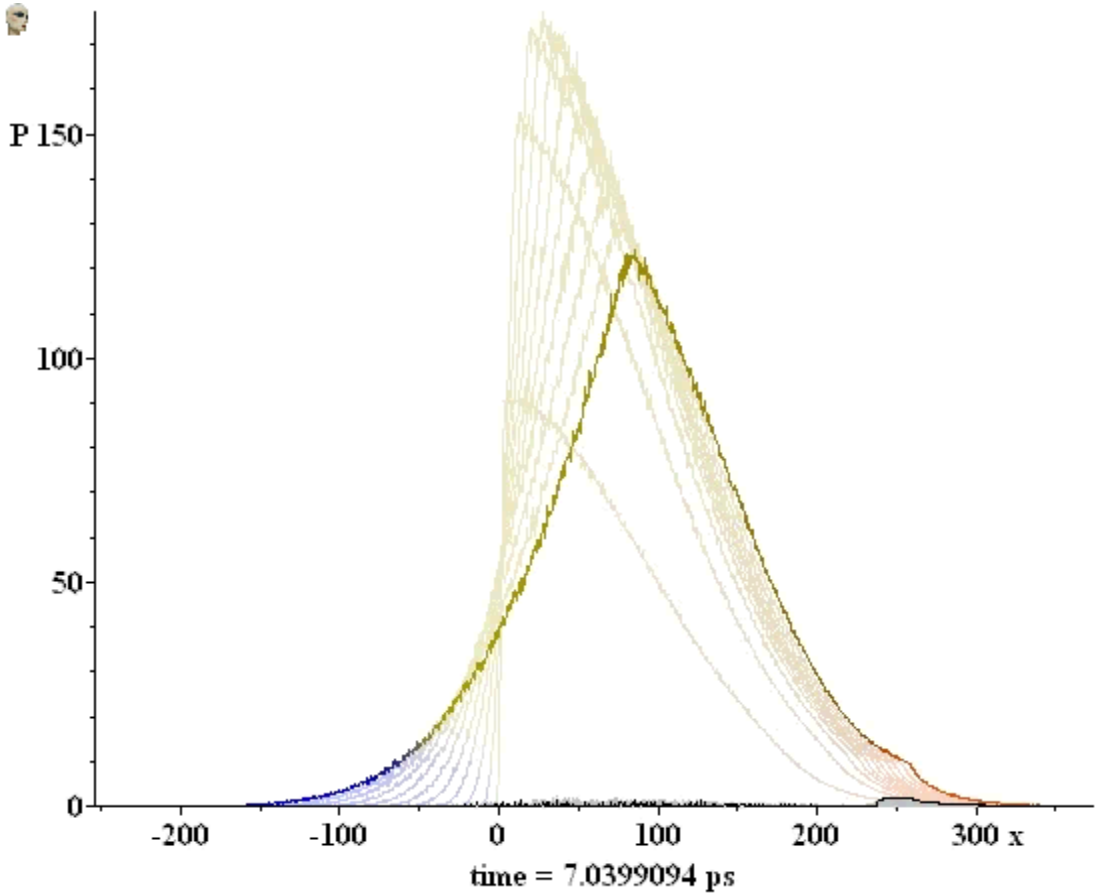
Compression wave at short times. Pressure profiles [GPa]



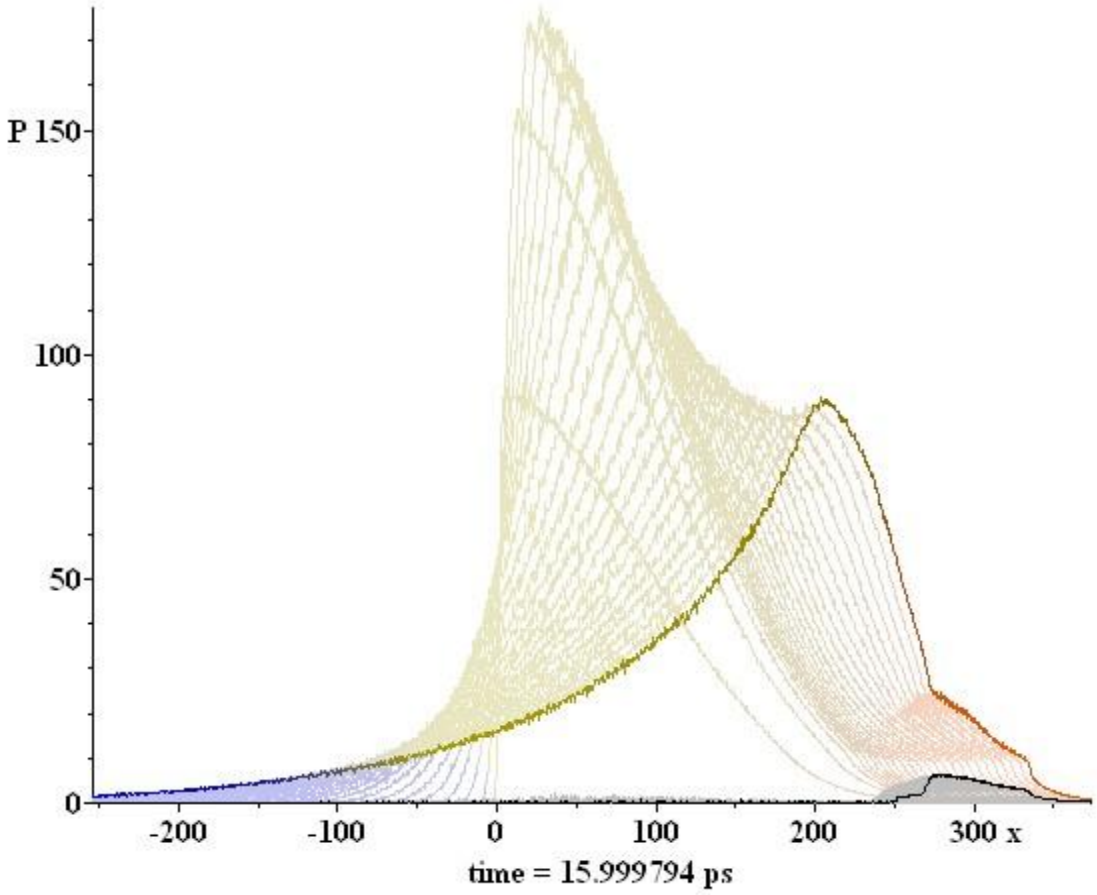
Compression wave at short times. Pressure profiles [GPa]



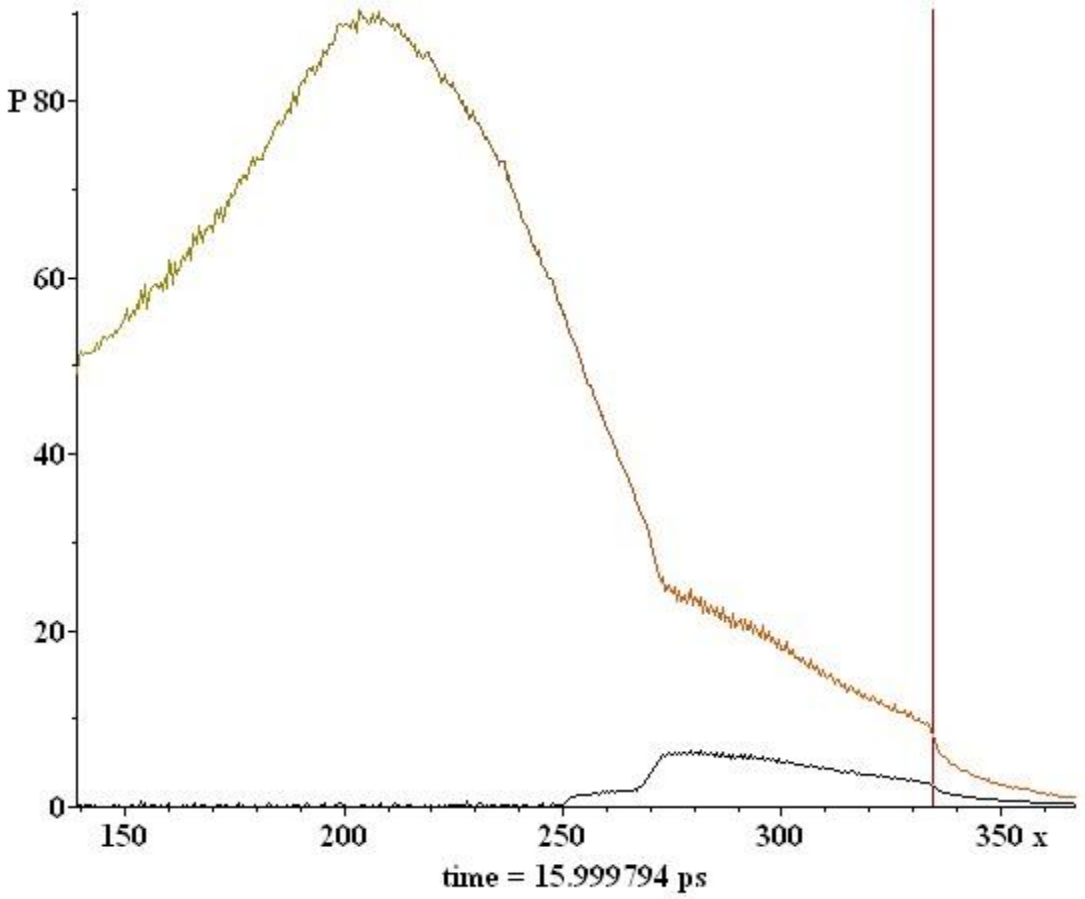
Steepening of pressure profile. (MD calculations)



Steepening of pressure profile. (MD calculations)

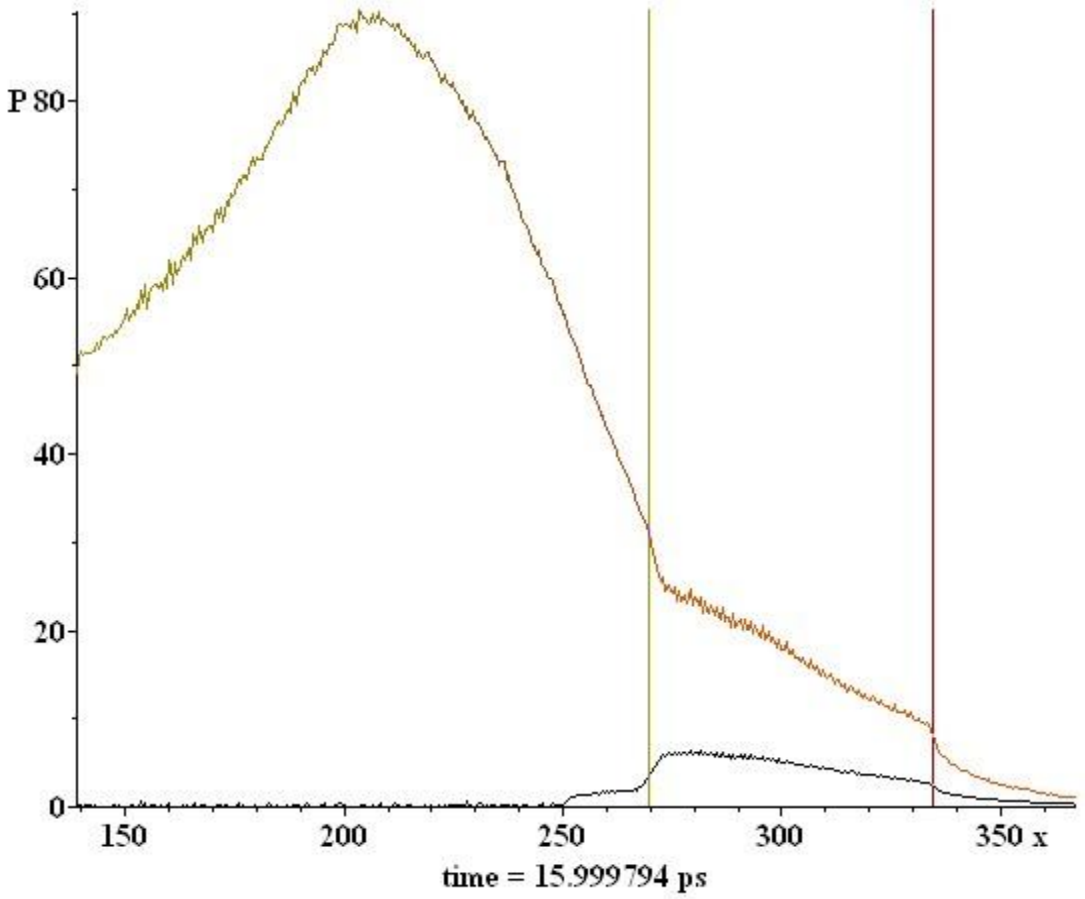


Areas with the greatest steepness of the pressure profile at t=16ps.
Elatic shock wave.



