ГОСУДАРСТВЕННАЯ КОРПОРАЦИЯ ПО АТОМНОЙ ЭНЕРГИИ «РОСАТОМ»

Physical Models of Heterogeneous Crystalline High Explosive Detonation

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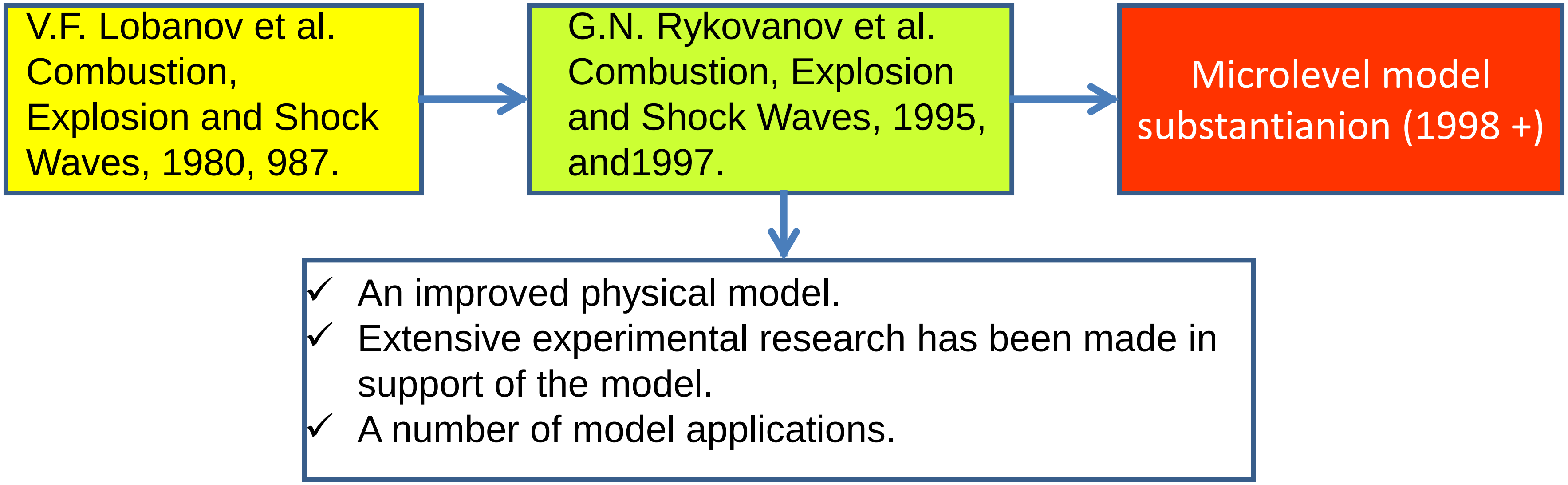
Introduction

- There are a lot of detonation models, which, as Roger Cheret pointed out, are entrenched in the cold war, i.e. they are developing independently.
- Practically all recent models of polymer-bonded crystalline explosives rest on the “hotspot” concept varying only in terms of its interpretations.
- In this paper, we review the research made using one of these models (Ural-Siberian Model - USM) since 1998.



V.F. Lobanov et al. Combustion, Explosion and Shock Waves, 1980, 987.

G.N. Rykovanov et al. Combustion, Explosion and Shock Waves, 1995, and1997.

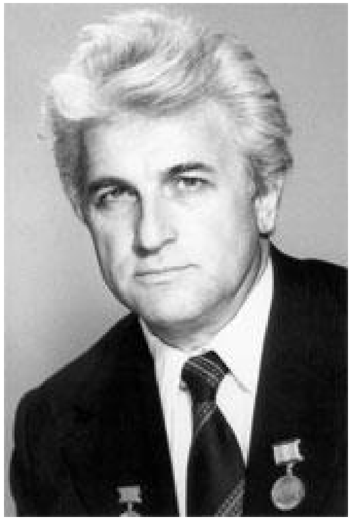
Microlevel model substantianion (1998 +)

- ✓ An improved physical model.
- ✓ Extensive experimental research has been made in support of the model.
- ✓ A number of model applications.

