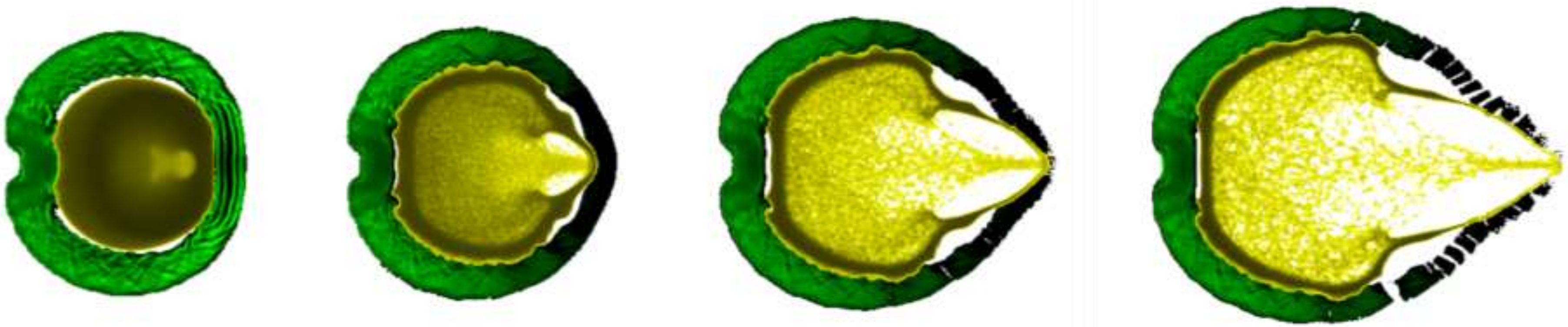
XIV Zababakhin Scientific Talks, Snezhinsk, March 18-22 (2019)

A STATE CORPORATION "ROSATOM" COMPANY

DUKHOV ALL-RUSSIAN RESEARCH INSTITUTE OF AUTOMATICS (VNIIA)

The models of boron carbide and steel for simulations of experiments on explosive compression of spherical shells using computational fluid dynamics



S. A. Dyachkov, S. Yu. Grigoryev,

A. N. Parshikov, V. V. Zhakhovsky

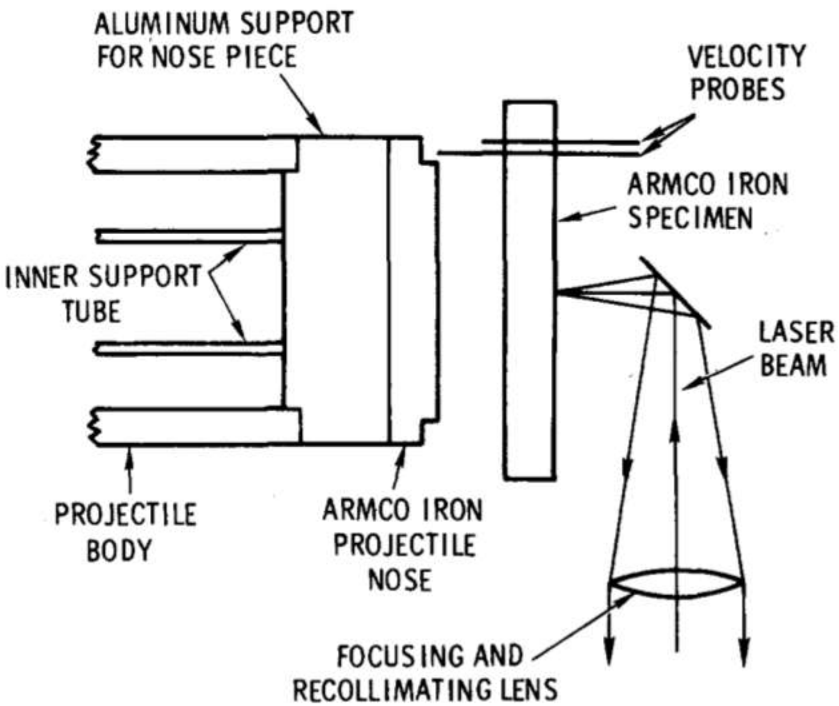
Motivation

- Simulations of material response to shock compression require complex models
- Material models are usually fitted to data obtained in uniaxial shock loading tests
- Do these models valid for simulations of complex engineering prototypes in three dimensional case?

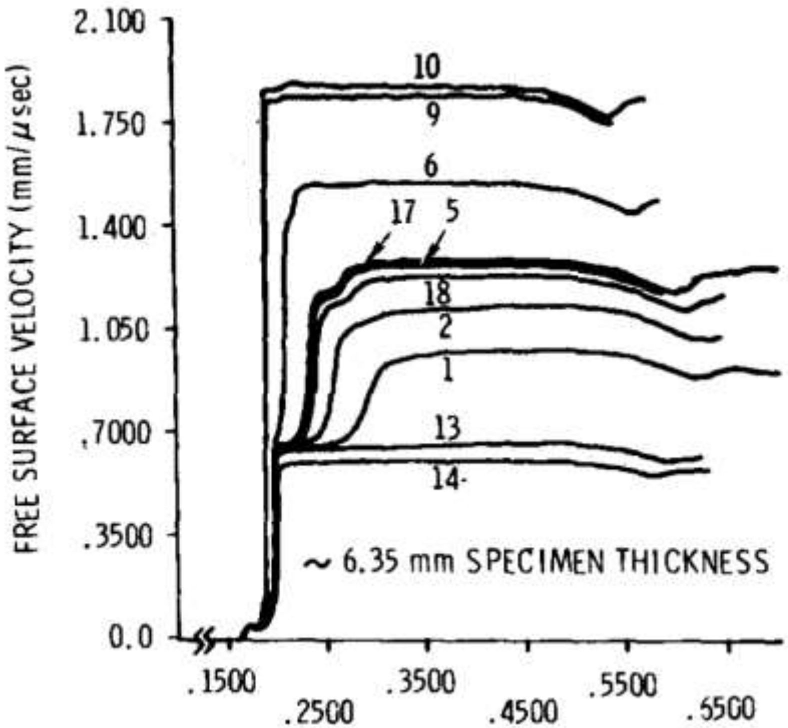
Experiments

Uniaxial compression of iron

Experiment setup



VISAR measurements

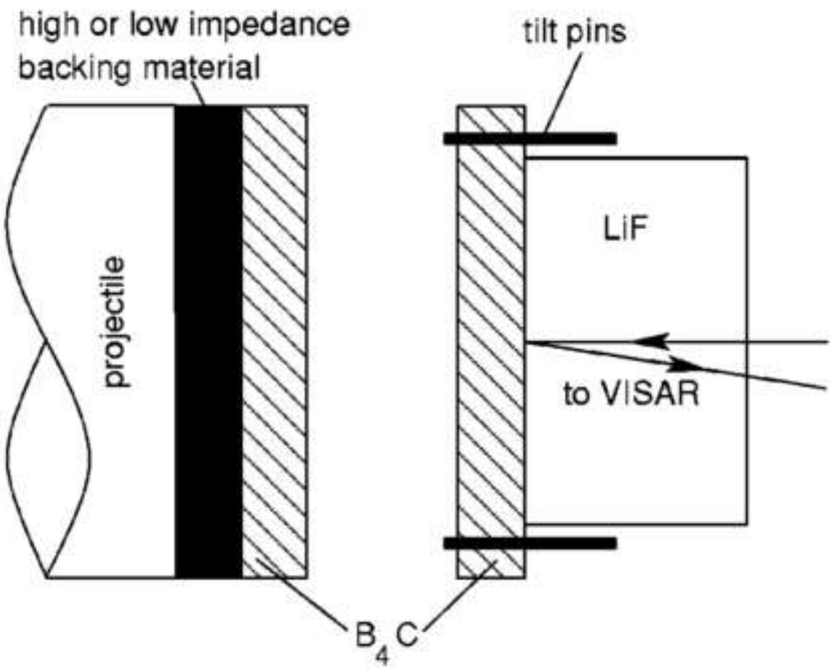


- An impactor and a target are ARMCO iron plates of 6.35 mm width
- An elastic precursor is observed at all loading conditions
- Region of phase transition is observed in free surface velocity profile for impact velocities higher that 0.67 km/s (test 13 and so on)
- Impacts (test 9, 10) with high velocity do not show the region of phase transition

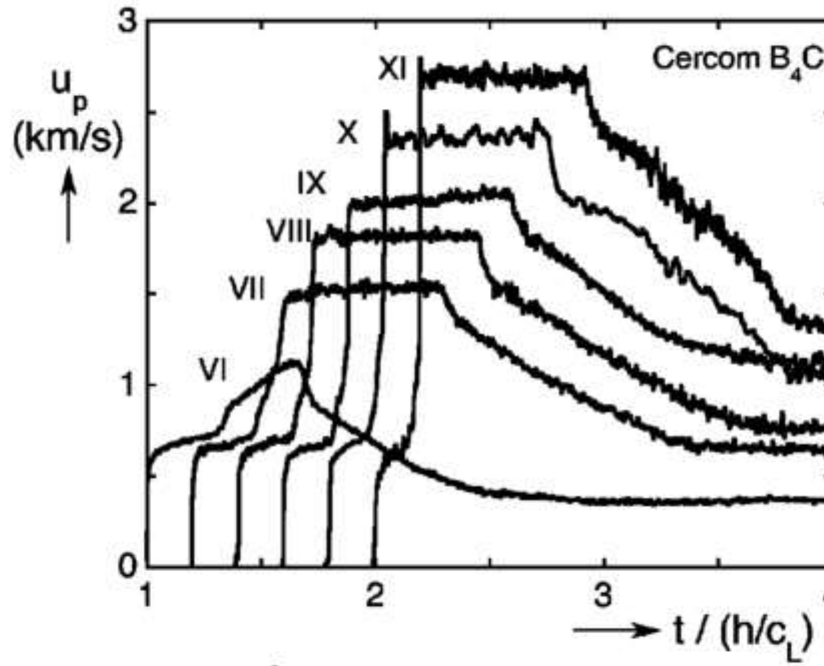
Barker L. M., Hollenbach R. E. Journal of Applied Physics **45** 4872 (1974)