Black line – shear stress

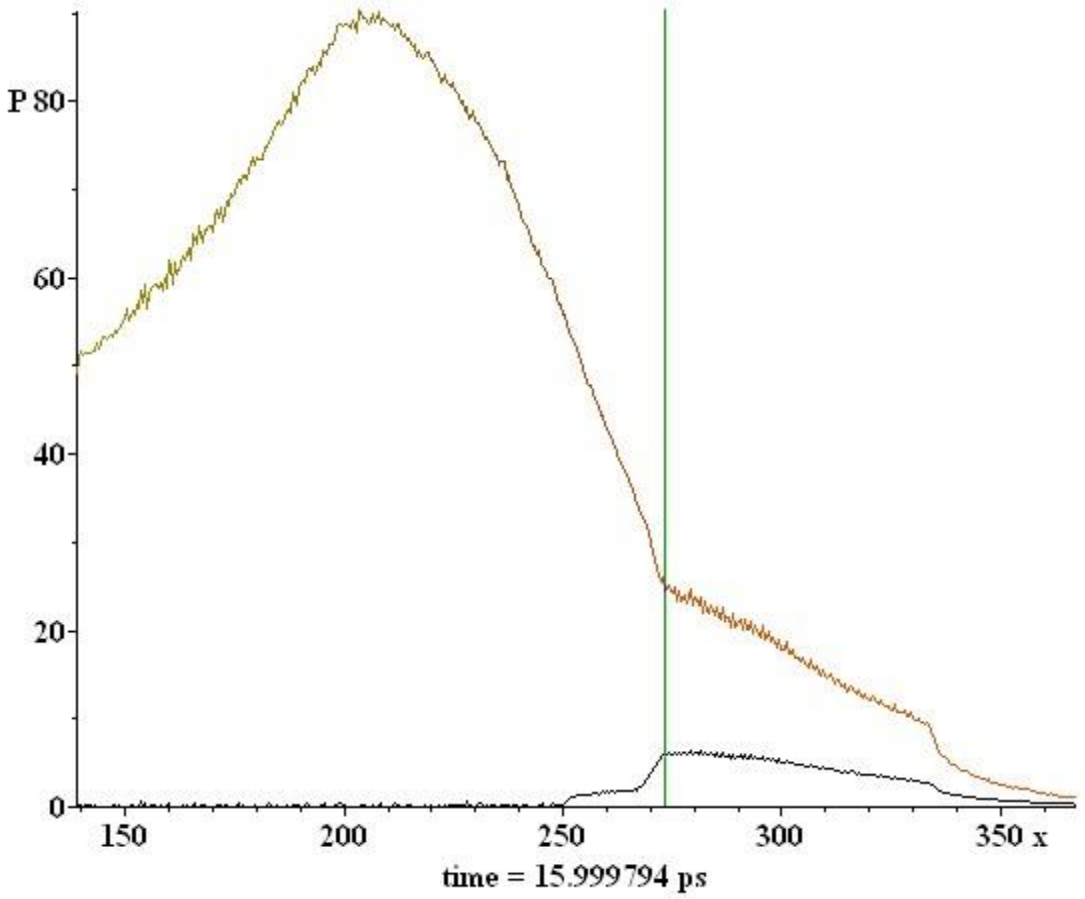
Areas with the greatest steepness of the pressure profile at t=16ps.
Plastic wave.



Black line – shear stress

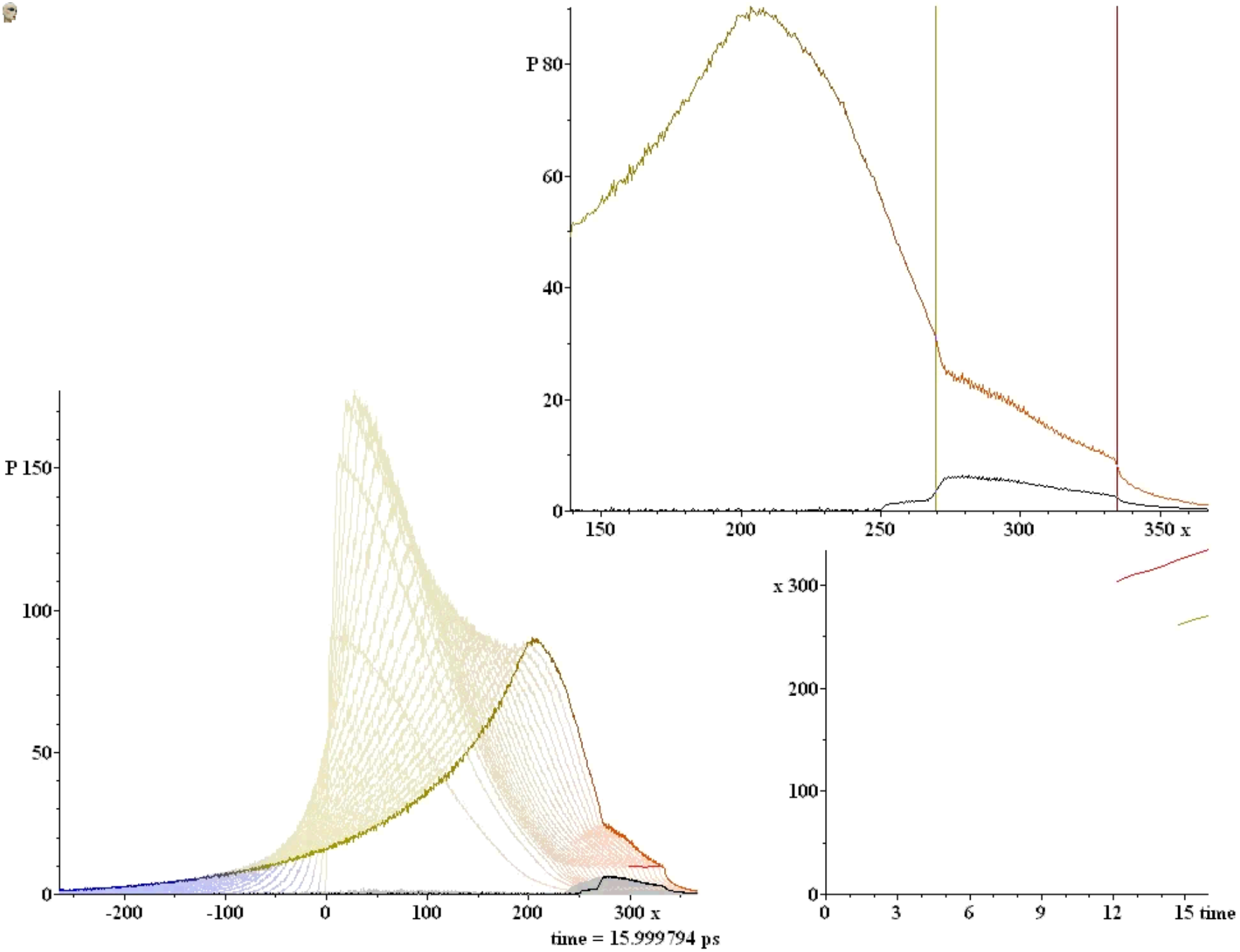
Areas with the greatest steepness of the pressure profile at t = 16ps.

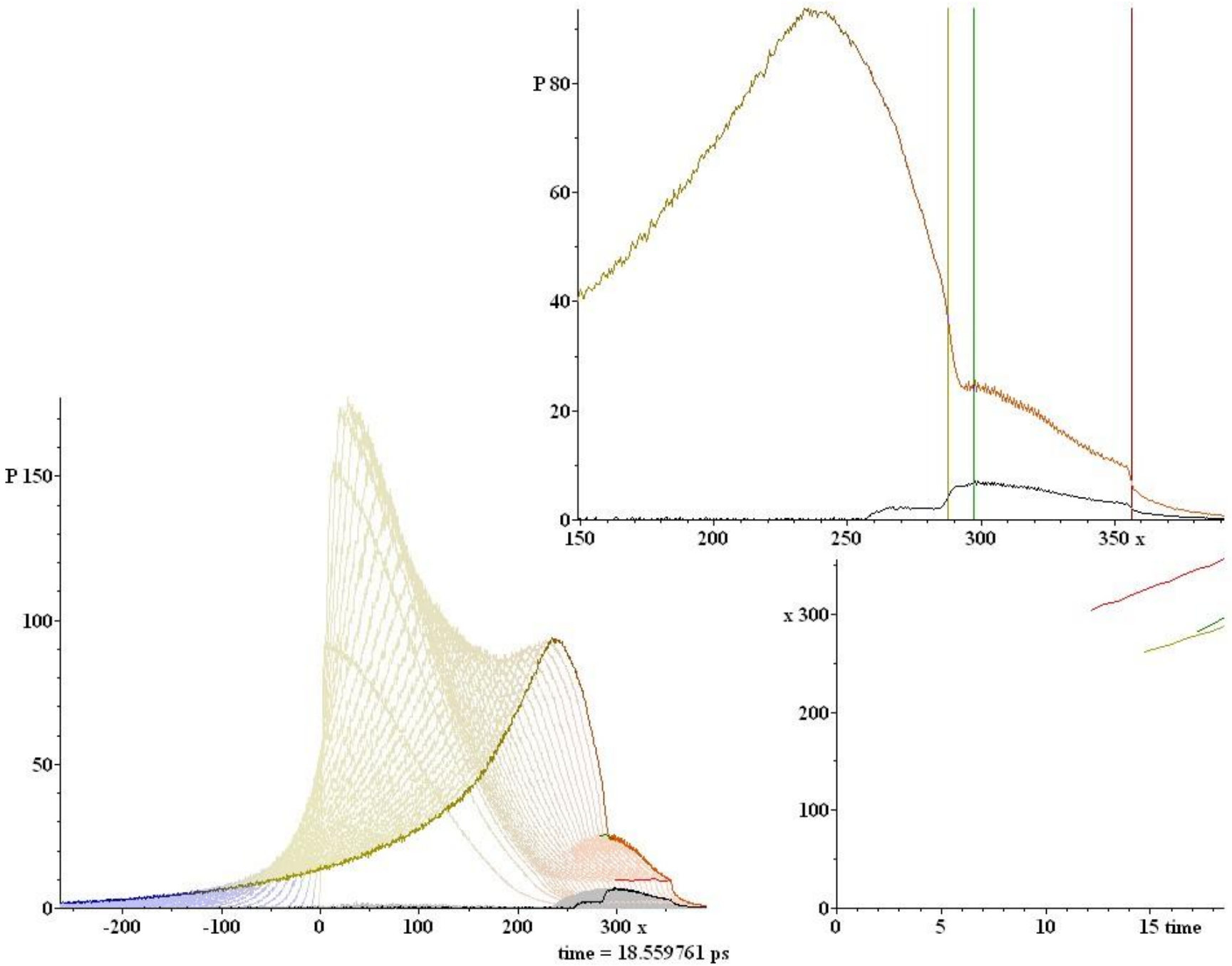
The break in the profile at the boundary of the elastic and plastically deformed zones.