Holy Grail of the detonation theory is the basic question in terms of the relationship between HE molecular structure and detonation properties

- Whereas condensed high explosive (HE) detonation have been studied and applied for many years, little is still known of the detonation process microphysics (“Mystery of Detonation” - Simpson et al, LLNL).
- But it is well-known that the detonation properties are determined not only by the molecular structure but also by the HE mesostructure and the same explosive compound demonstrates different properties in different physical states:
  - ✓ monocrystalline,
  - ✓ cast,
  - ✓ microcrystalline bulk,
  - ✓ microcrystalline pressed,
  - ✓ microcrystalline plasticized.
- In the beginning of the 90-s of the 20th century, Boris G. Loboiko gave the following opinion: “A significant progress will be achieved, if one succeeds in some understanding of the relationship between the HE microstructure and its detonation properties”.

Boris G. Loboiko



Boris Grigorievich Loboiko (1937-2018)

a prominent physical scientist and experimenter.

The key lines of his research:

- generation of high explosives (HE),
- investigation on HE physics, engineering, processing technology, and safety.

Doctor of Technical Science, Professor, Honored Worker of Science of the RF, winner of the State Prizes of the USSR and RF.

Regular participant of Zababakhin Scientific Talks, the founder and first head of Section 2 “Explosive and Detonation Phenomena”.

According to my personal impressions, he possessed an uncanny ability to set fundamental problems as “simple” questions:

1. Why some substances are explosive? (Why do high explosives explode?)
2. Why does TATB possess abnormal low sensitivity?
3. Why is the chemical reactions’ rate determined by temperature (Arrhenius law) but the effective (macrokinetic) reaction rate in kinetics detonation models is normally specified as the pressure function?
4. How can we perform ab initio (from first principles) calculations of macrokinetic reactions’ rate?
5. **………..**

The basic concept is the detonation process scale hierarchy

MICRO

Sizes of molecules

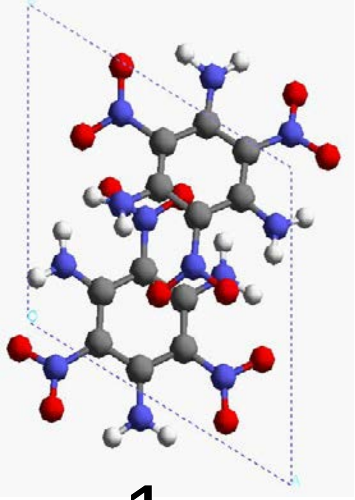
Chemical reaction time.

MESO

Sizes of microcrystals. Time of their shock-wave induced combustion

MACRO

Sizes of HE charge. Explosion time



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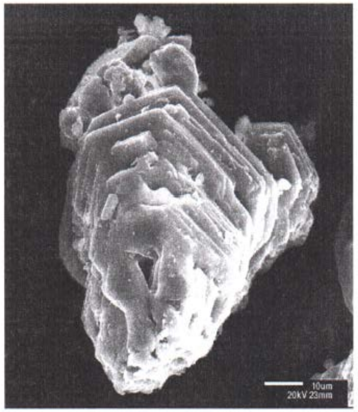


10^5

10^{10}

Due to profound difference between the space-time scales of these three levels the problem should be decomposed to study each level separately, and the obtained results should be further used to construct higher-level models.