Uniaxial compression of boron carbide

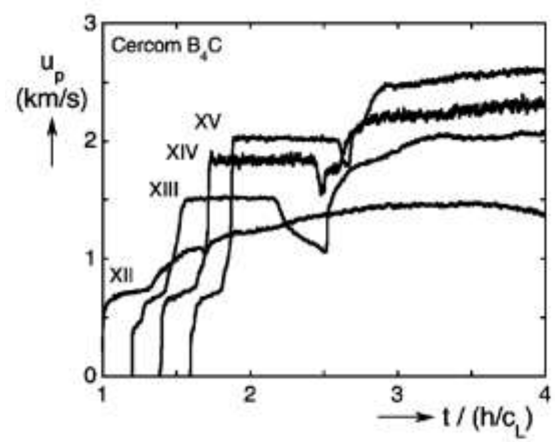
Experiment setup



VISAR measurements



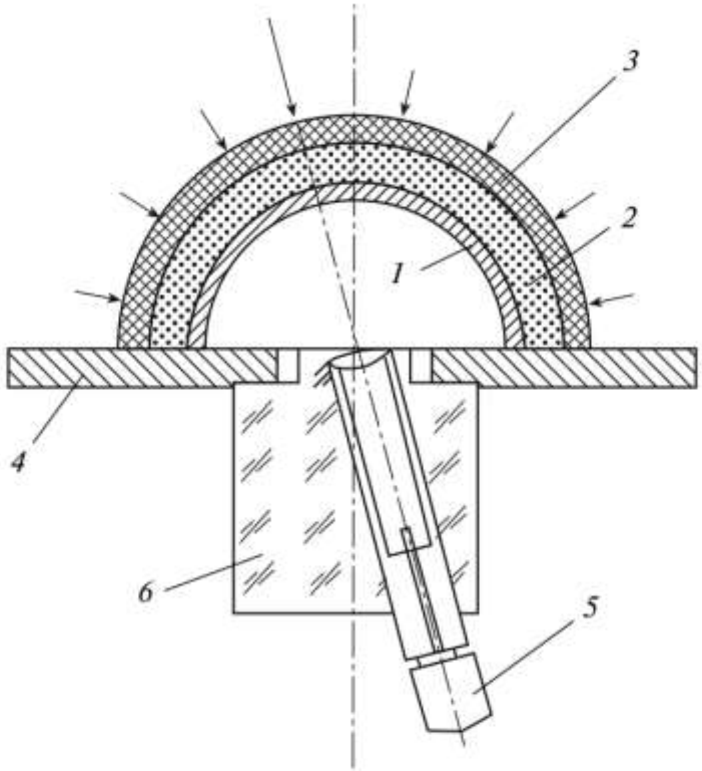
- Impactor and target are of boron carbide (B_4C).
- Some tests include backing of light or heavy material. A LiF window is attached behind a target.
- VISAR measurements of B_4C/LiF interface velocity are obtained.



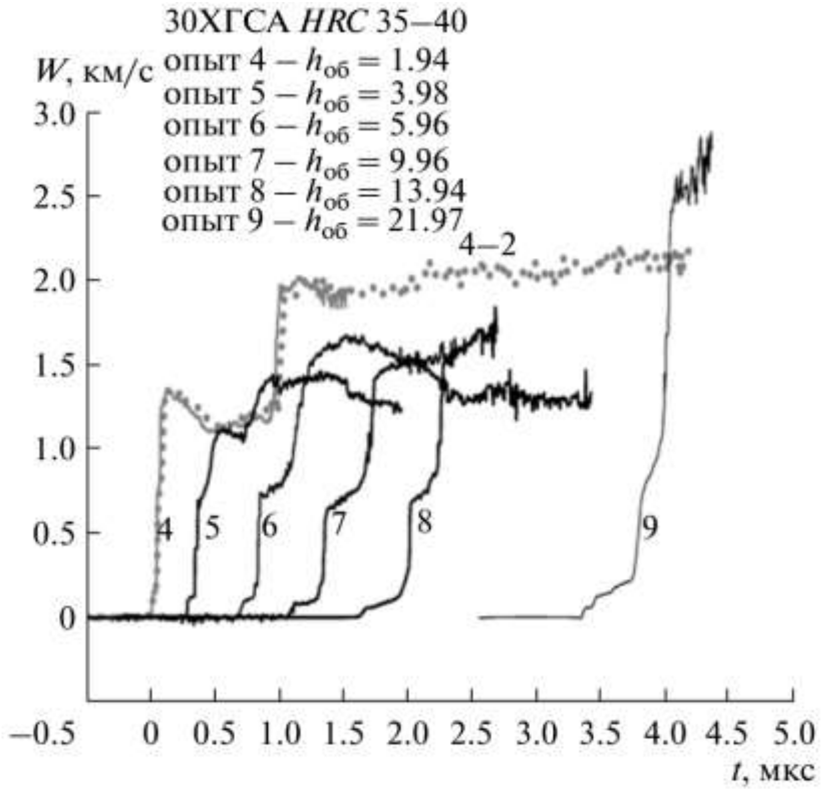
T. J. Vogler, W. D. Reinhart, L. C. Chhabildas, Journal of Applied Physics **95,** 4173 (2004)

Spherical compression of steel shells

Experiment setup



Laser interferometer

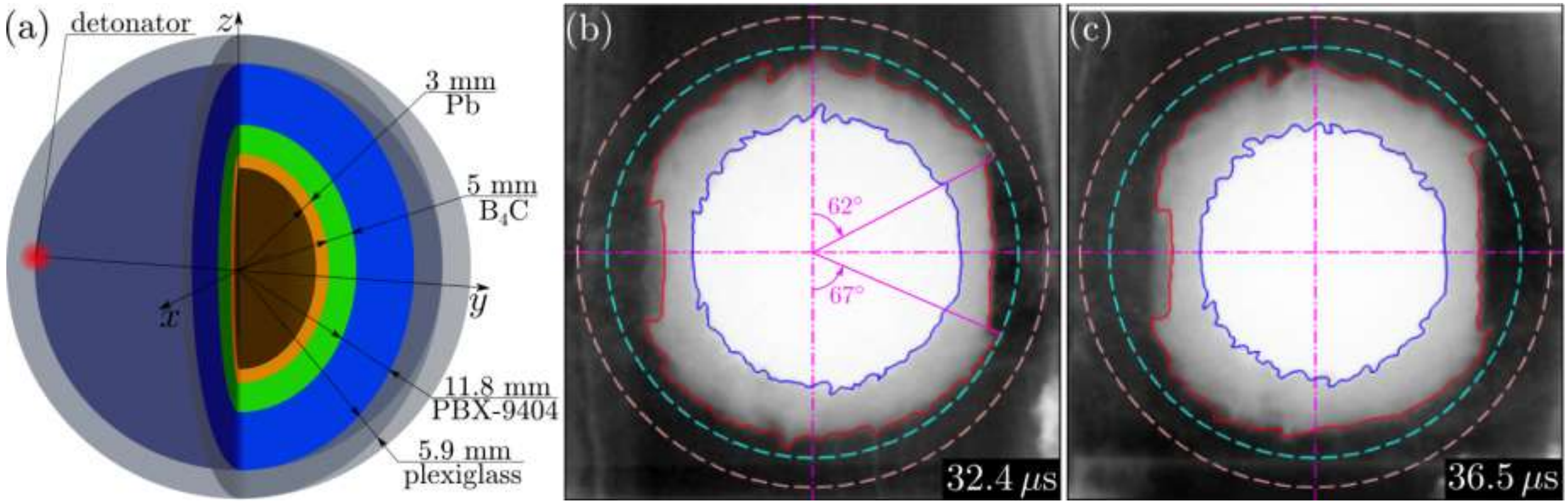


1 – Steel shell
2 – Spherical HE layer (HMX-based composition)
3 – System of detonators
4 – Aluminum protecting plaste
5 – Laser measurements device

A set of velocity profiles of an inner free surface of steel plates of various width.
α-ε phase transition can be observed in steel.

Е. А. Козлов, С. А. Бричиков, Д. С. Боярников [и др.] Физика металлов и металловедение. Прочность и пластичность. Т. 112. С. 412–428 (2011)

Spherical compression of the boron carbide shell



Setup (RFNC-VNIIEF)

V. A. Arinin, G. Ya. Karpenko, V. V. Kovaldov,
A. V. Nefedov, K. N. Panov, S. Yu. Sogrin

- Maximal outer radius 57.8 mm
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- HE PBX-9404 shell (11.8 mm width)
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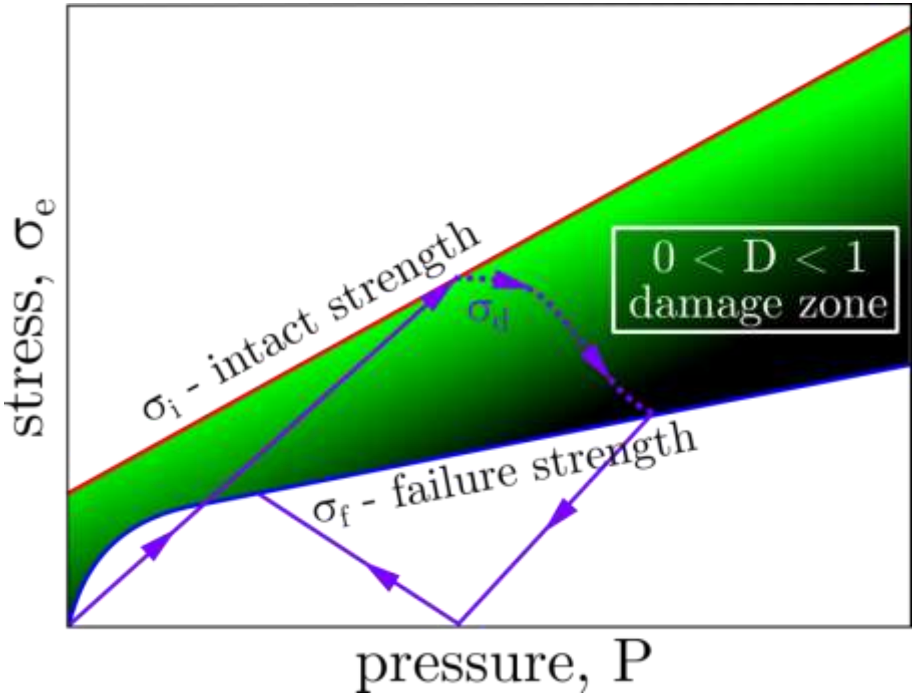
Results

- X-ray snapshots are taken at 32.4 and 36.5 μs after detonation
- Outer boundaries of the boron carbide (B_4C) and lead (Pb) shells are visible
- A crater is formed near detonator
- Detonation wave converges at the rear side of the B_4C shell which becomes flattened
- Inner and outer surface of the B_4C shell has visible perturbations

Simulation of boron carbide

B_4C failure: a change in strength properties

Johnson-Holmquist (JH) model



Strength limit in ceramics:

$$\sigma_d = \sigma_i - D(\sigma_i - \sigma_f)$$

Accumulation of damage:

$$D = \sum \frac{\Delta \varepsilon_p}{\varepsilon_p^f}$$

plastic strain increment

total plastic strain to failure

Stress deviator correction: the von Mises criterion

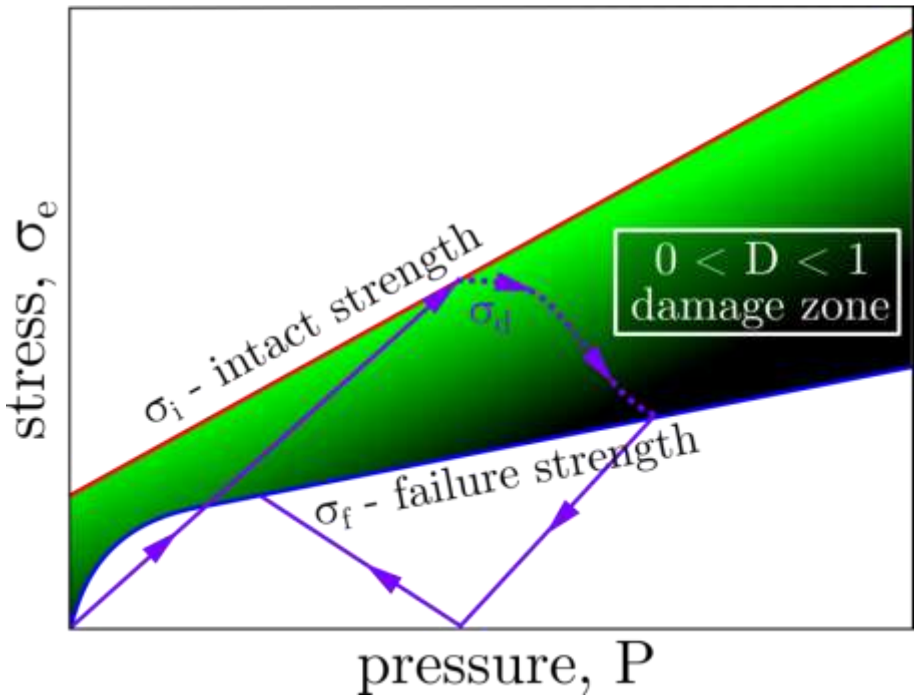
$$\hat{\sigma}_e = \sqrt{\frac{1}{2}\left[\left(\hat{S}_{xx} - \hat{S}_{yy}\right)^2 + \left(\hat{S}_{yy} - \hat{S}_{zz}\right)^2 + \left(\hat{S}_{xx} - \hat{S}_{zz}\right)^2 + + 6\left(\hat{S}_{xy}^2 + \hat{S}_{yz}^2 + \hat{S}_{xz}^2\right)\right]}$$