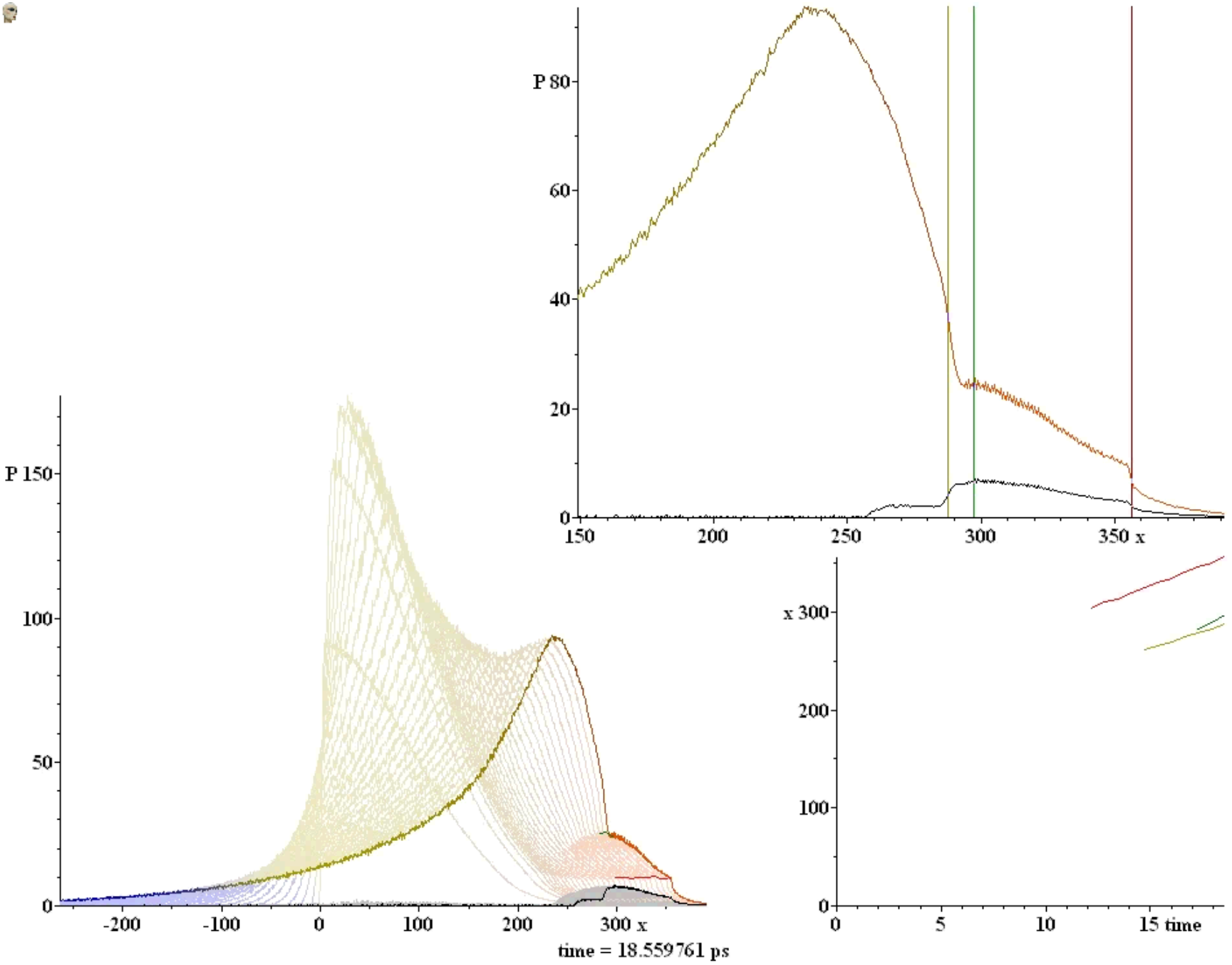


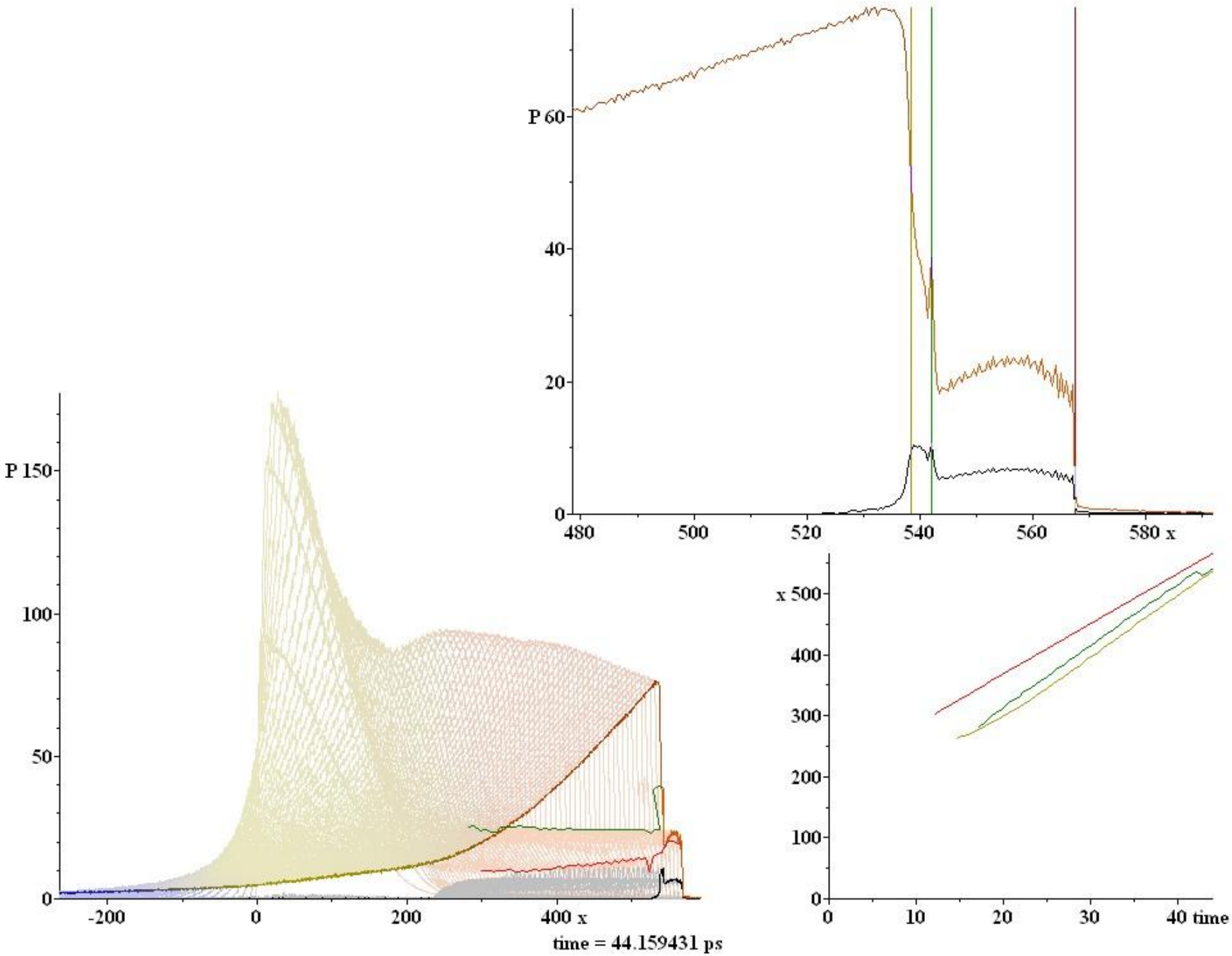
Black line – shear stress

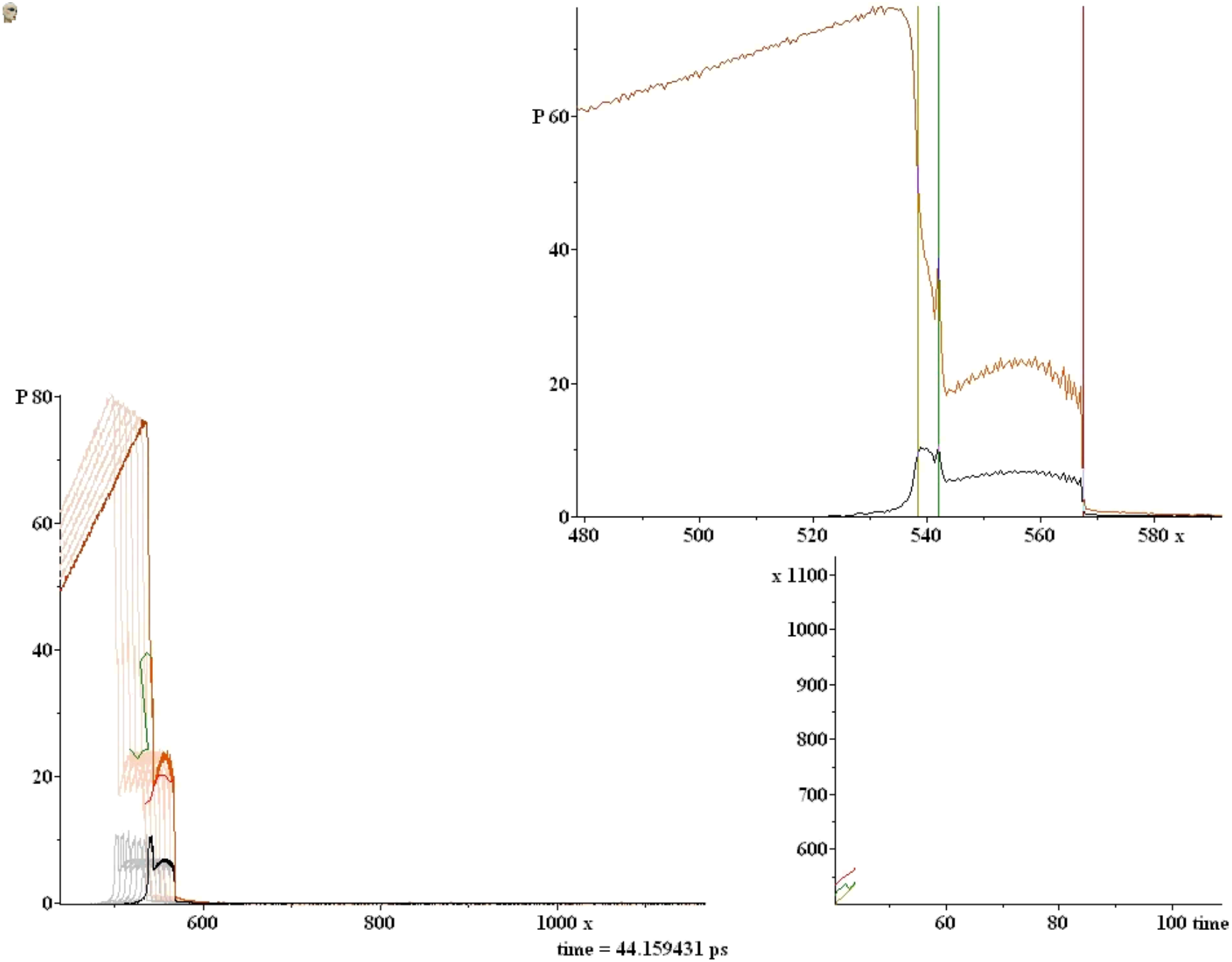
$c_{pl} = \sqrt{K/\rho}$ $c_{el} = \sqrt{K + 4G/3)/\rho}$