Macrolevel is macrokinetics of their chemical reactions and equation of state

РФЯЦ–ВНИИТФ

$$\frac{d\rho}{dt} + \rho \cdot \nabla \vec{u} = 0$$

$$\frac{d\vec{u}}{dt} = -\frac{1}{\rho} \nabla P$$

$$\frac{d\varepsilon}{dt} + P\frac{d}{dt}\left(\frac{1}{\rho}\right) = Q$$

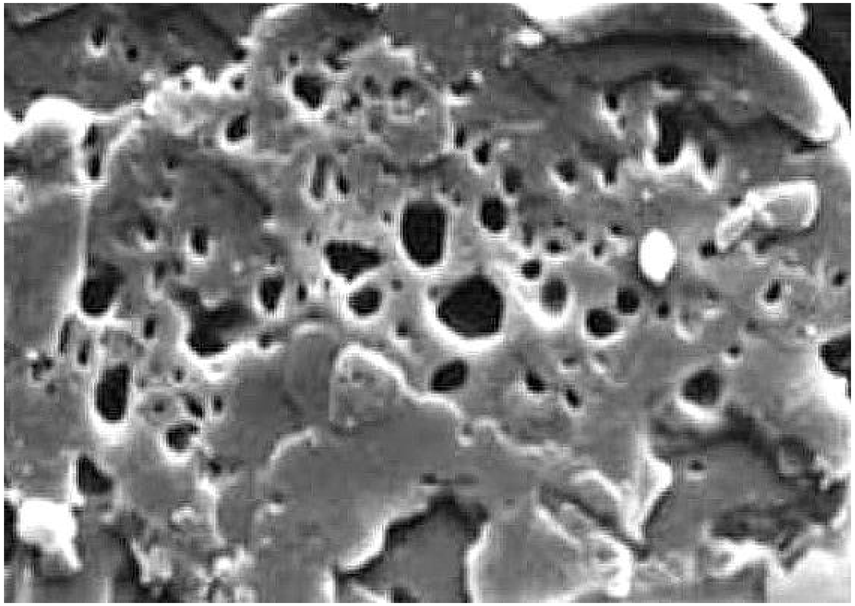
- Q – energy release in chemical reactions. It is normally taken that

  $Q = -\ q_0 \cdot d\xi/dt$, where

  q_0 – HE caloric content,

  ξ – HE concentration.
- $P(\rho,\varepsilon)$ – reactive medium EOS
- The micro- and mesolevels information is delivered to the microlevel <u>only by</u> $\xi(t)$ and $P(\rho,\varepsilon)$.