если $\hat{\sigma}_e > \sigma_d$: $S_{\alpha\beta} = \frac{\sigma_d}{\hat{\sigma}_e} \hat{S}_{\alpha\beta}$, $\sigma_e = \sigma_d$

G. R. Johnson, T. J. Holmquist, Journal of Applied Physics **85,** 8060 (1999)

B_4C failure: a change in strength properties

Improved Johnson-Homquist model



Strength limit in ceramics:

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Accumulation of damage:

$$D = \sum \frac{\Delta\varepsilon_p}{\varepsilon_p^f}$$

plastic strain increment

total plastic strain to failure

How to evaluate $\Delta\varepsilon_p$?

uncorrected corrected

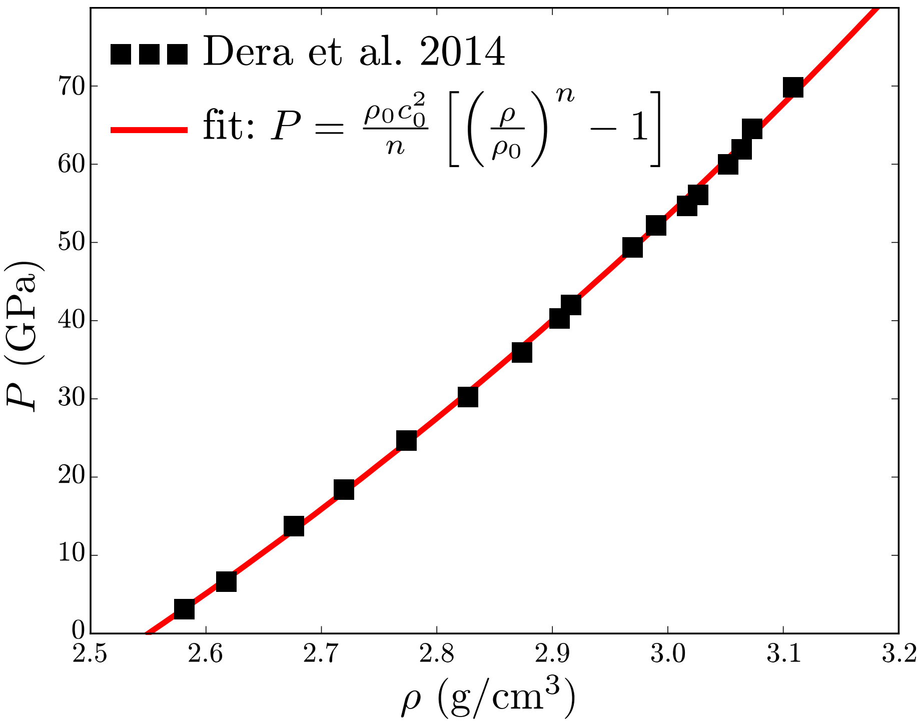
Wilkins: $\Delta\varepsilon_p = \dfrac{\hat{\sigma}_e - \sigma_e}{3G}$ shear modulus

What about ε_p^f ?

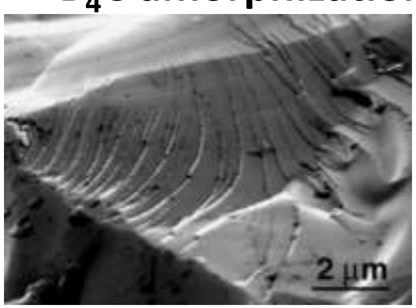
JH – empirical expression $\varepsilon_p^f = D_1(P^* + T^*)^{D_2}$

our consistent definition $\varepsilon_p^f = \max \Delta\varepsilon_p = \dfrac{\sigma_i - \sigma_f}{3G}$

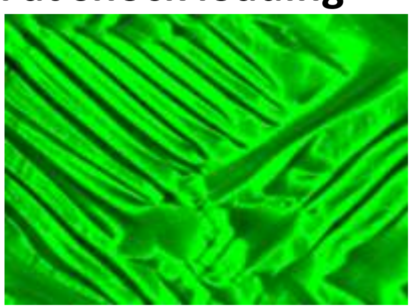
B_4C equation of state



B_4C amorphization at shock loading



Mingwei Chen et al.
Science 299, 1563 (2003)



Local failure bands
appear in a simulation

Mie-Gruneisen form

$$P_{\mathrm{EoS}} = P_r + \Gamma\rho(e - e_r)$$

Local amorphization accompanied with “bulking”:

B – bulk modulus,

$$\mu = \rho/\rho_0 - 1$$

$$\Delta P^{t+\Delta t} = -B\mu + \sqrt{(B\mu + \Delta P^t)^2 + 2\beta B \Delta U}$$

Elastic energy loss during failure:

$$\Delta U = \frac{\left(\sigma_d^2\right)_t}{6G} - \frac{\left(\sigma_d^2\right)_{t+\Delta t}}{6G}$$

Total pressure:

$$\boldsymbol{P}_{\mathbf{total}} = \boldsymbol{P}_{\mathbf{EoS}} + \boldsymbol{\Delta P}$$

SPH-simulation with high spatial resolution

Function and its gradient interpolation

$$f(\mathbf{r}) = \sum_{j=1}^{N} f_j \Delta V_j W(|\mathbf{r} - \mathbf{r}_j|, h)$$

Fluid dynamics equations approximation (CSPH)

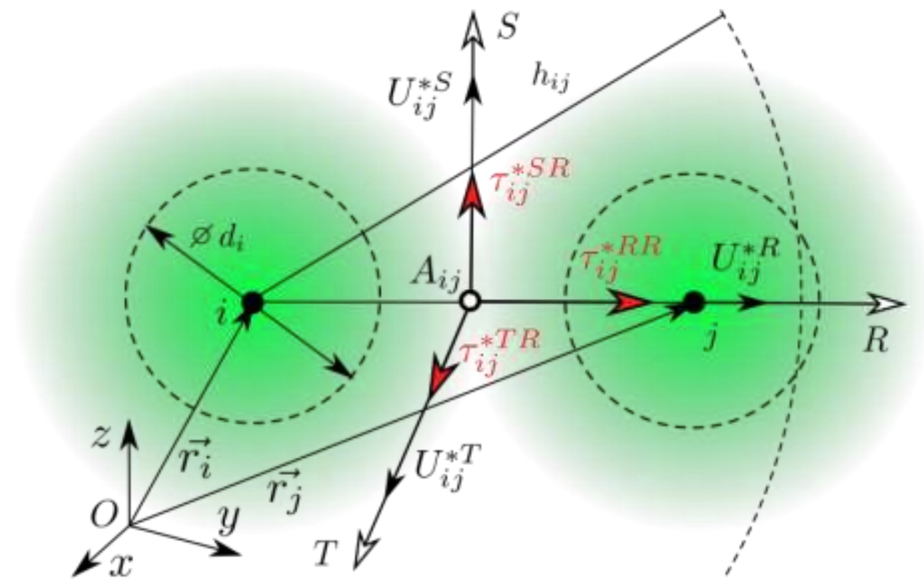
A. N. Parshikov, S. A. Medin. J. Comp. Phys. ***180*** *353-382 (2002)*

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = 2\rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} (\mathbf{U}_i - \mathbf{U}_{ij}^*) \cdot \nabla W_{ij}$$

$$\frac{\mathrm{d}\mathbf{U}_i}{\mathrm{d}t} = -\frac{2}{\rho_i} \sum_{j=1}^{N} \frac{m_j}{\rho_j} P_{ij}^* \nabla W_{ij}$$

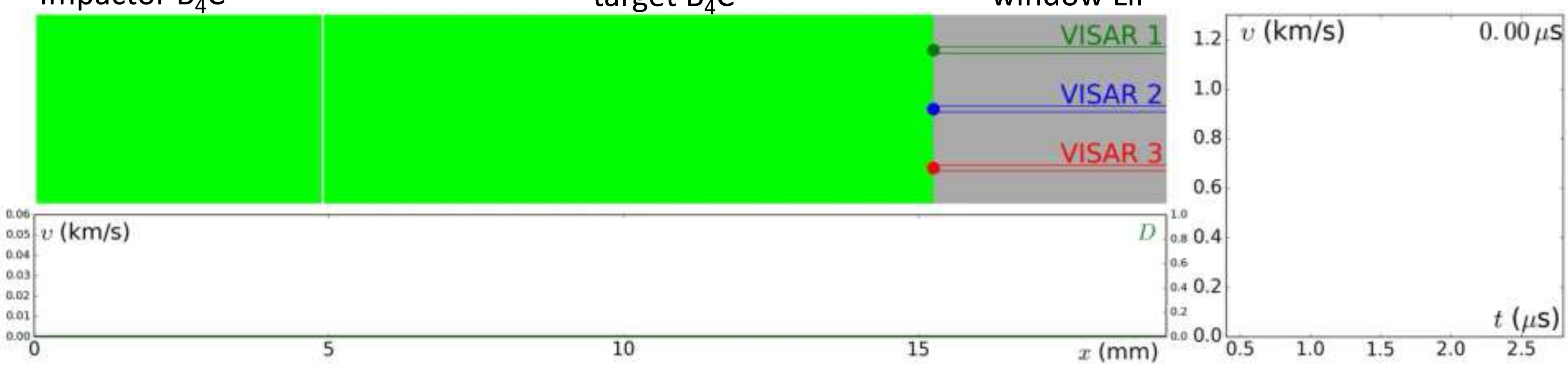
$$\frac{\mathrm{d}e_i}{\mathrm{d}t} = \frac{2}{\rho_i} \sum_{j=1}^{N} \frac{m_j}{\rho_j} P_{ij}^* (\mathbf{U}_i - \mathbf{U}_{ij}^*) \cdot \nabla W_{ij}$$