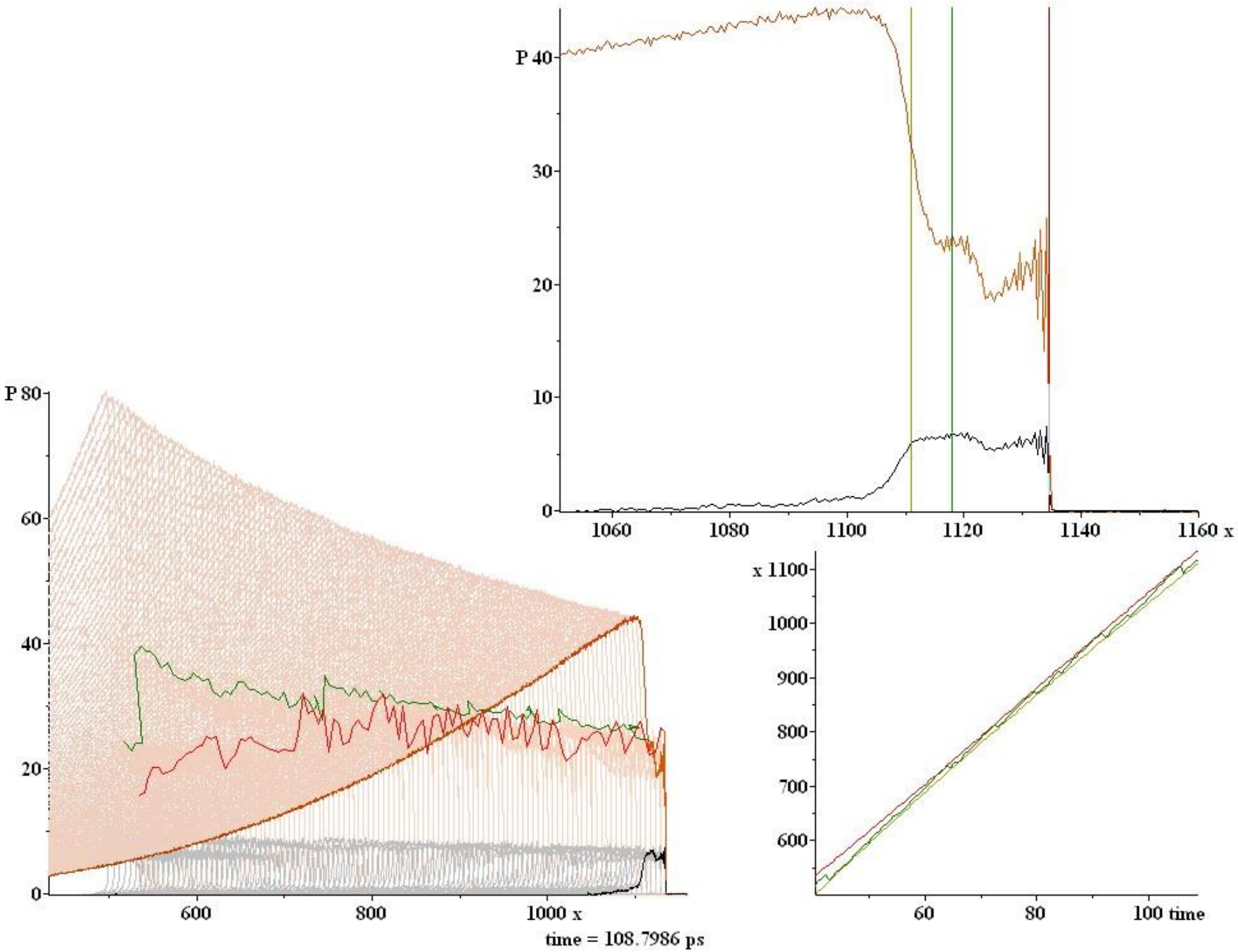

P 80
60
40
20
0
150
200
250
300
350 x
P 150
100
50
0
-200
-100
0
100
200
300 x
time = 15.999794 ps
x 300
200
100
0
0
3
6
9
12
15 time

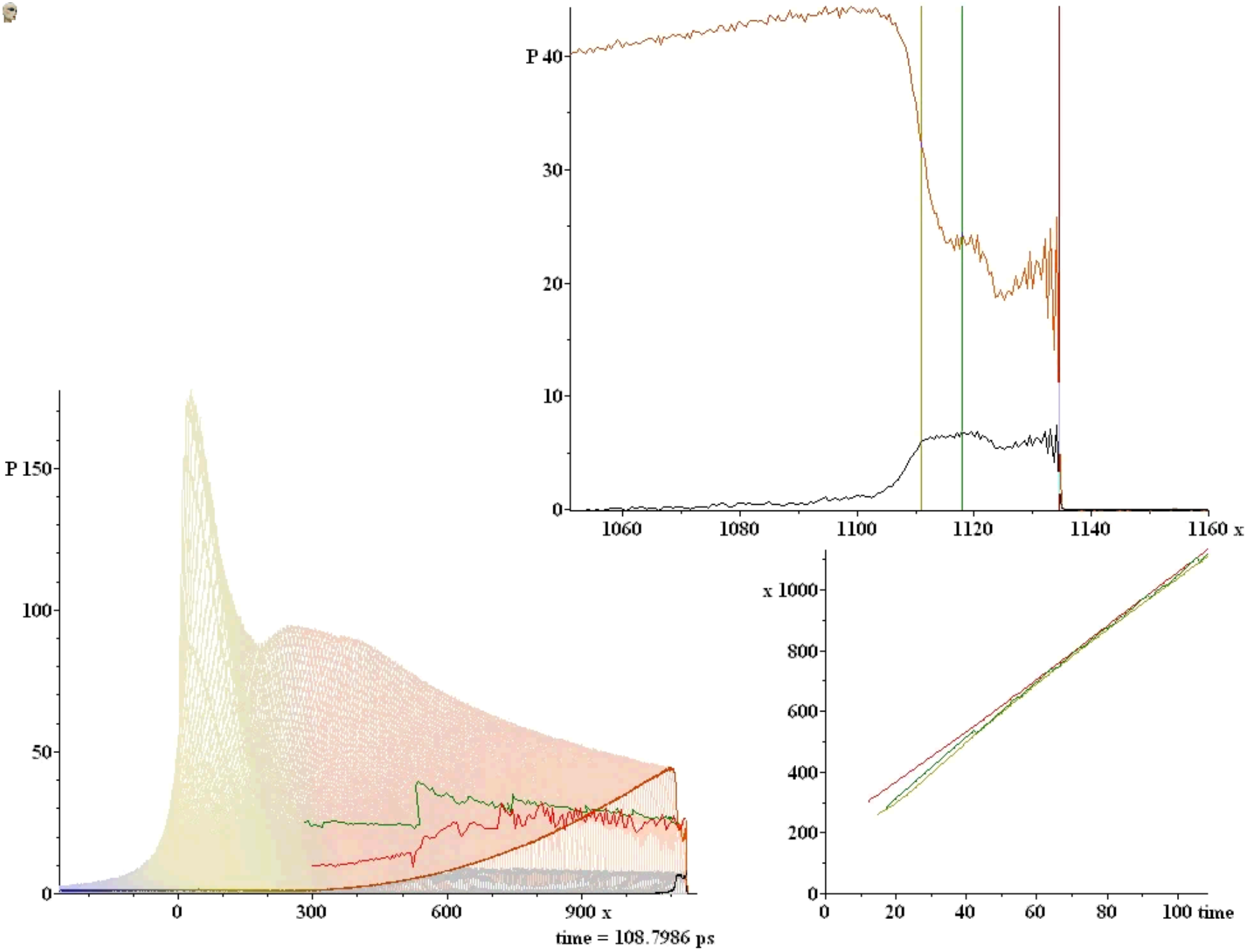

P 80
60
40
20
0
150
200
250
300
350 x
P 150
100
50
0
-200
-100
0
100
200
300 x
time = 18.559761 ps
x 300
200
100
0
0
5
10
15 time

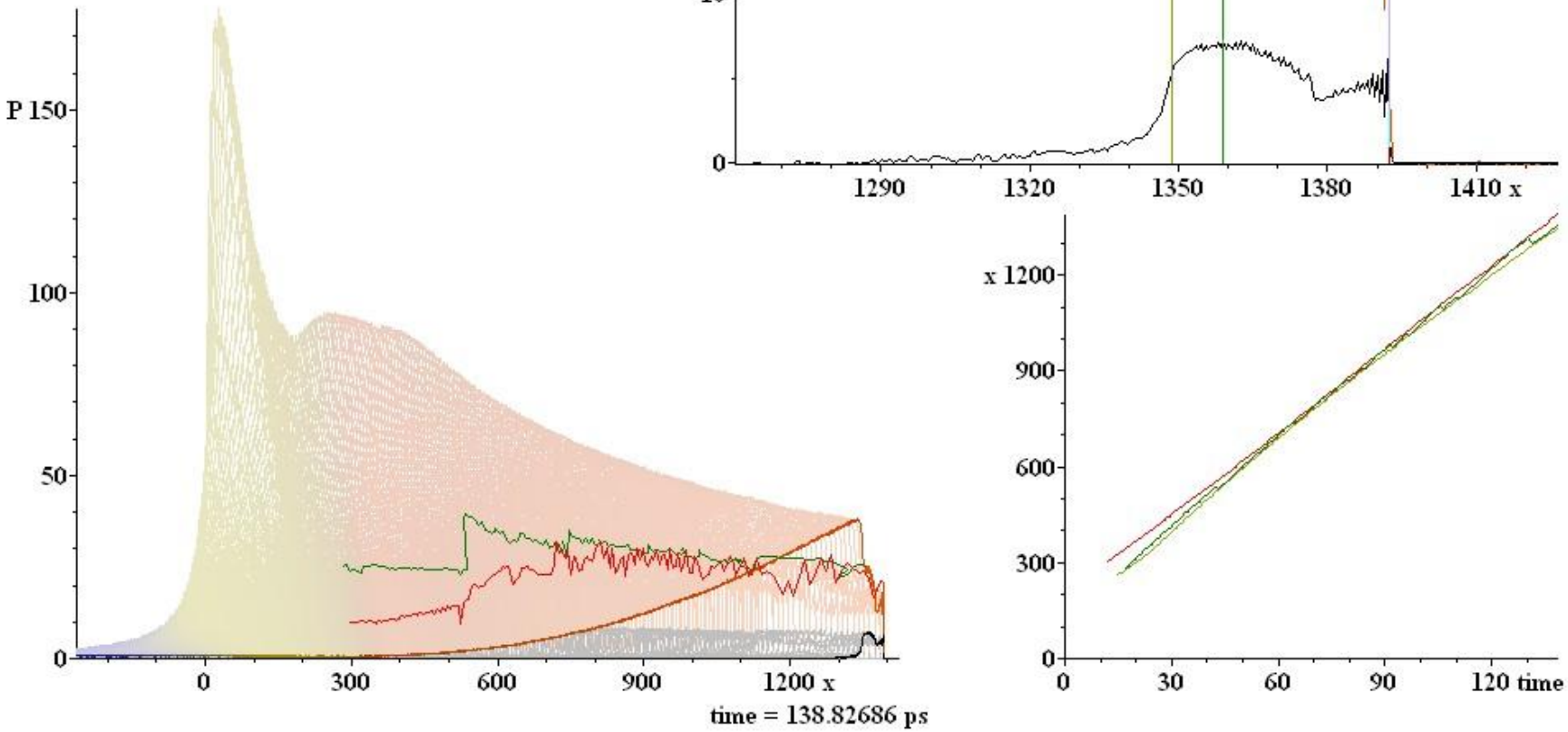

P 80
60
40
20
0
150
200
250
300
350 x
P 150
100
50
0
-200
-100
0
100
200
300 x
time = 18.559761 ps
x 300
200
100
0
0
5
10
15 time

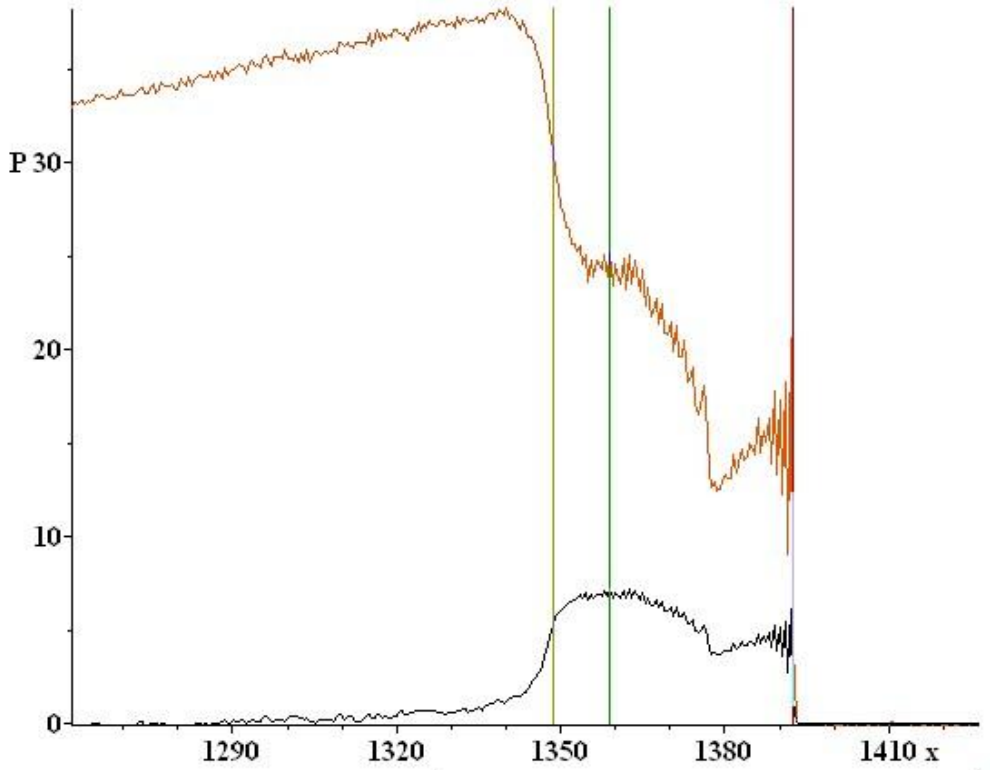

P 60
40
20
0
480
500
520
540
560
580 x
P 150
100
50
0
-200
0
200
400 x
time = 44.159431 ps
x 500
400
300
200
100
0
0
10
20
30
40 time