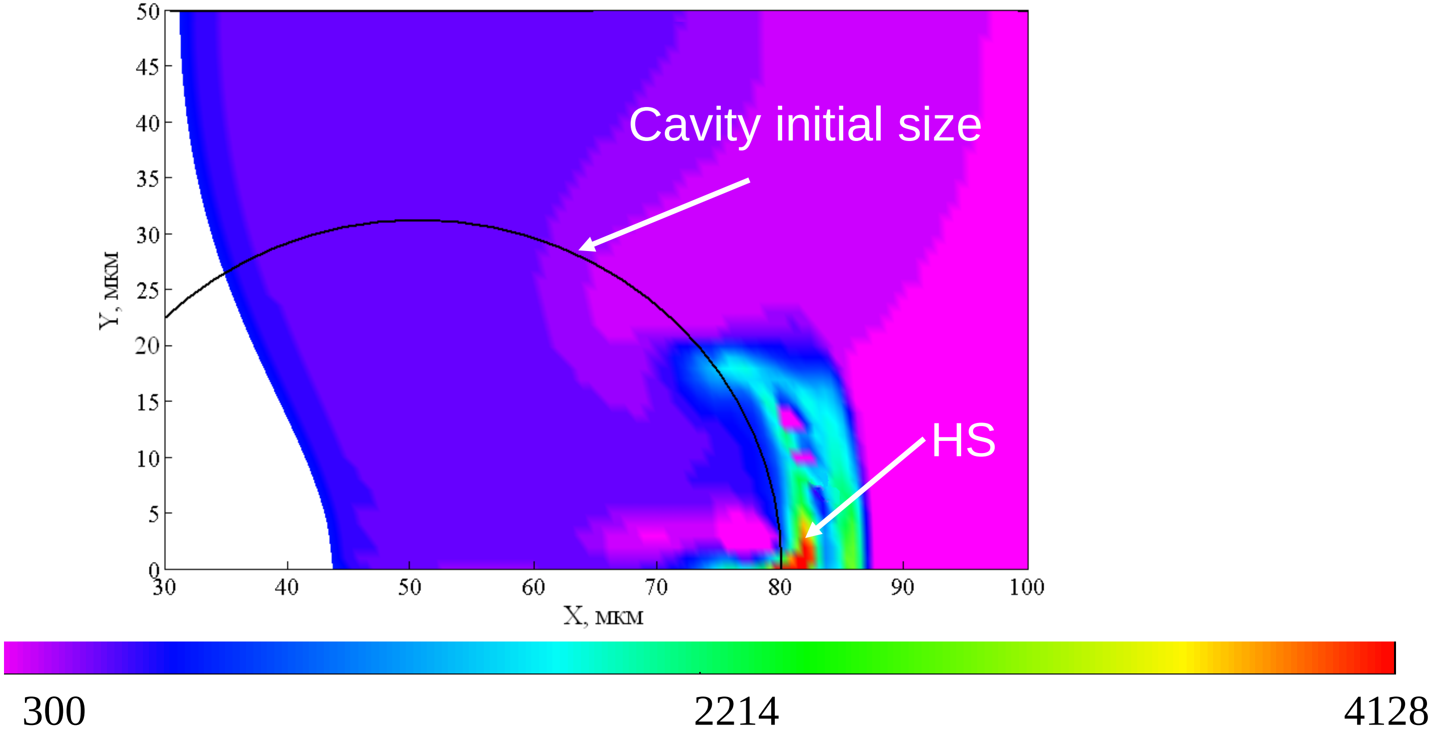
Mesolevel makes the “hotspot” concept



And, by the way, monocrystalline TATB, does not appear to be high explosive – stationary detonation in it cannot occur.

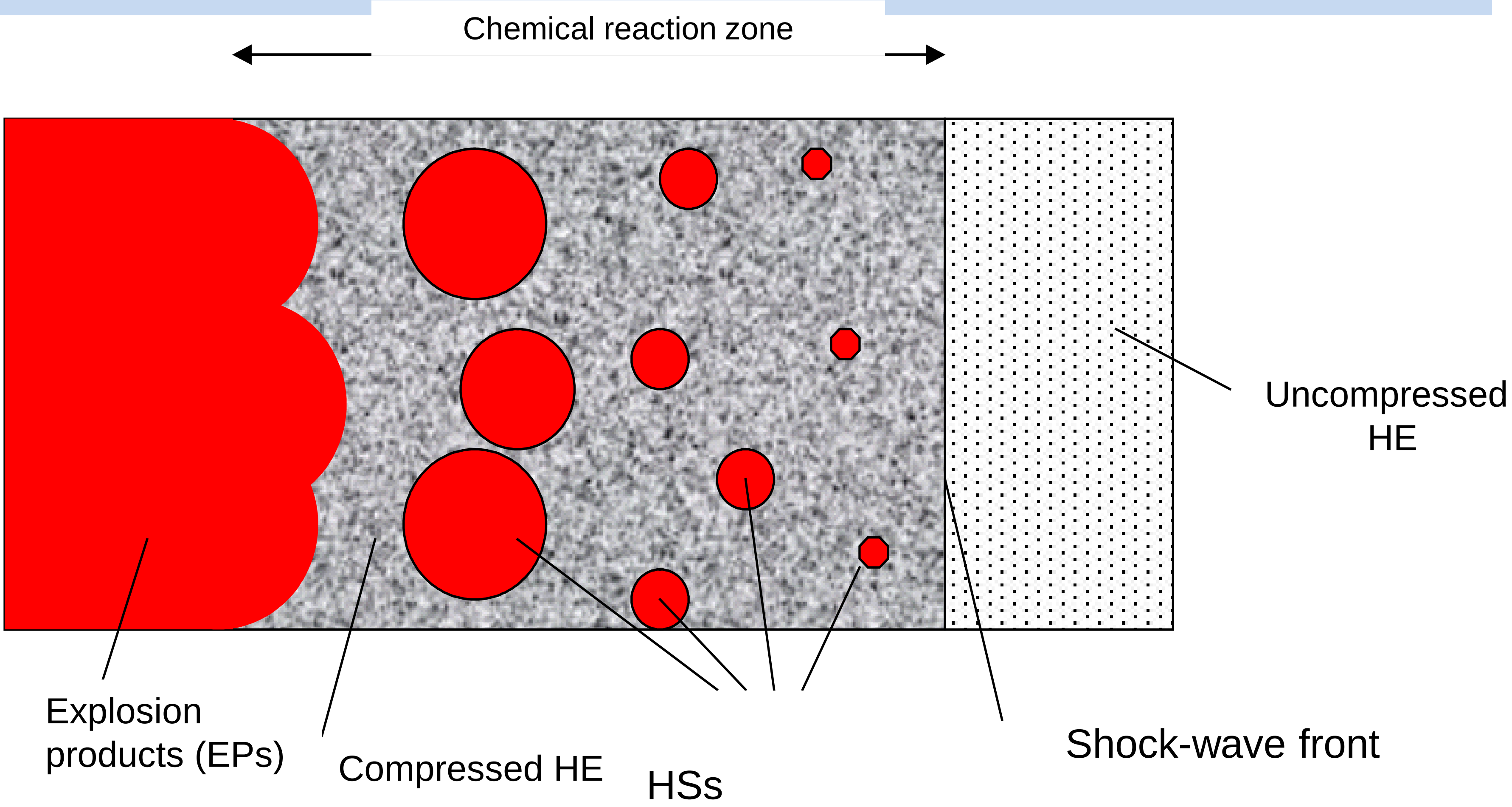
- Critical pressure of RDX detonation initiation:
  - ✓ > 30 GPa for monocrystalline,
  - ✓ 3 GPa for pressed microcrystalline samples.
- Structure of HE samples recovered after shock-wave.
- Conclusion – in heterogeneous HE, the reaction starts in combustion microsources –”hotspots” (HPs) and the combustion waves are propagating inside the HE.
- And this, too, is verified by calculations of the void collapse in the HE after the shock-wave propagation.