Riemann problem solution at interparticle contacts



Uniaxial compression of boron carbide samples

Impactor B_4C target B_4C window LiF

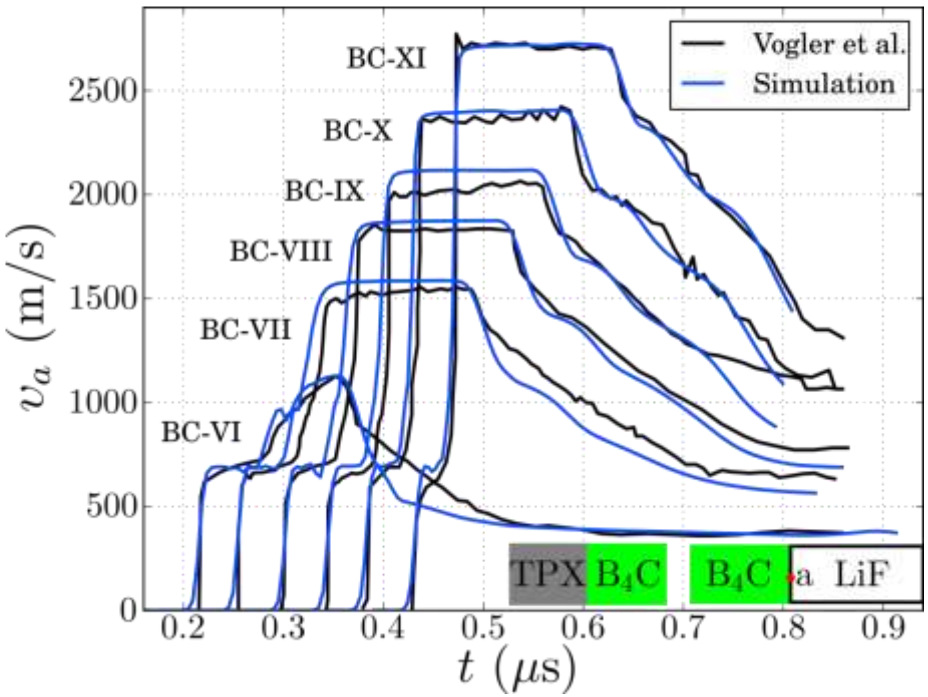


Эксперимент: D. E. Grady and R. L. Moody, Tech.Rep. SAND96-0551 (1996)

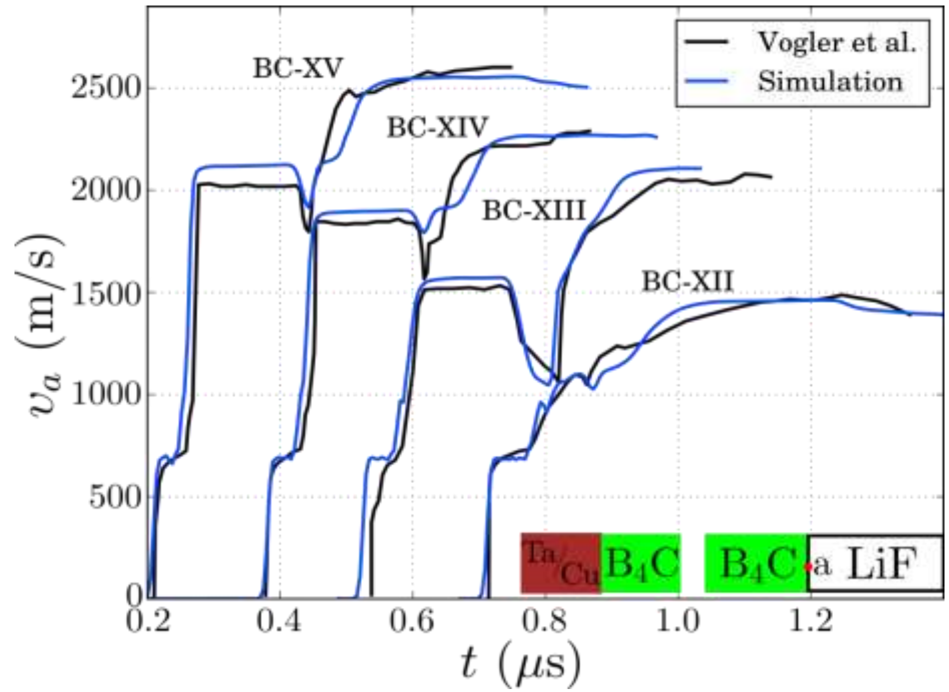
Расчет: S. A. Dyachkov et al., Journal of Applied Physics ***124*** *085902 (2018)*

SPH-simulation of Vogler et al. tests

Release tests



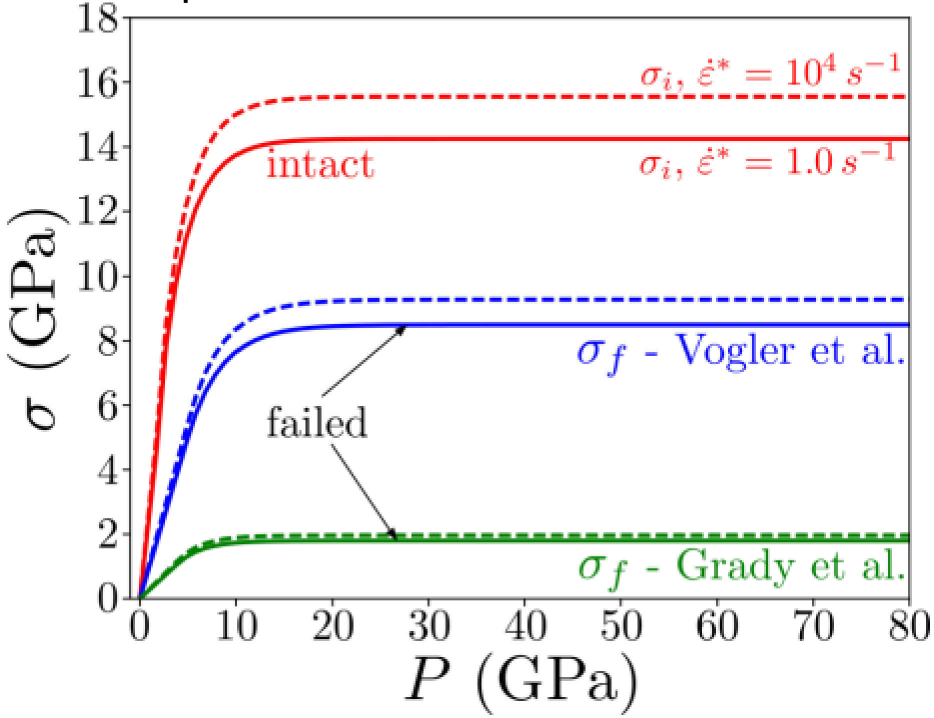
Reshock tests



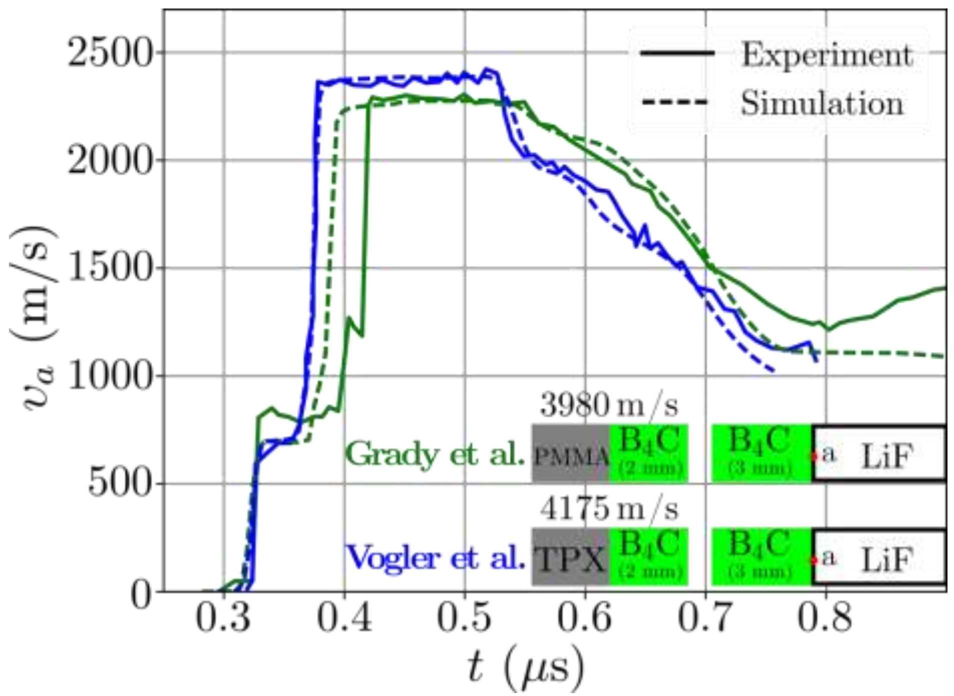
- A single set of parameters for boron carbide model is valid for the all tests
- Agreement with experiments is excellent in a wide range of compressions