P 60
40
20
0
480
500
520
540
560
580 x
P 80
60
40
20
0
600
800
1000 x
time = 44.159431 ps
x 1100
1000
900
800
700
600
60
80
100 time

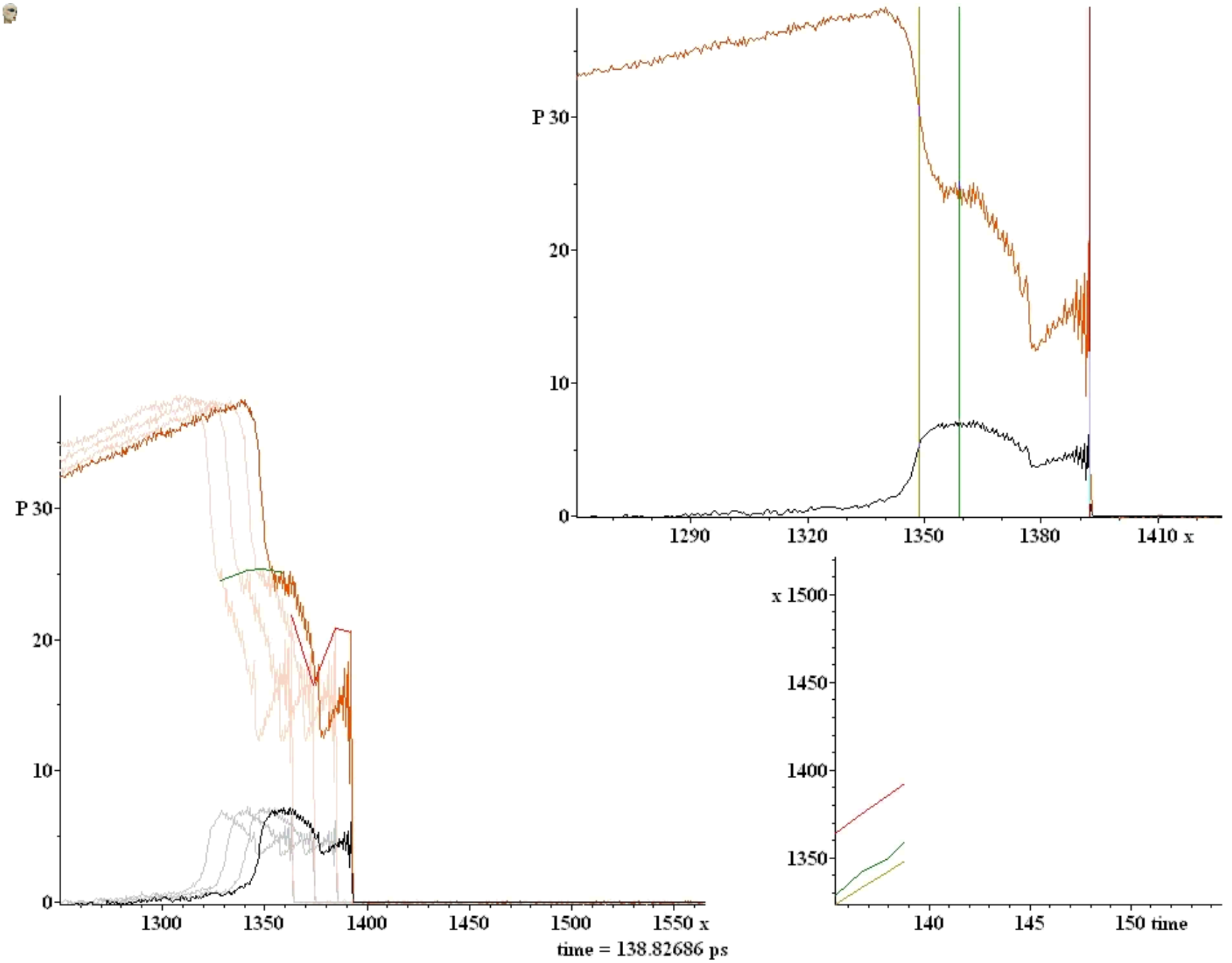

P 40
30
20
10
0
1060
1080
1100
1120
1140
1160 x
P 80
60
40
20
0
600
800
1000 x
time = 108.7986 ps
x 1100
1000
900
800
700
600
60
80
100 time

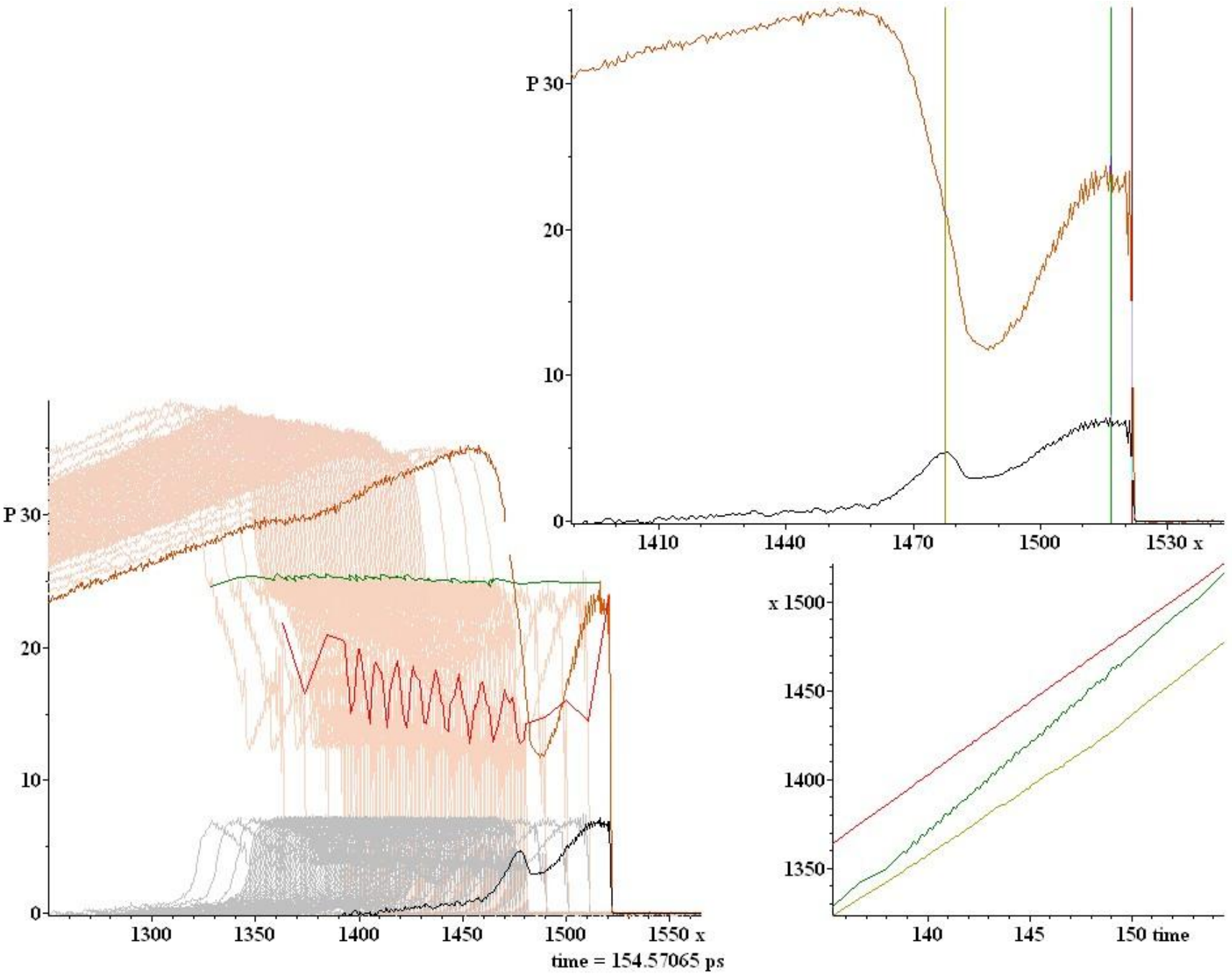

P 40
30
20
10
0
1060
1080
1100
1120
1140
1160 x
P 150
100
50
0
0
300
600
900 x
time = 108.7986 ps
x 1000
800
600
400
200
0
0
20
40
60
80
100 time