HE temperature after the shock-wave passing through the cavity



- ✓ A lot of calculations of shock-wave induced void collapse has been reported since the classic paper by Charles L. Mader.
- ✓ An overall conclusion: the HS initiation hydrodynamic mechanism dominates at high pressures P ≥ 10 GPa. At the same time,
  - ✓ “HS” volume << amount of the unreacted shock-compressed HE.
  - ✓ time of reaction in HSs << combustion wave propagation time.

Combustion propagation from HSs under shock-wave initiated detonation



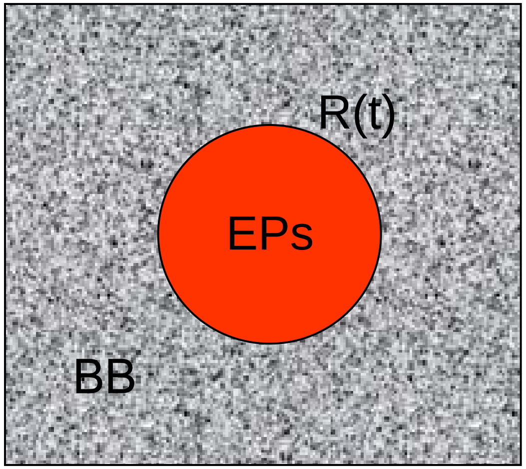
- ✓ Reaction time $\Delta\tau \approx \delta/D$, where δ is half of the average distance between the neighboring HSs, D is the combustion wave propagation velocity.
- ✓ The combustion geometry undergoes changes: the combustion waves propagate from individual HSs until they join together.

Microkinetics is governed by the USM three factors

$$-\frac{d\xi}{dt} = F \cdot N^{1/3} \cdot D$$

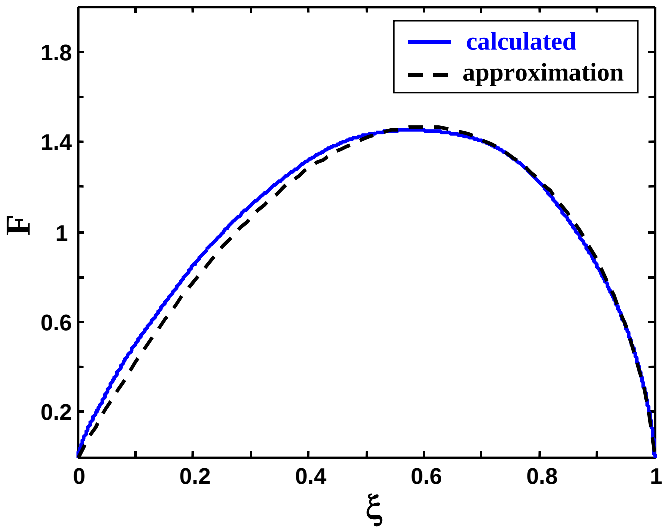
- ➢ *ξ – HE concentration,*
- ➢ *F* – geometry factor (the changeover from “outward combustion” to “combustion waves joining together”),
- ➢ N – reaction HSs concentration ($N^{-1/3}$ – average distance between them),
- ➢D – velocity of the combustion wave propagating from HSs.