B_4C strength affects wave profiles

B_4C strength may vary



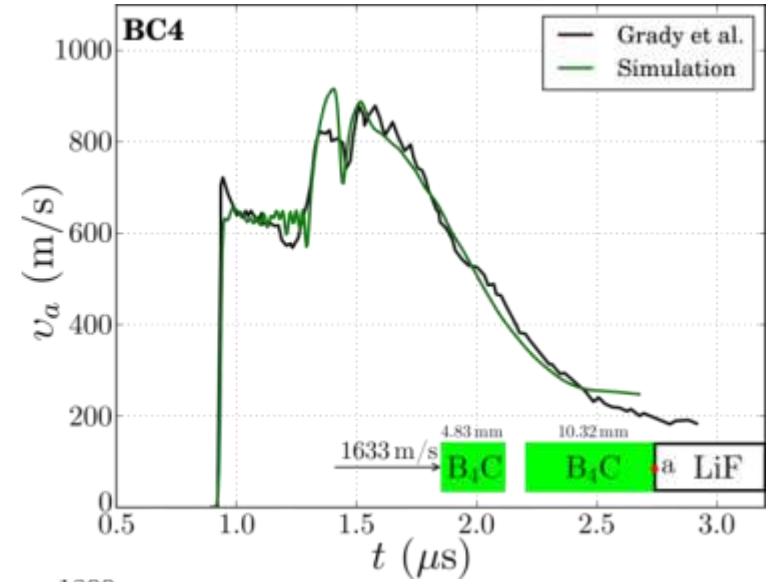
Wave profiles in B_4C of various kind

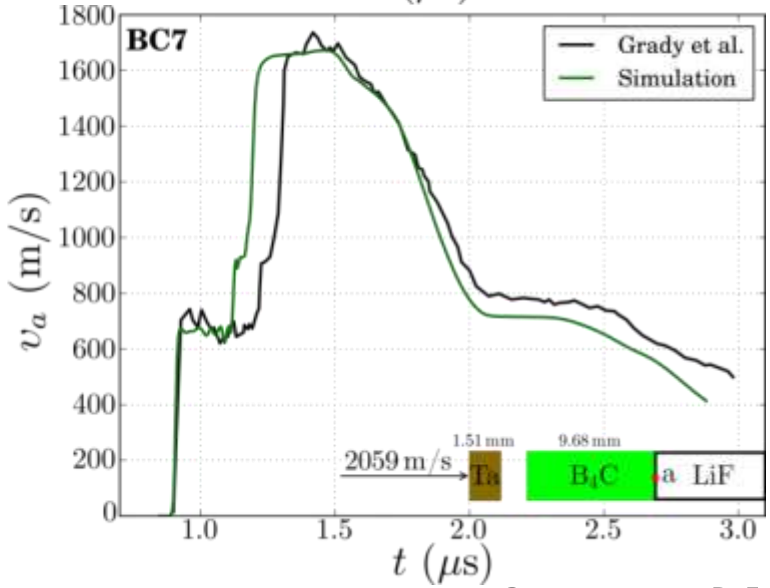


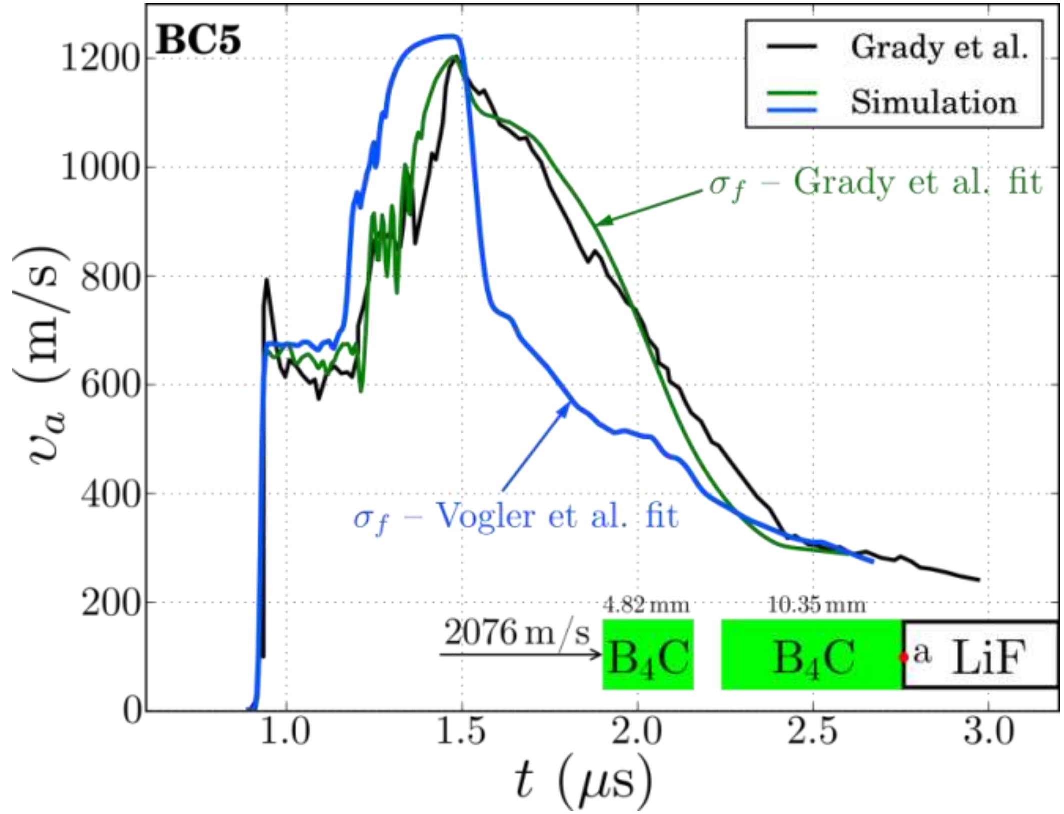
- Different manufacturing technology of boron carbide affects its dynamic response to uniaxial shock loading
- Simulations show that various B_4C samples have all properties in common, except for σ_f
- By adjusting $\sigma_f(P)$ for a particular kind of boron carbide, it is possible to achieve a very good agreement with plate impact experiments
- σ_f may possibly be defined using molecular dynamics

*Расчет: S. A. Dyachkov et al., Journal of Applied Physics **124** 085902 (2018)*

SPH-simulation of Grady et al. tests







- All Grady et al. tests are described better with the reduced values of σ_f
- Simulation of BC5 tests with σ_f fitted to Vogler et al. data provides a rather distinct wave profile

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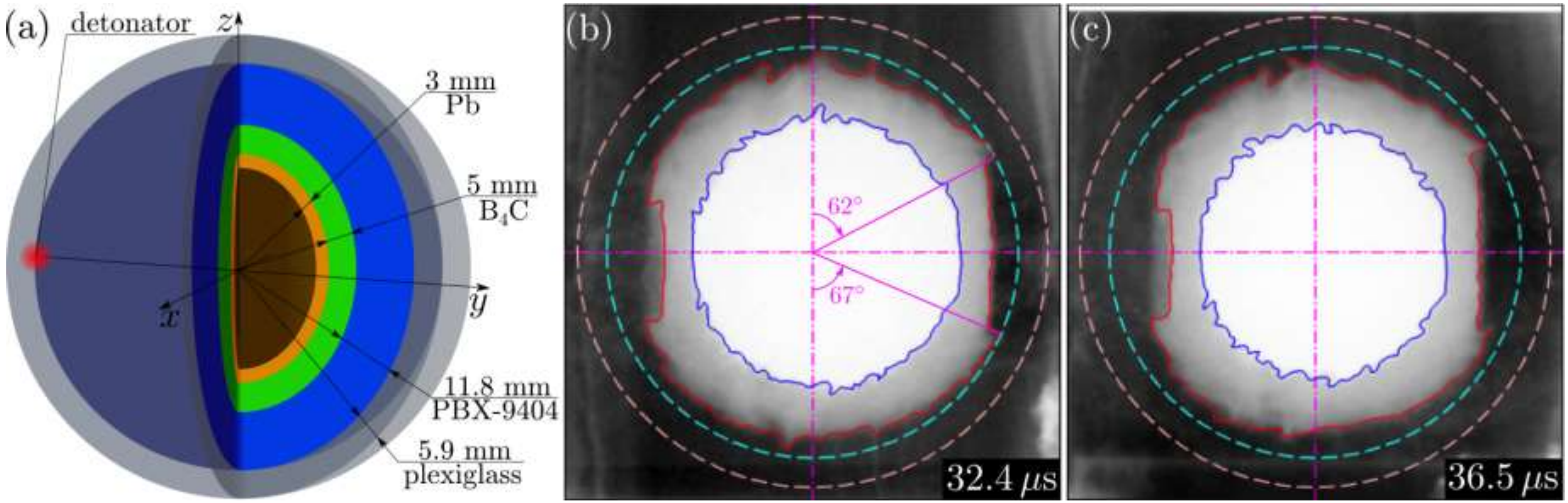
Spherical compression of the boron carbide shell