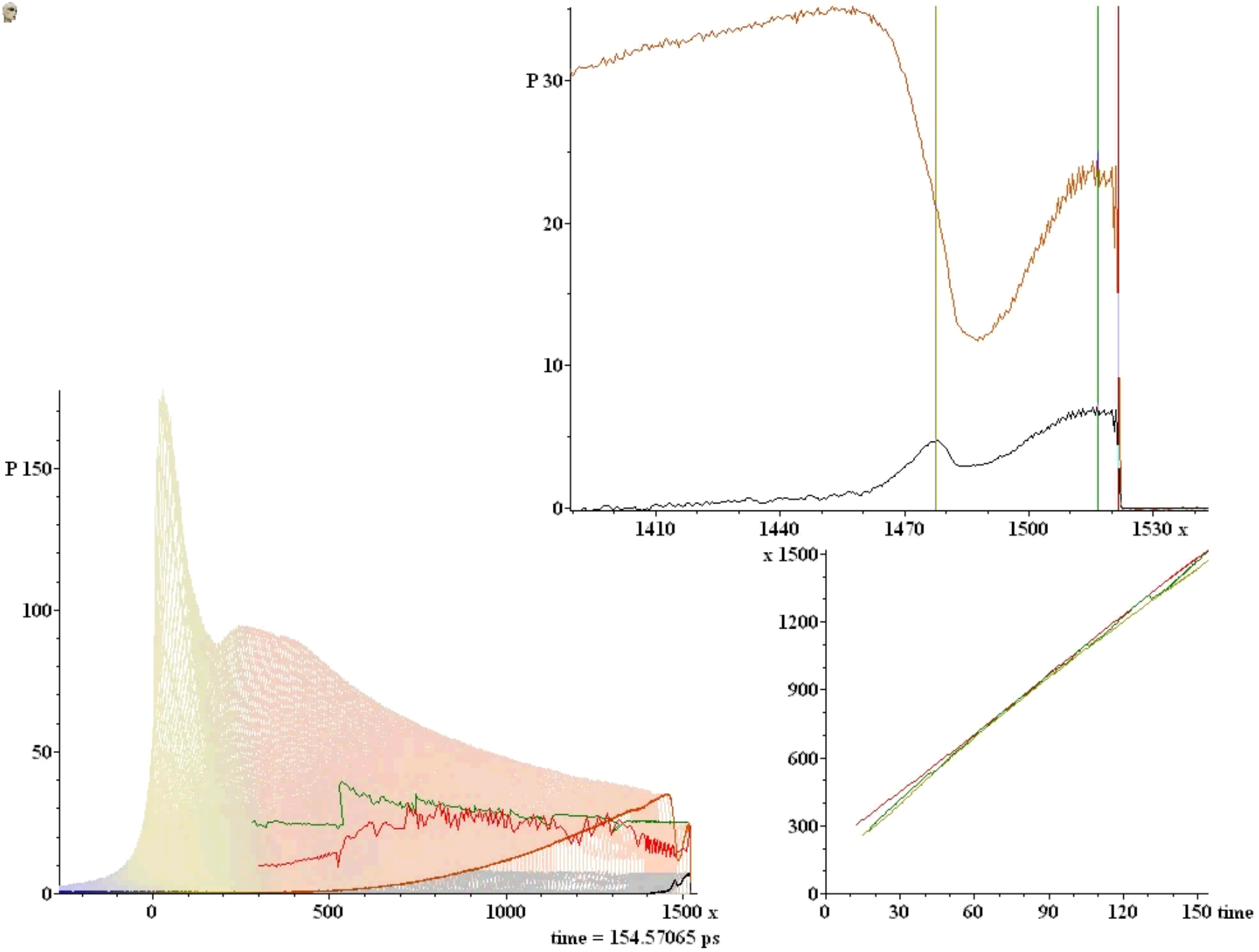

P 150
100
50
0
0
300
600
900
1200 x
time = 138.82686 ps

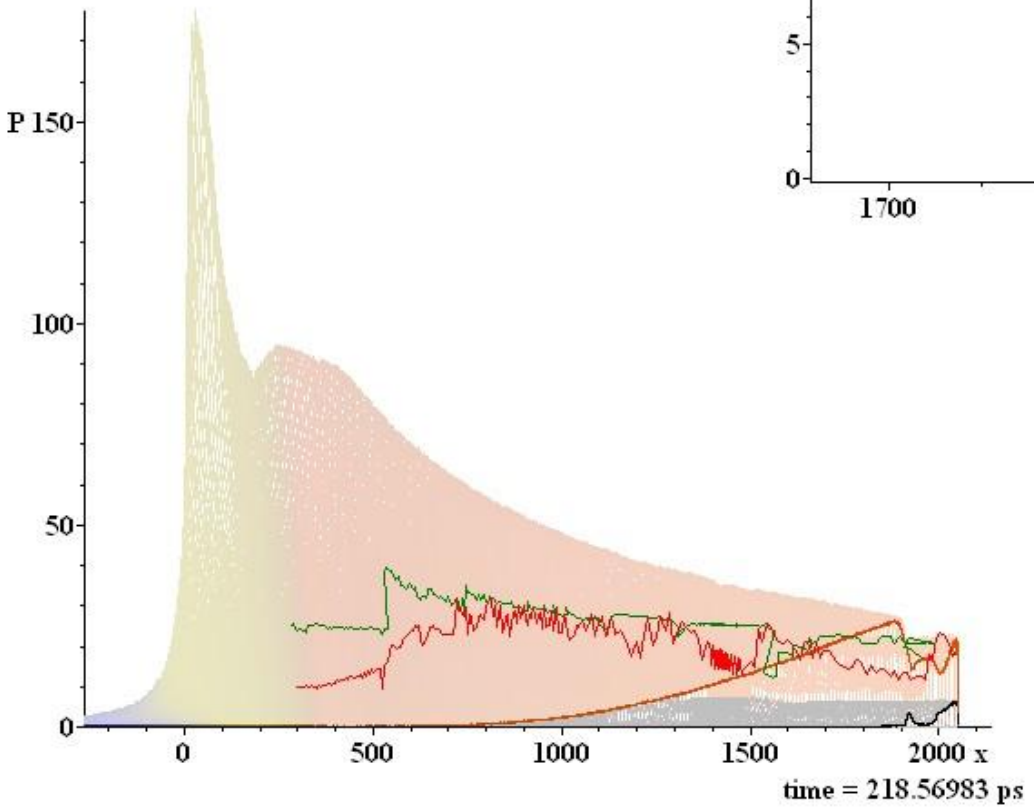

P 30
20
10
0
1290
1320
1350
1380
1410 x

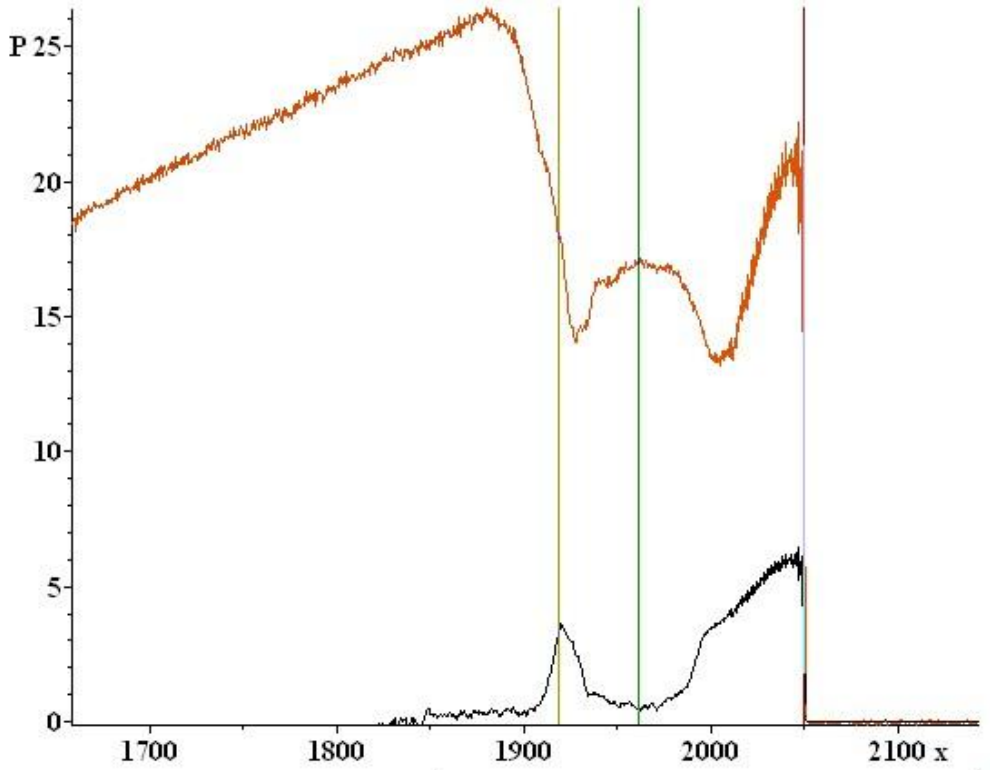
x 1200
900
600
300
0
0
30
60
90
120 time

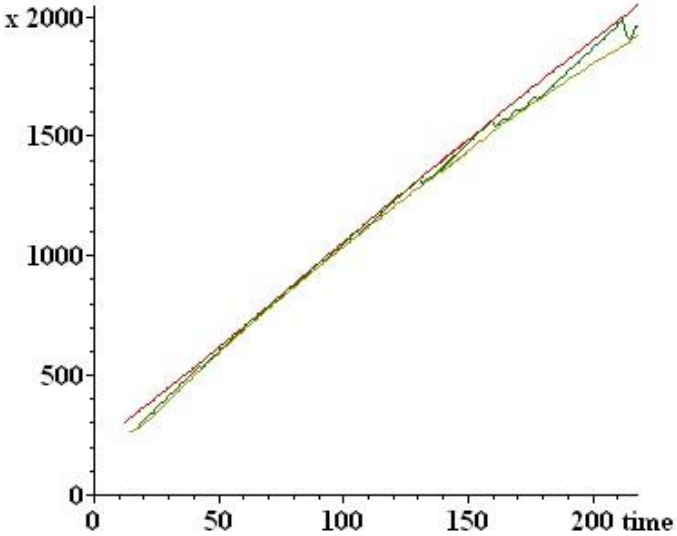

P 30
20
10
0
1290
1320
1350
1380
1410 x
P 30
20
10
0
1300
1350
1400
1450
1500
1550 x
time = 138.82686 ps
x 1500
1450
1400
1350
140
145
150 time

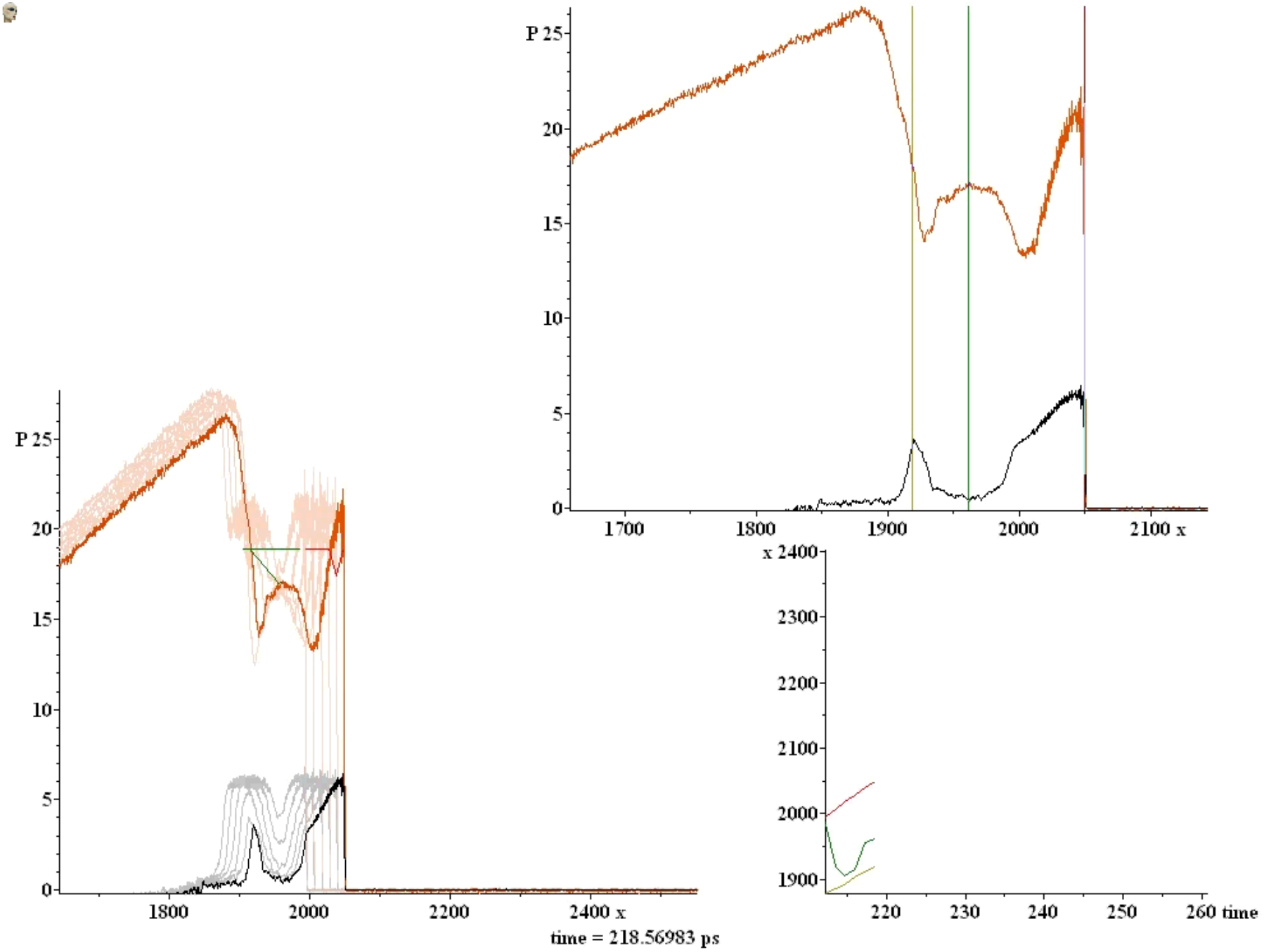

P 30
20
10
0
1410
1440
1470
1500
1530 x
P 30
20
10
0
1300
1350
1400
1450
1500
1550 x
time = 154.57065 ps
x 1500
1450
1400
1350
140
145
150 time