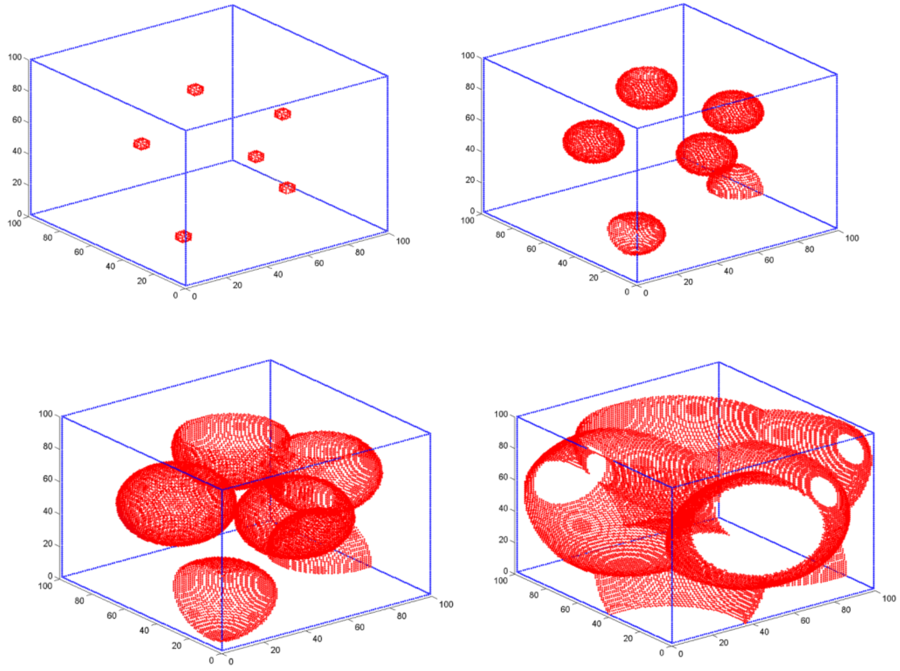
- ❑ HSs are randomly distributed over the HE.
- ❑ burnup = the EPs mass-to-full mass ratio (HE + EP).



The approach involves calculation of these three factors having obvious physical meaning based on the HE micro-and- mesostructures, i.e. ab initio calculations.

Geometry factor estimate





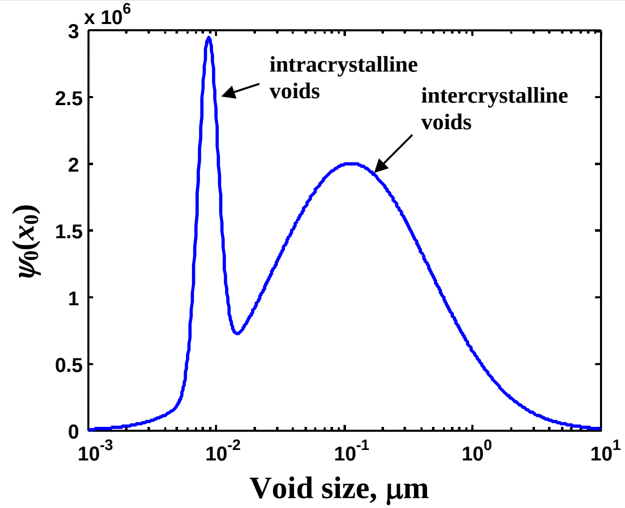
$$F(\xi) = \frac{-d\xi/dt}{N^{1/3} \cdot D}$$