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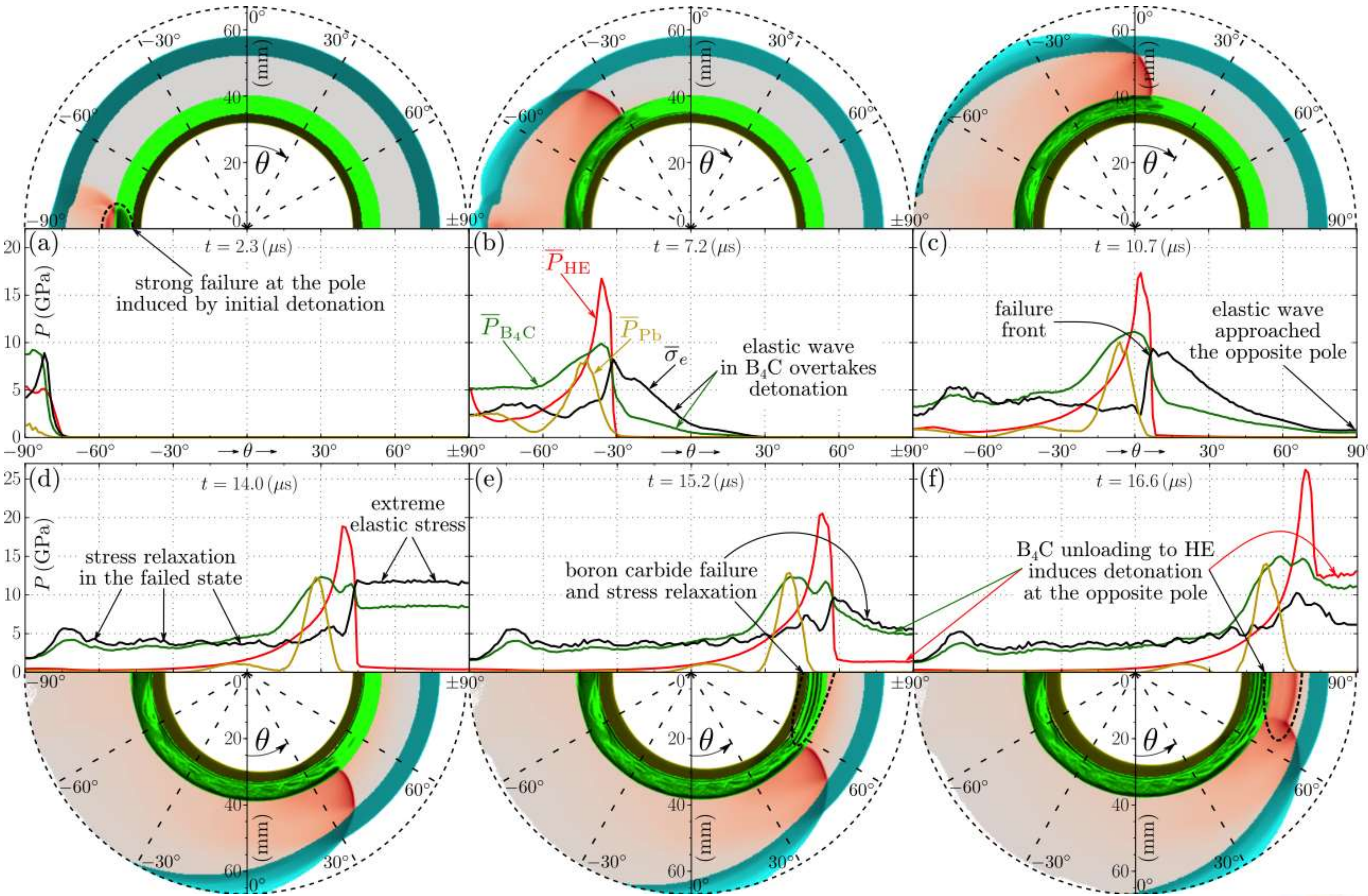
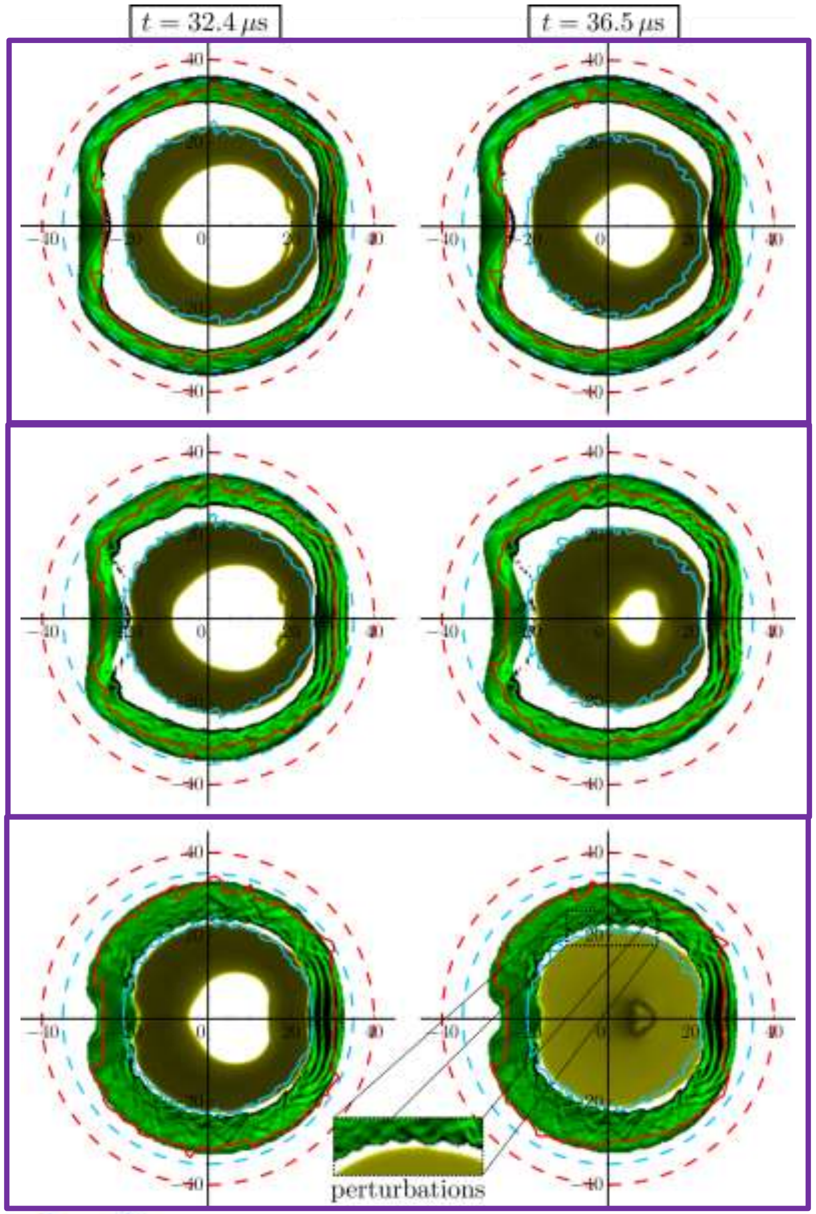
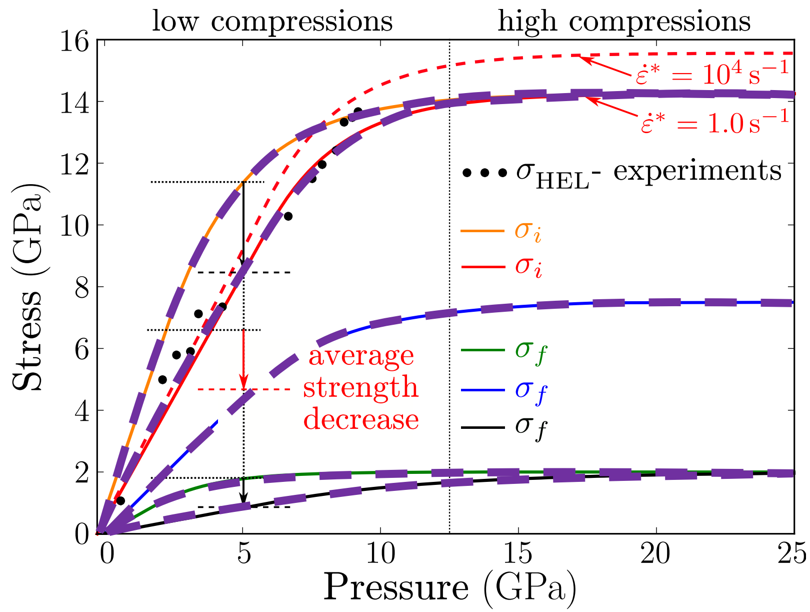
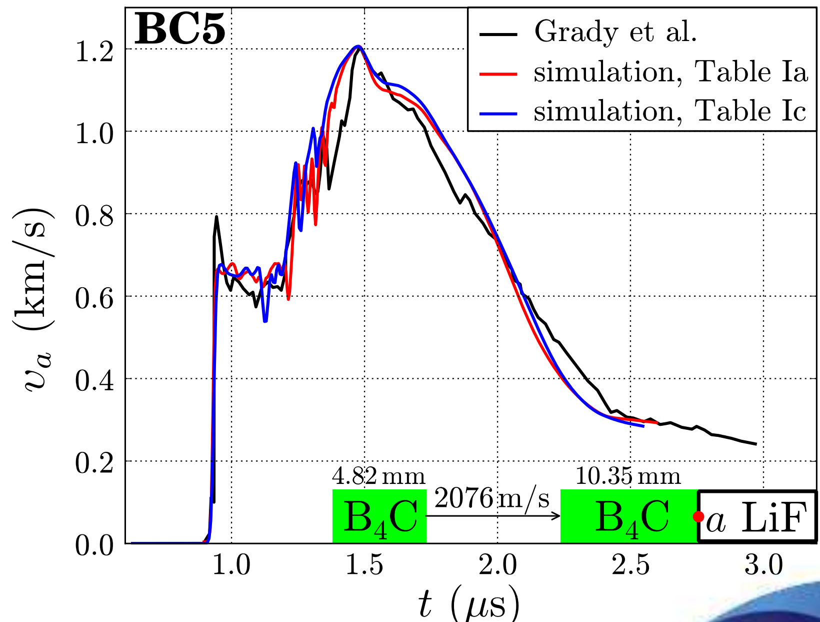
SPH-simulation of the experiment