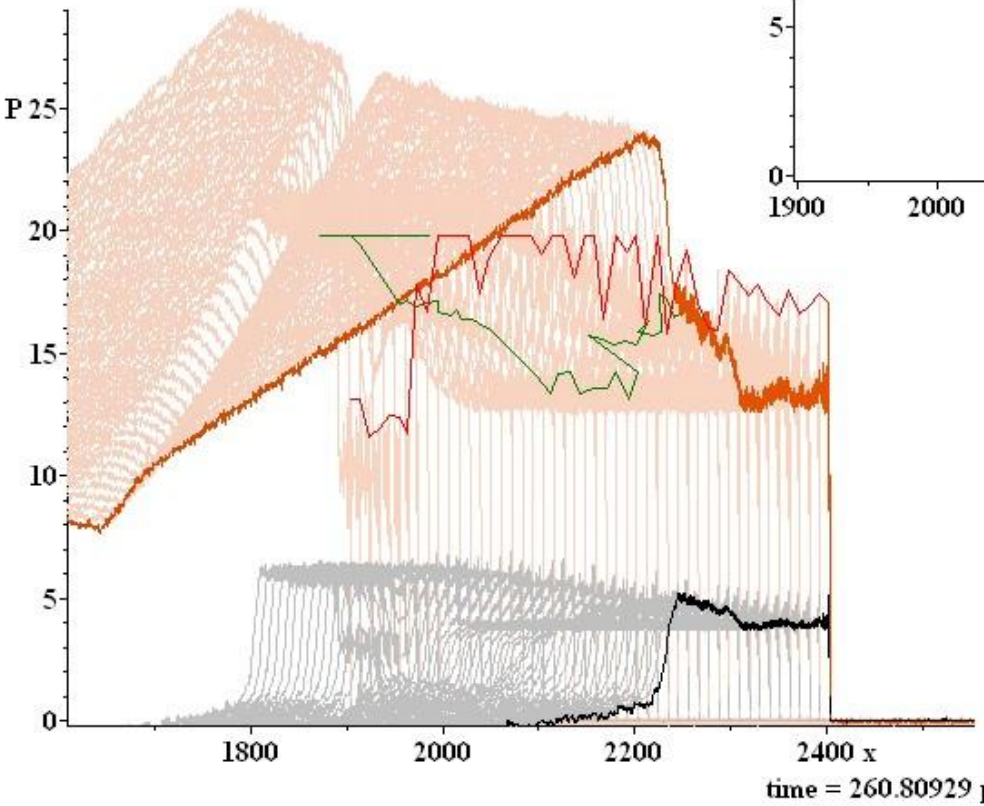

P 30
20
10
0
1410
1440
1470
1500
1530 x
P 150
100
50
0
0
500
1000
1500 x
time = 154.57065 ps
x 1500
1200
900
600
300
0
0
30
60
90
120
150 time


P 150
100
50
0
0
500
1000
1500
2000 x
time = 218.56983 ps

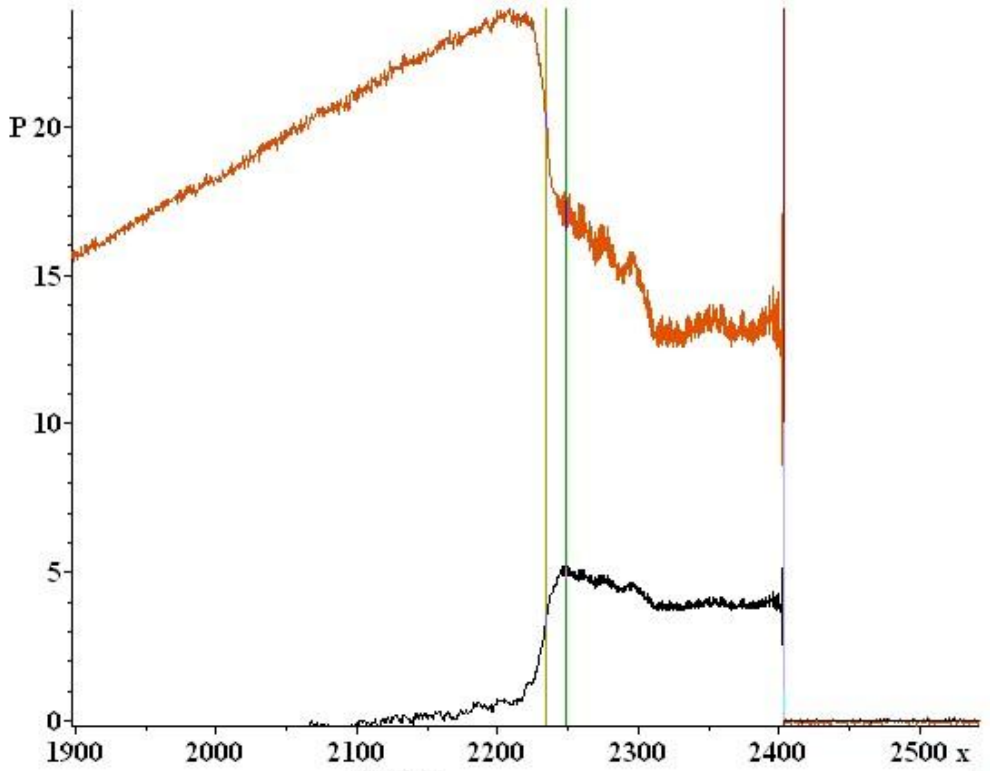

P 25
20
15
10
5
0
1700
1800
1900
2000
2100 x

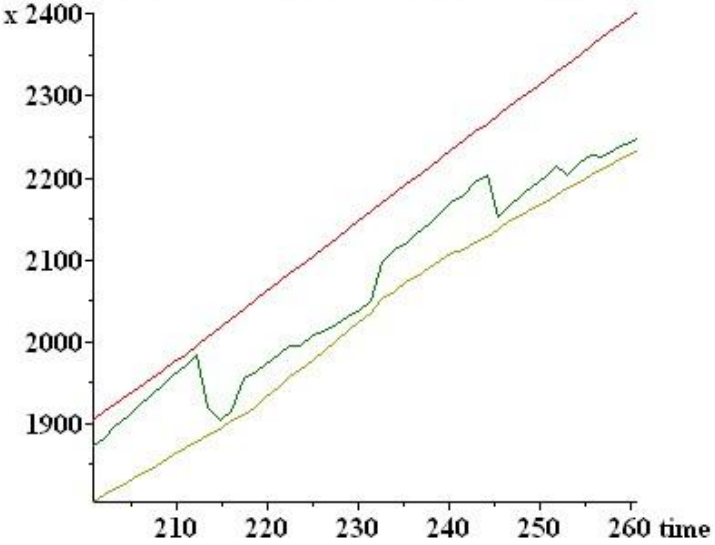

x 2000
1500
1000
500
0
0
50
100
150
200 time

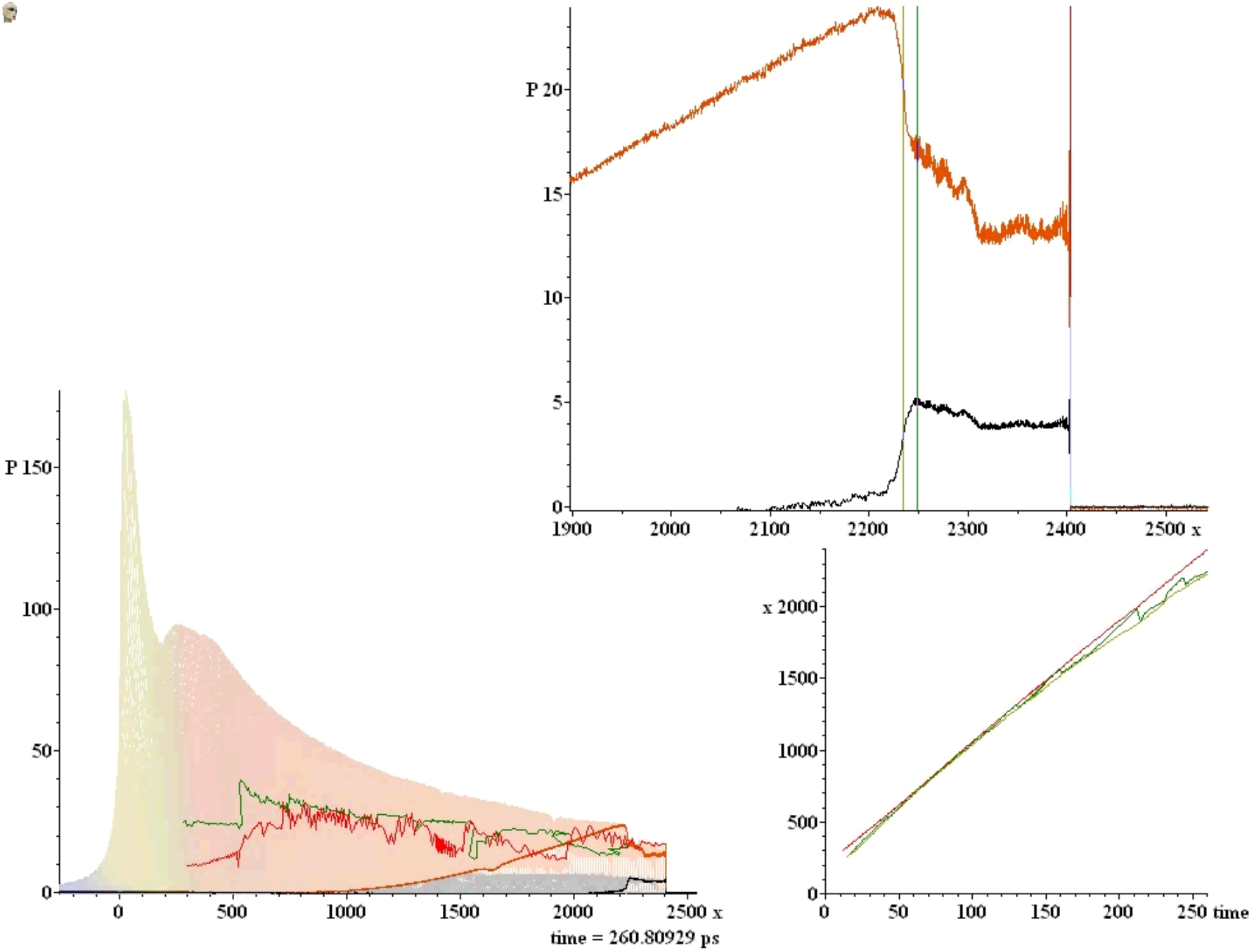

P 25
20
15
10
5
0
1700
1800
1900
2000
2100 x
P 25
20
15
10
5
0
1800
2000
2200
2400 x
time = 218.56983 ps
x 2400
2300
2200
2100
2000
1900
220
230
240
250
260 time