$$F(\xi) \approx K \cdot \xi^{n} \cdot (1-\xi)^{m}$$

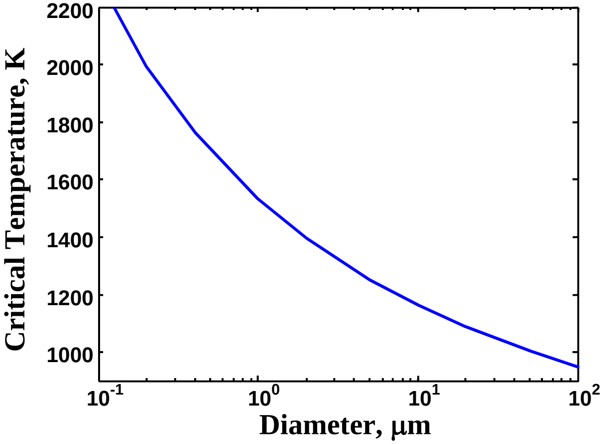
$$K = 4.5,\ n = 1,\ m = 2/3$$

Propagation of combustion from the HSs randomly distributed in space.
Model (purely geometrical) problem:
D=const, ρ=const.

HSs density can be calculated based on the initial void size distribution (Combustion, Explosion and Shock Waves, 2009, # 1)



Size distribution of porous in HE LX-17
(T.M. Wiley, T.Van Buuren et al 2006).



$$T_{cr}\left[K\right]=\frac{A}{d^{\gamma}}$$

A=1400
γ = 0.08

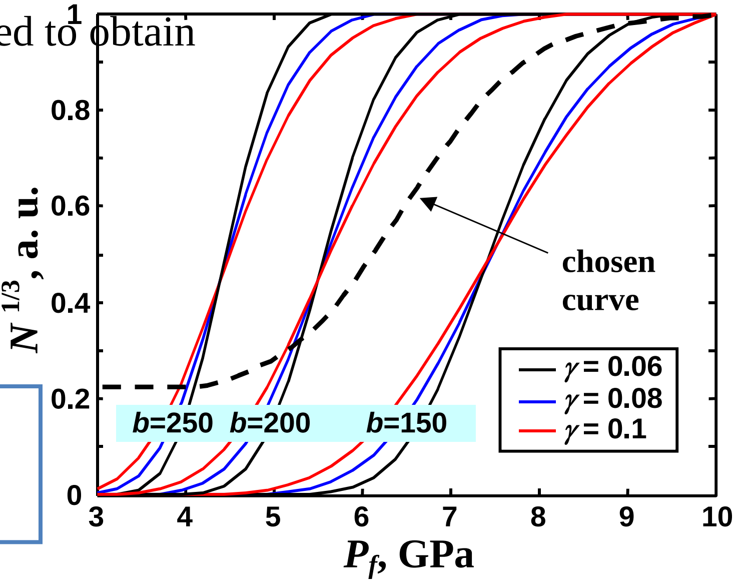
Critical HS temperature as a function of the size (C.M. Tarver, 1996).

Calculation of the shock wave passing through the void can be used to obtain the HS size, temperature, and density (they depend on P at the front, initial size, and initial density of voids).

Estimate – Ths ≈ T_0 + b*P_f , b = 150 – 250.

x ≈ k*x_0, k = 0.1

$$N\left(P_f\right)\sim\int_{d_{cr}\left(T_{\text{ГТ}}\right)}^{\infty}\psi(x)\cdot dx$$ *(Yu.A. Aminov, Yu.R. Nikitenko, 2002)*



1. **At $P_f \geq 10$ GPa – HS saturation and fast ignition, decomposition kinetics is only determined by the HS increase.**
2. **At $P_f \leq 5$ GPa non-hydrodynamic mechanism.**

Combustion wave propagation velocity is the primary factor responsible for polymer-bonded TATB (PTATB) detonation kinetics

- **V.G. Morozov's paradox**

✓ Macrokinetic time of the reaction is the time taken for the combustion waves propagating from the neighboring HSs to join together: $\boldsymbol{\Delta\tau \approx \delta/D}$**,** where δ is half of the average distance between the neighboring HSs. At $\delta \approx 10 – 100$ μm (on the order of HE microcrystalline size) and detonation initiation time $\Delta\tau \approx 0.1 \div 1$μs , an estimate of ***D*** **~ 100 m/s** is obtained.