SPH-simulation of the experiment





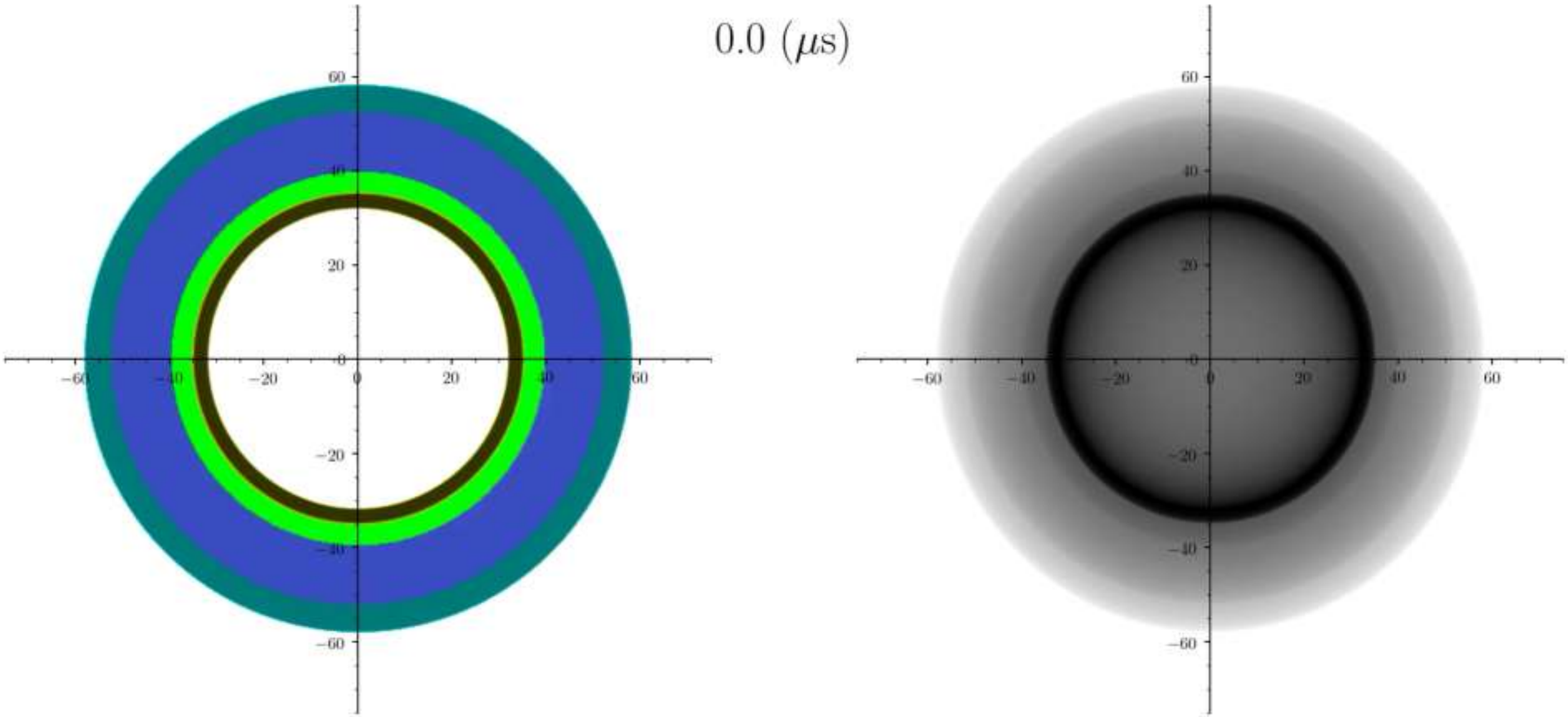


SPH-simulation of the experiment

Explosive compression of boron carbide and lead shells with a single detonator

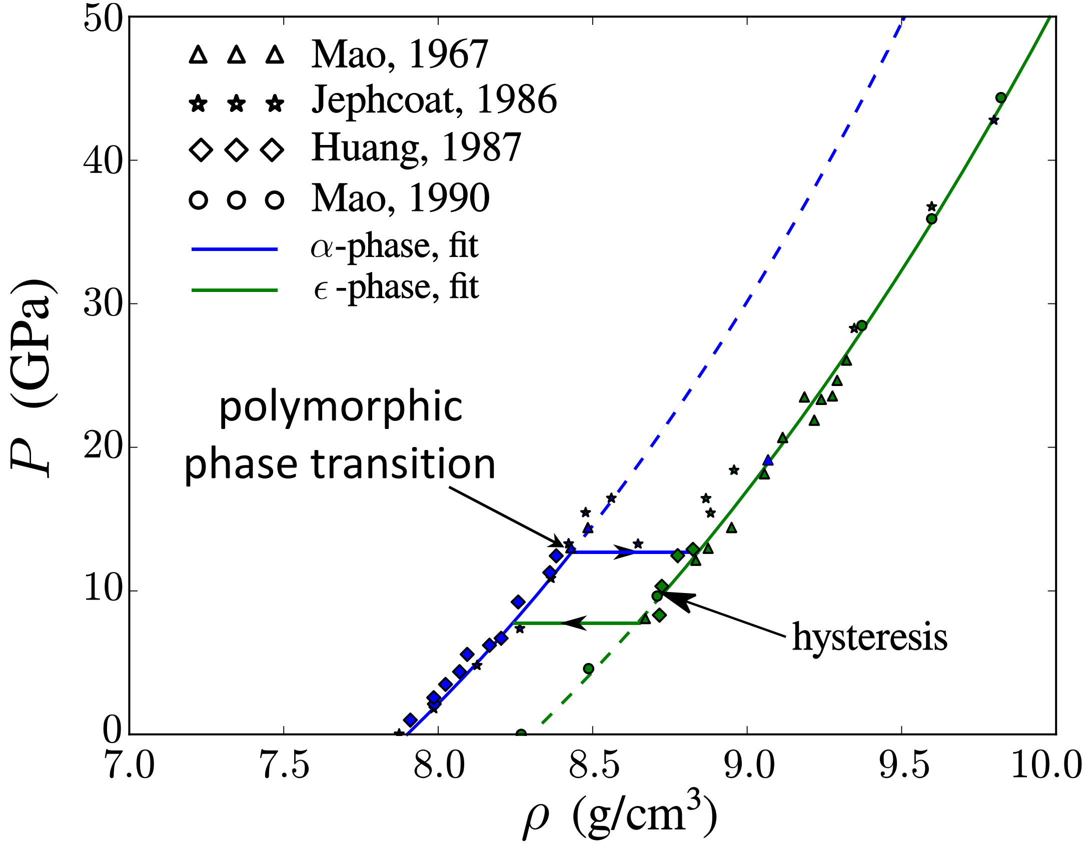
color map of the slice

column density



Simulation of iron and steel

Iron model



Mie-Gruneisen form

$$P_{\text{EoS}} = P_r + \Gamma\rho(e - e_r)$$

α-phase fit

$$P_{r\alpha}(x) = \rho_{0\alpha}c^2 \frac{1-x}{[1-s_\alpha(1-x)]^2}$$

$$e_{r\alpha}(x) = \frac{P_{r\alpha}}{\rho_{0\alpha}}\frac{1-x}{2} \qquad x = \rho_0/\rho$$

ε-phase fit

$$P_{r\varepsilon}(x) = \rho_{0\varepsilon}c^2 \frac{1-x}{[1-s_\varepsilon(1-x)]^2}$$

$$e_{r\varepsilon}(x) = \frac{P_{r\varepsilon}}{\rho_{0\varepsilon}}\frac{1-x}{2} \qquad x = \rho_0/\rho$$

hysteresis

$$P_{r\alpha}(\rho_{0\alpha}/\rho_1^{\alpha\varepsilon}) = 13\,\text{GPa}, \quad P_{r\varepsilon}(\rho_{0\varepsilon}/\rho_2^{\alpha\varepsilon}) = 13\,\text{GPa}$$

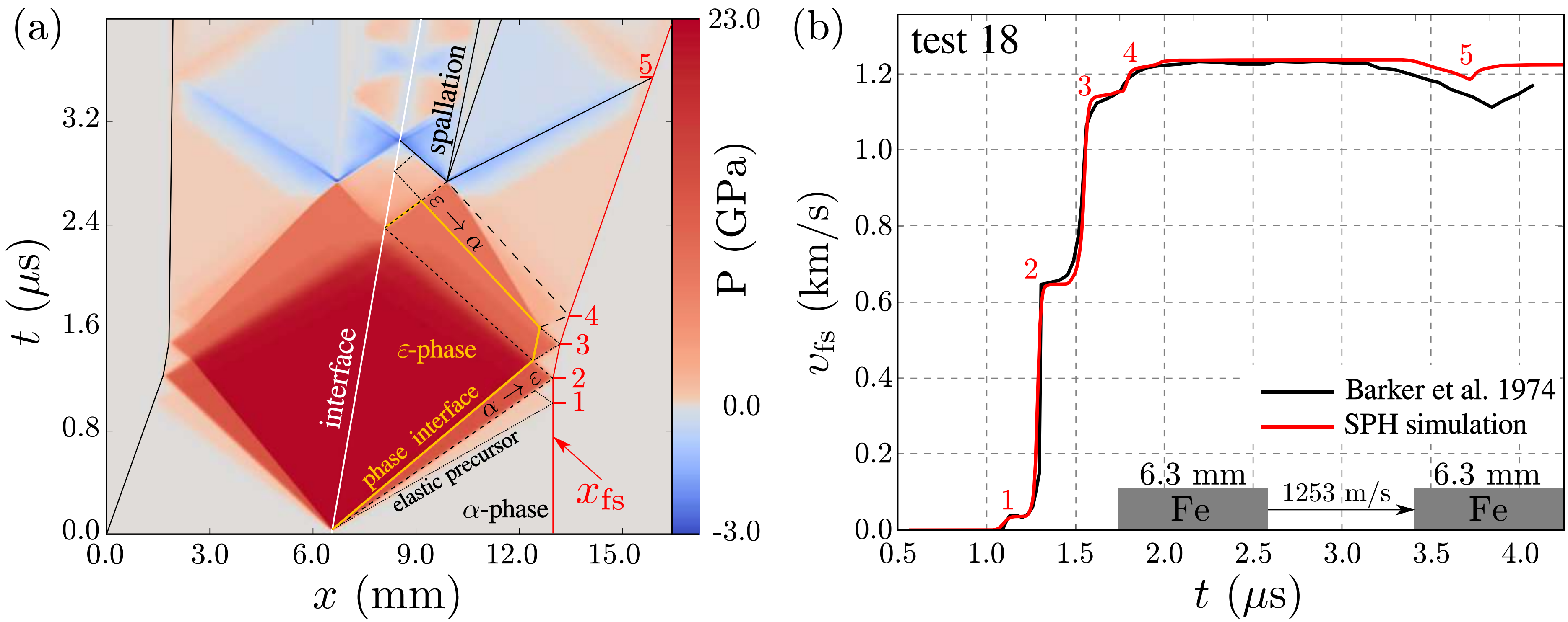
$$P_{r\varepsilon}(\rho_{0\varepsilon}/\rho_1^{\varepsilon\alpha}) = 8.5\,\text{GPa}, \quad P_{r\alpha}(\rho_{0\alpha}/\rho_2^{\varepsilon\alpha}) = 8.5\,\text{GPa}$$

- Reference energy and pressure follow from the linear hugoniot approximation: $u_s = c + su_p$
- Different phases have the densities $\rho_{0\alpha}$ and $\rho_{0\varepsilon}$, respectively
- Hysteresis is taken into account: reverse phase transition in iron appears at lower pressure
- Constant yield strength model represents elastic-plastic properties

УрС: Kerley G. I. Tech. Rep.: SAND93-0027: Sandia National Laboratories (1993)

SPH-simulation of uniaxial compression of iron

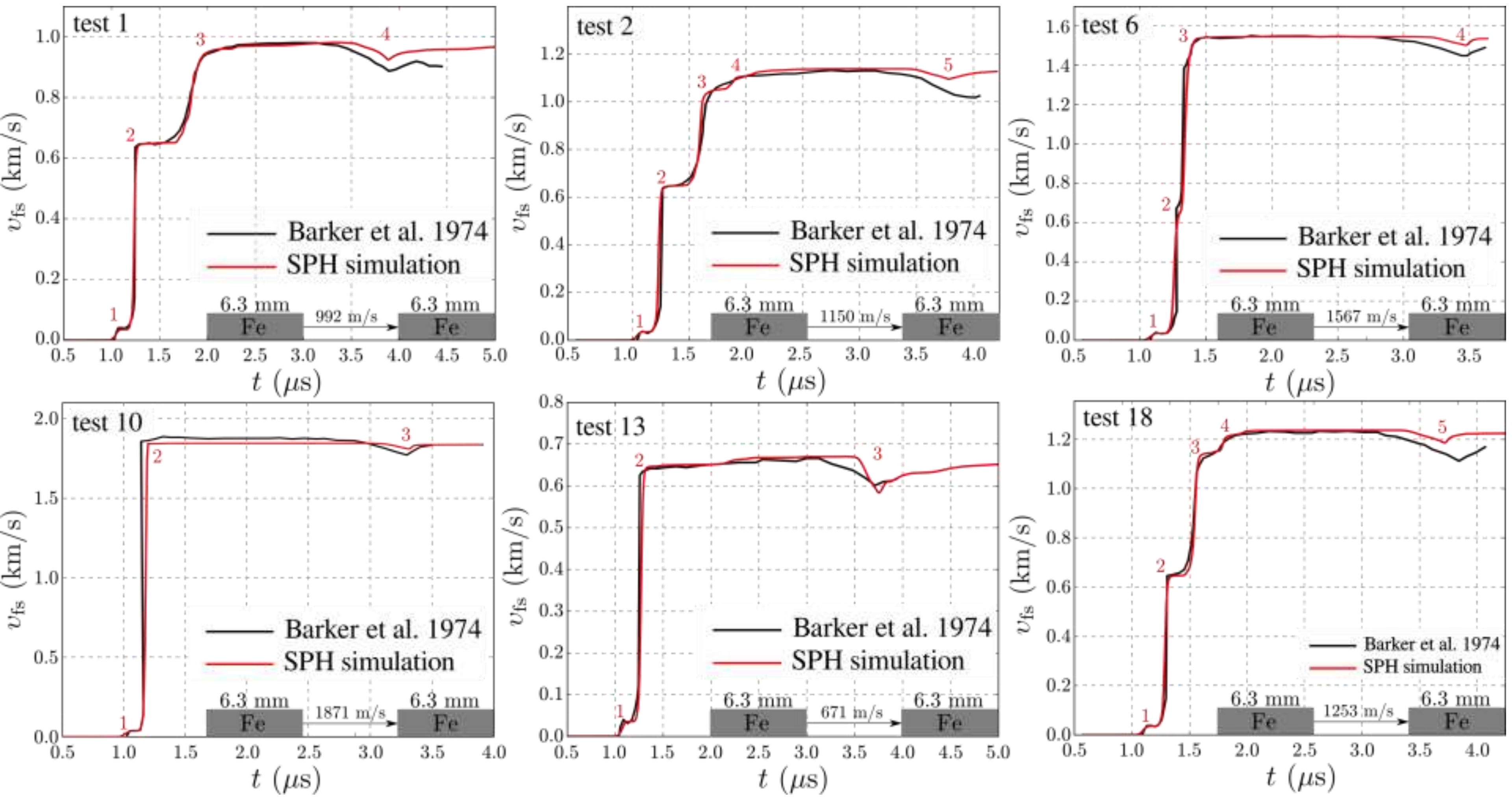
Details



- The most interesting case appears when shock pressure is ~ 25 GPa
- 1 – elastic precursor reaches the free surface of target
- 2-3 – α-ε phase transition takes place
- 3-4 – is a result of hysteresis during ε-α reverse transition
- 5 – spallation

Barker L. M., Hollenbach R. E. Journal of Applied Physics **45** 4872 (1974)