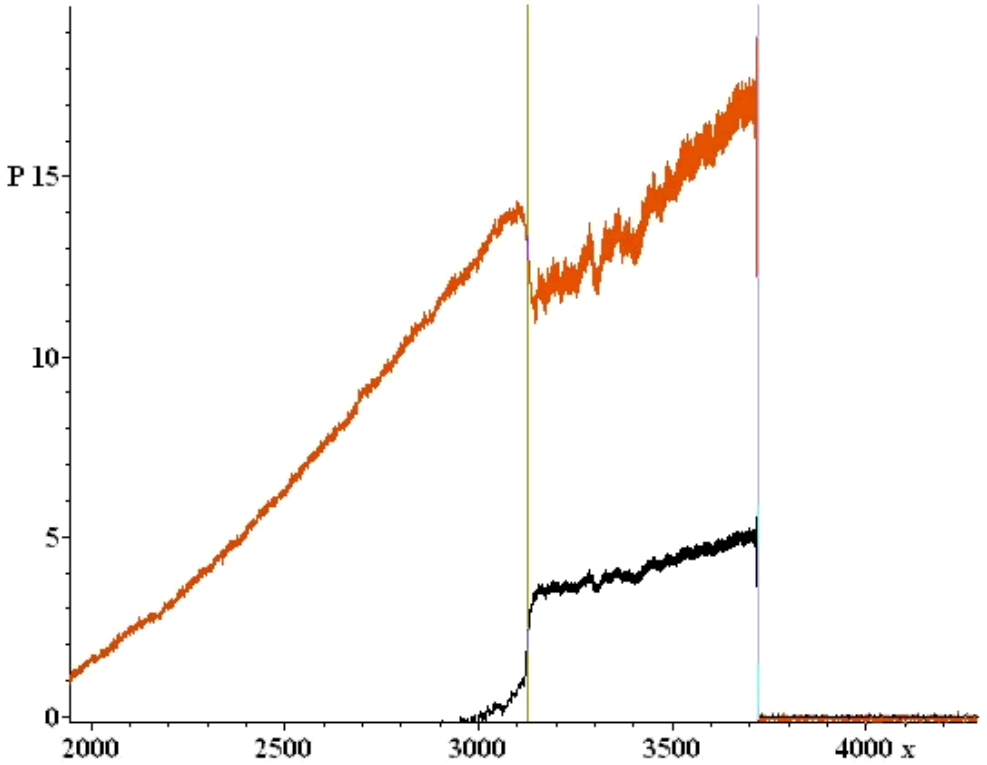


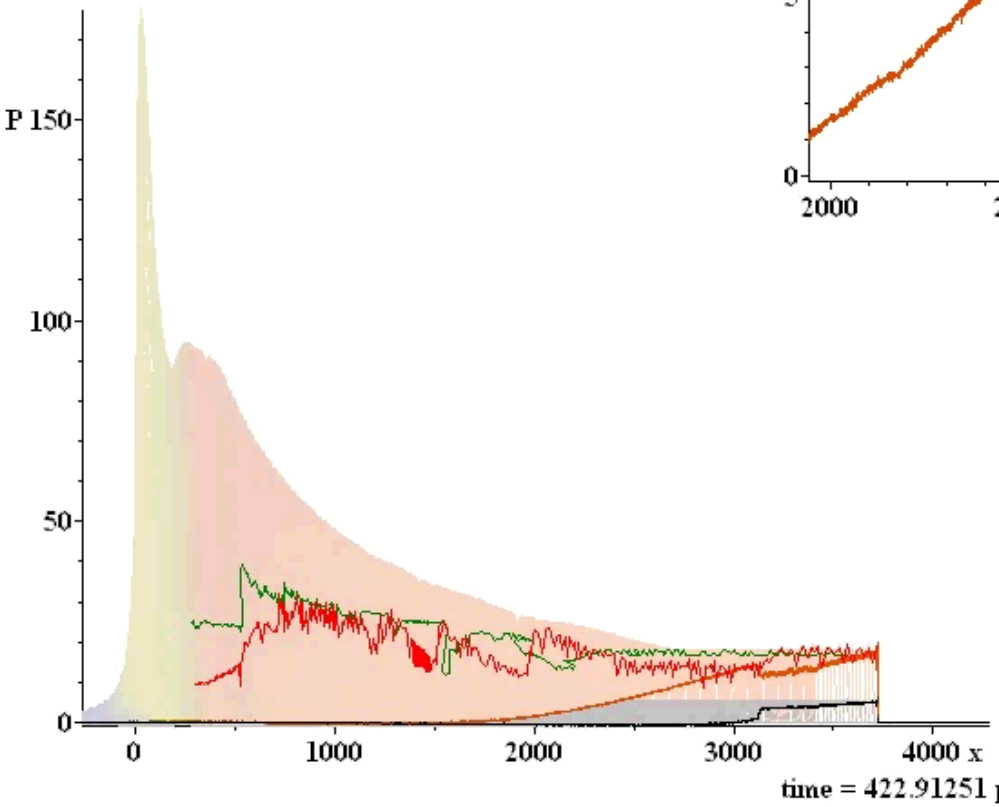
time = 260.80929 ps

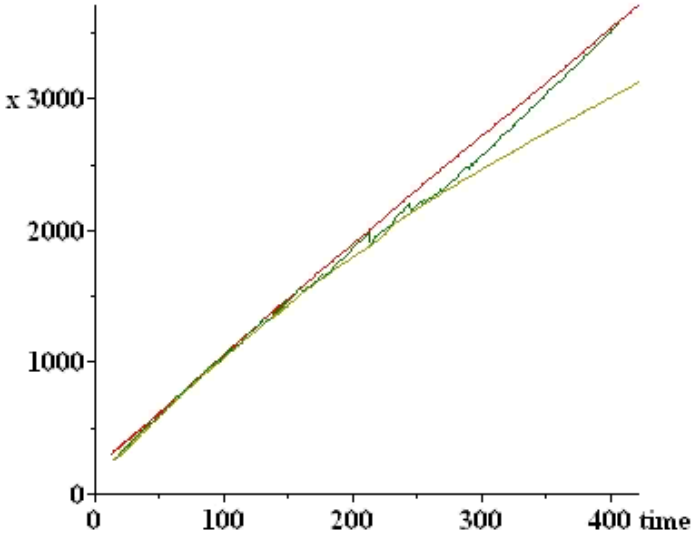


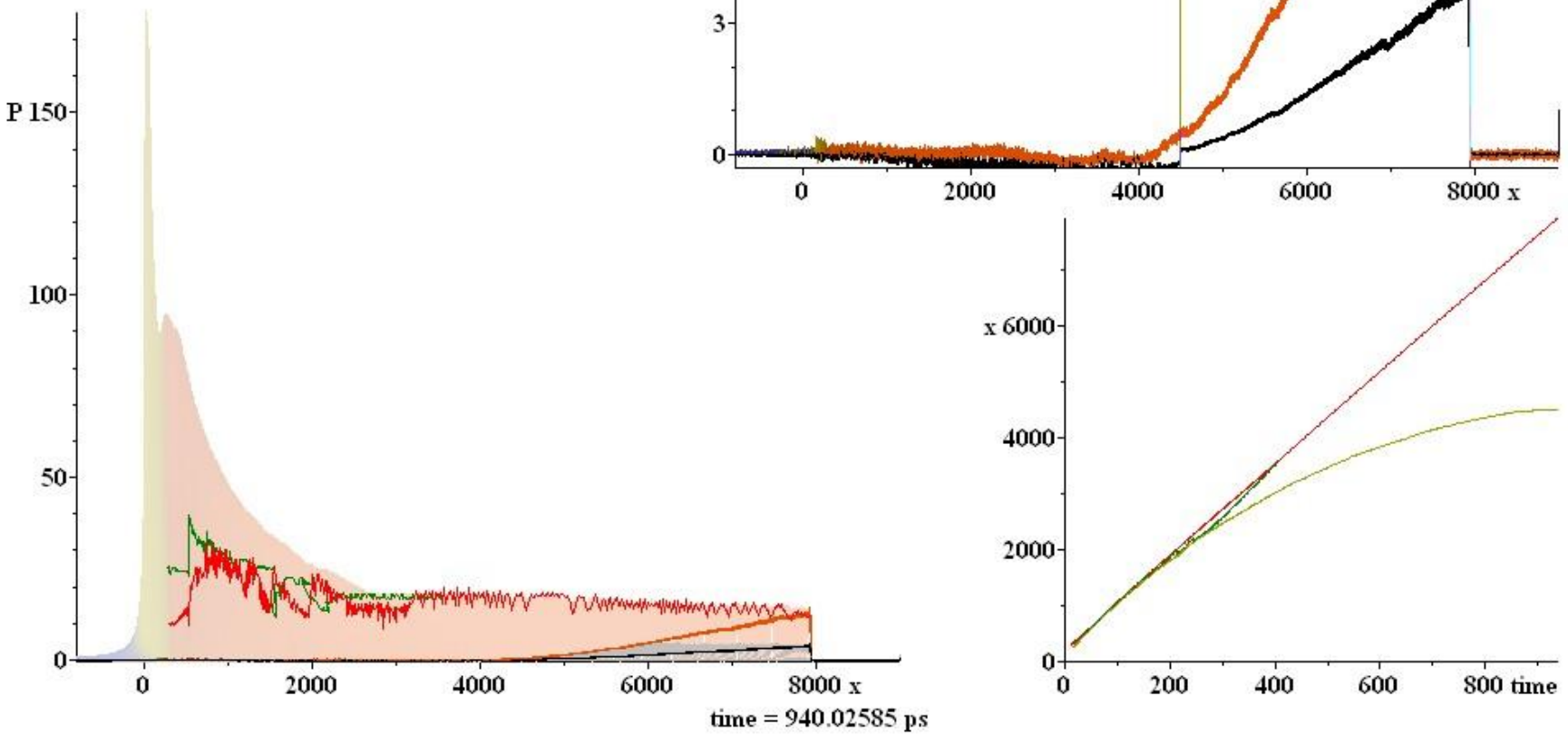



P 20
15
10
5
0
1900
2000
2100
2200
2300
2400
2500 x
P 150
100
50
0
0
500
1000
1500
2000
2500 x
time = 260.80929 ps
x 2000
1500
1000
500
0
0
50
100
150
200
250 time

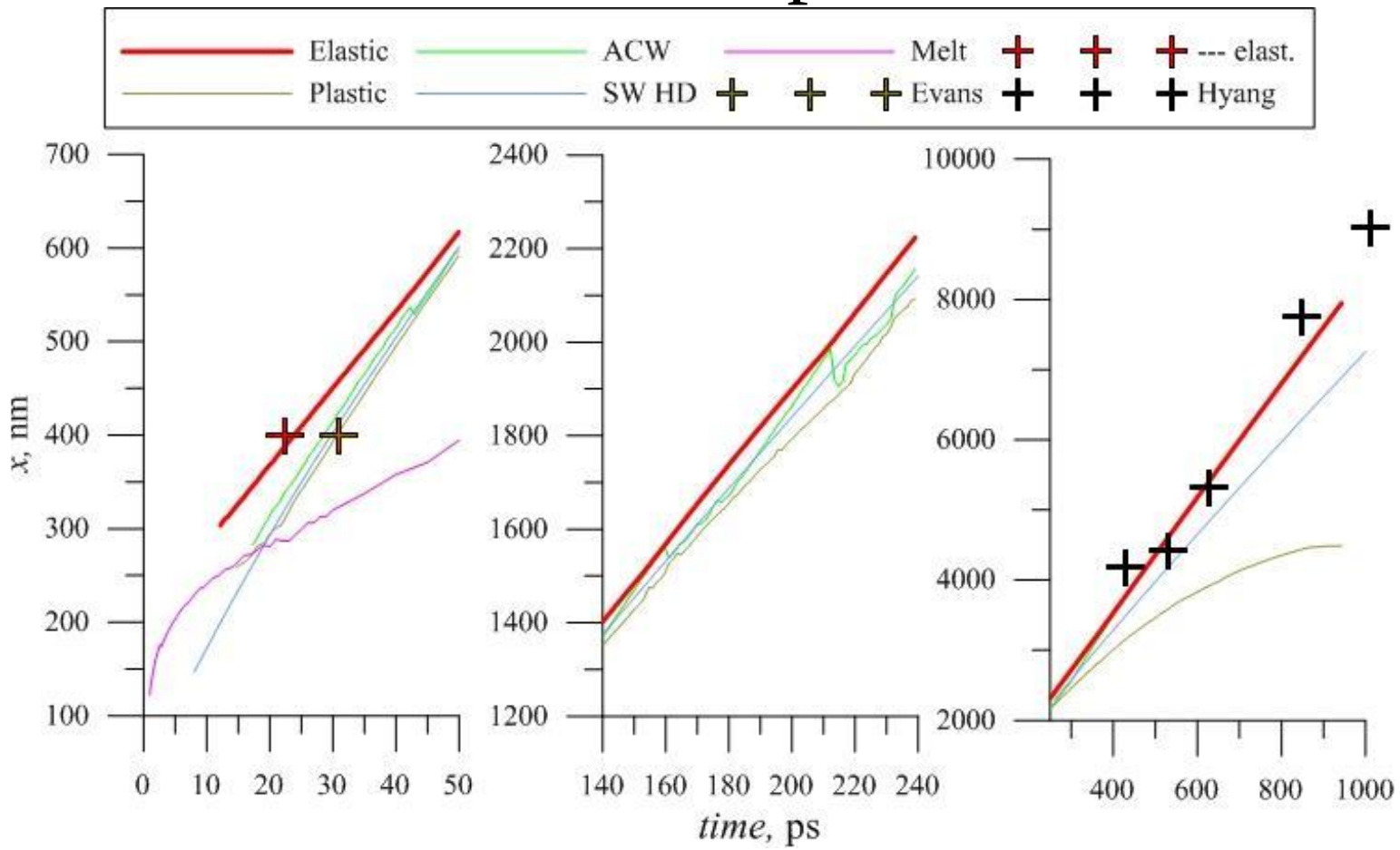

P 15
10
5
0
2000
2500
3000
3500
4000 x


P 150
100
50
0
0
1000
2000
3000
4000 x
time = 422.91251 ps


x 3000
2000
1000
0
0
100
200
300
400 time


P 12
9
6
3
0
0
2000
4000
6000
8000 x
P 150
100
50
0
0
2000
4000
6000
8000 x
time = 940.02585 ps
x 6000
4000
2000
0
0
200
400
600
800 time

Positions of elastic and plastic SW in time



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