SPH-simulation of uniaxial compression of iron

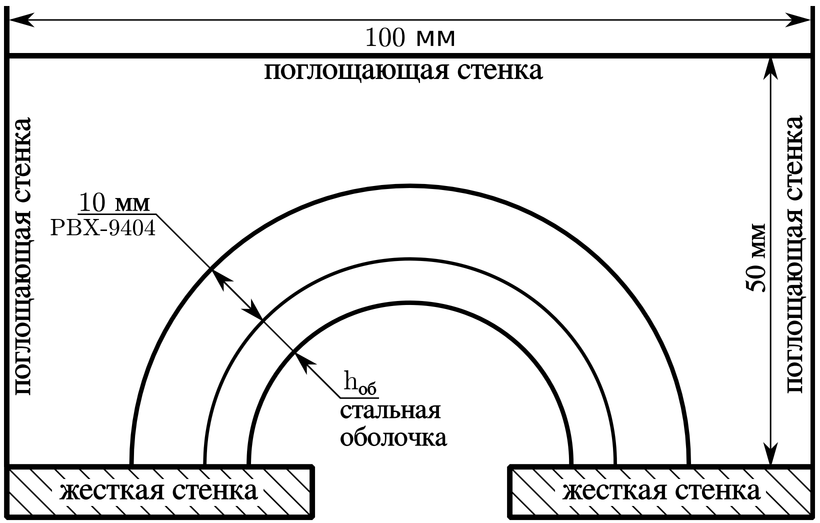


Elastic precursor, phase transition, and spall appear in our simulations

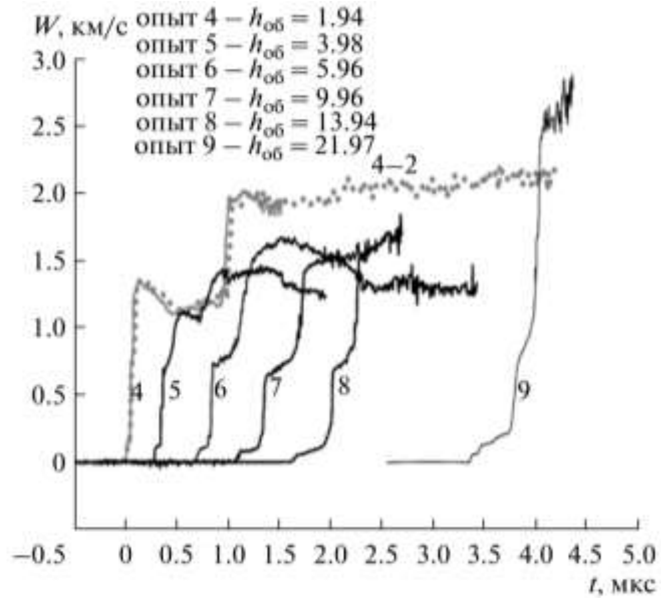
Barker L. M., Hollenbach R. E. Journal of Applied Physics **45** 4872 (1974)

SPH-simulation of steel shells compression

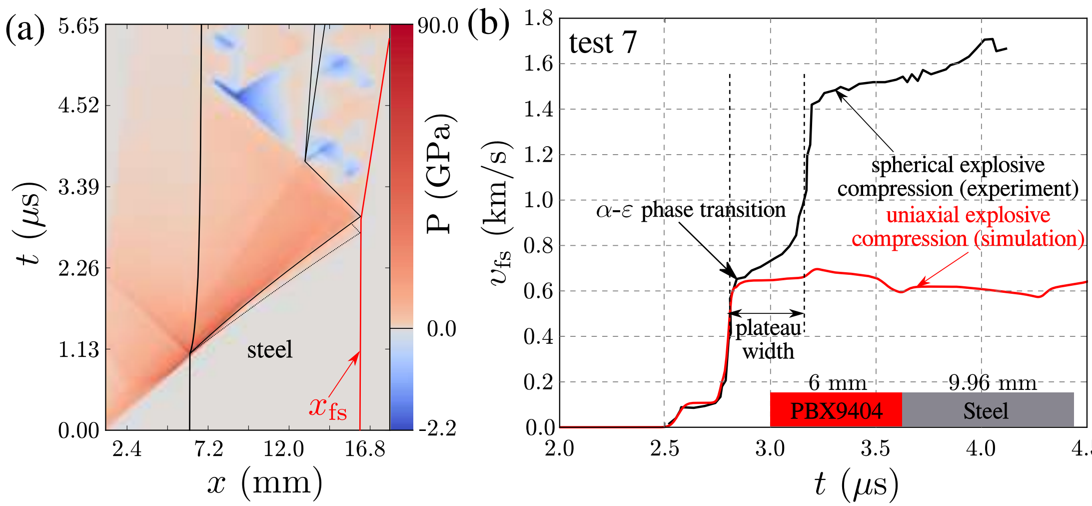
Problem setup



Laser interferometer measurements



Uniaxial explosive compression



Details of the waves structure are available only in a test with uniaxial loading.

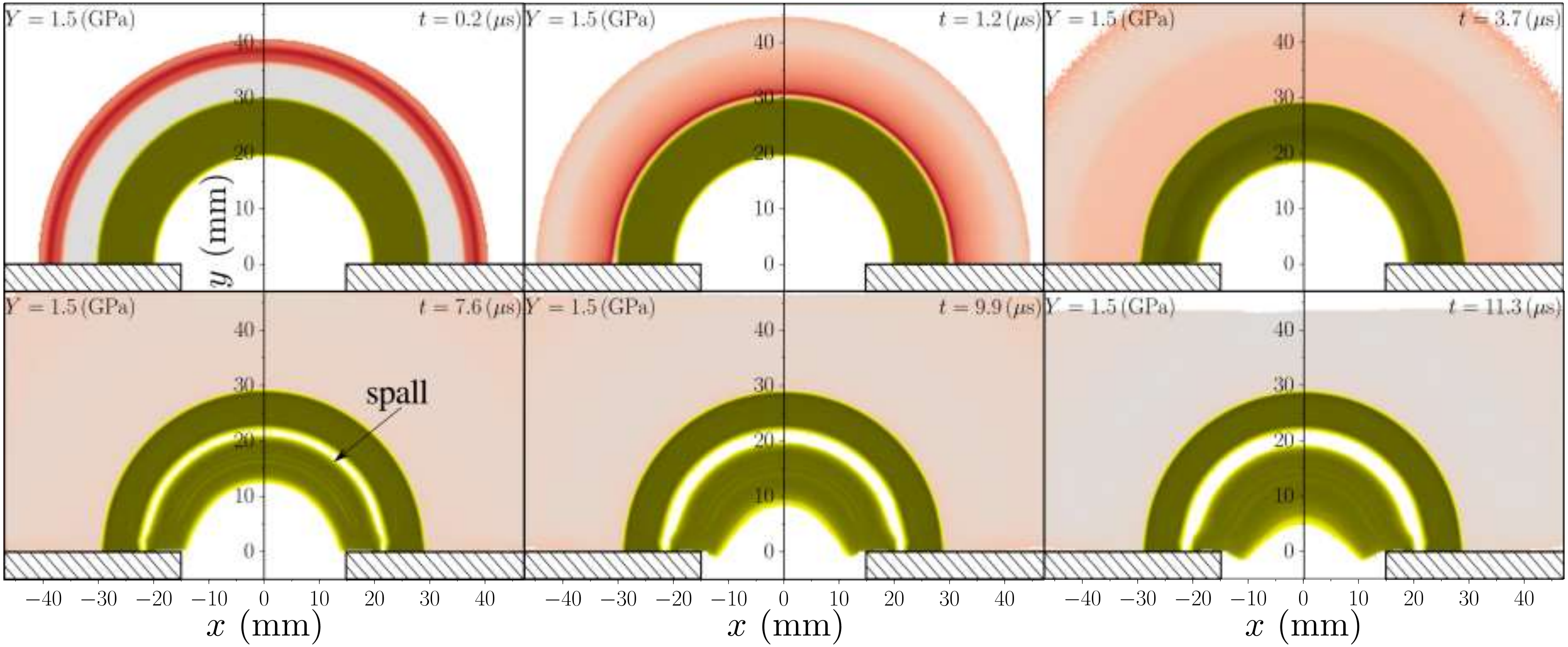
<u>There are 2 important results</u>:

- α-ε phase transition should be taken into account for steel;
- steel has the higher yield strength.

Е. А. Козлов, С. А. Бричиков, Д. С. Боярников [и др.] Физика металлов и металловедение. Прочность и пластичность. Т. 112. С. 412–428 (2011)

SPH-simulation of steel shells compression

Steel shell convergence dynamics (test 7, h = 10 mm)

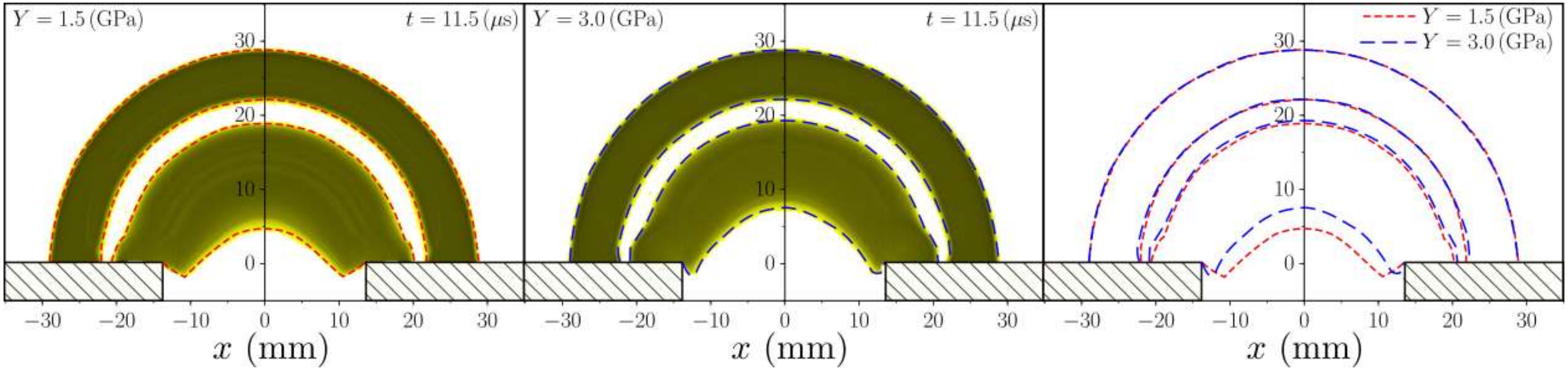


- Spallation appears in shells with width h > 4 mm
- The outer part of the shell stops after spallation
- The outer boundary of the outer part of the shell stops
- The inner boundary of inner part of the shell keep moving, but is guided by the yield strength

Е. А. Козлов, С. А. Бричиков, Д. С. Боярников [и др.] Физика металлов и металловедение. Прочность и пластичность. Т. 112. С. 412–428 (2011)

SPH-simulation of steel shells compression

Simulations with different yield strength (test 7 , h = 10 mm)



Saved experimental shells (test 7 , h = 10 mm)

Е. А. Козлов, С. А. Бричиков, Д. С. Боярников [и др.] Физика металлов и металловедение. Прочность и пластичность. Т. 112. С. 412–428 (2011)

Conclusions

Conclusions

- Models of boron carbide and steel are developed to simulate complex engineering prototypes under shock loading with pressures < 100 GPa
- The example with boron carbide explicitly shows that some of its model parameters cannot be properly defined using only uniaxial shock compression data
- Interesting feature of the spherical boron carbide shell behavior is revealed: the forward propagation of elastic waves may produce a secondary detonation of HE material
- In the models of iron and steel the polymorphic phase transition with hysteresis is taken into account. The related wave profile features are shown to be reproduced correctly in our simulations