✓ According to C. Tarver (11th Det. Symp., 1998), in TATB, ***D*** **≈ 0.5 - 1 m/s.**

- **Calculated velocity of the combustion wave is 2 orders of magnitude less as compared to estimates based on detonation experiments' results!**
- V.G. Morozov suggested that the energy transfer mechanism in the combustion wave was turbulent (more intensive than thermal conductivity).

Alternative proposal (Zababakhin Scientific Talks, 1998)

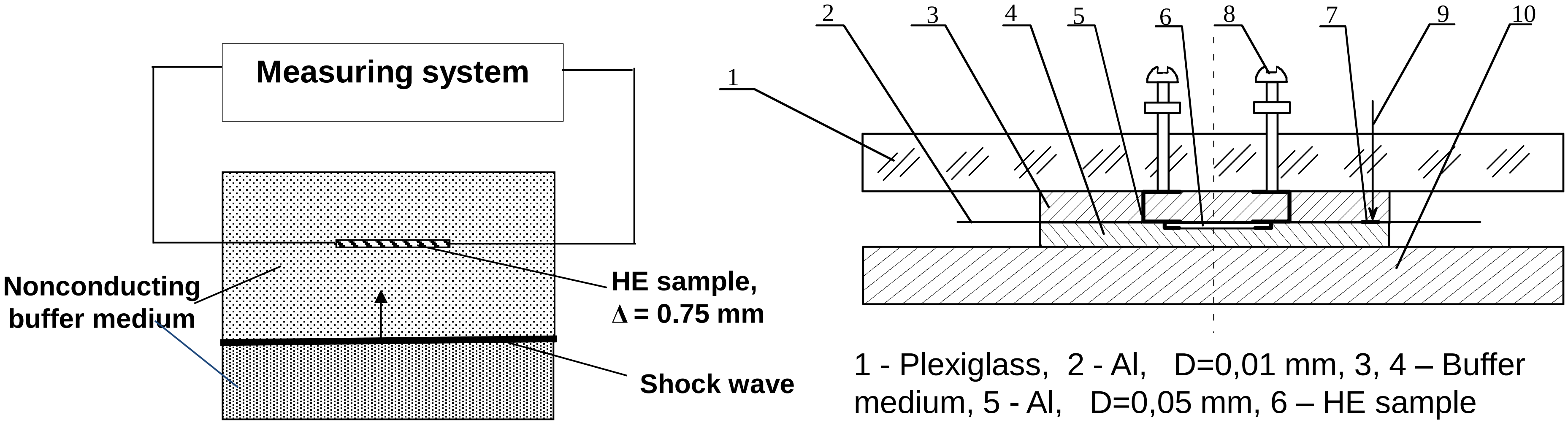
РФЯЦ–ВНИИТФ

- **Hypothesis** ("semiconductor detonation model"):
  - ✓ energy in the combustion wave is transferred by electron thermal conductivity.
  - ✓ TATB compressed and heated by the shock wave becomes a semiconductor, i.e. high concentration of electrons is generated in the conduction band.
- **How can we check this?**
  - ✓ Simulation of electron (zone) structure of HE molecular crystals.
  - ✓ Electrical conductivity is an indication of electron thermal conductivity, both "-conductivities" are proportional to concentration of electrons in the conduction band (Wiedemann-Franz law).
  - ✓ Measurement of HE electrical conductivity after shock wave passing-through (for example, "the shock wave was found to convert monocrystalline RDX into a semiconductor" at P=12.5 GPa, G.P. Chambers et al, SCCM, 2001).

Shock wave converts RDX into a semiconductor, a similar effect might be observed in TATB.

Arrangement of measurements of shock-compressed TATB electrical conductivity

M.M. Gorshkov, K.F. Grebenkin, V. T. Zaikin et al. Proc. 13th Int. Det. Symp. 2006

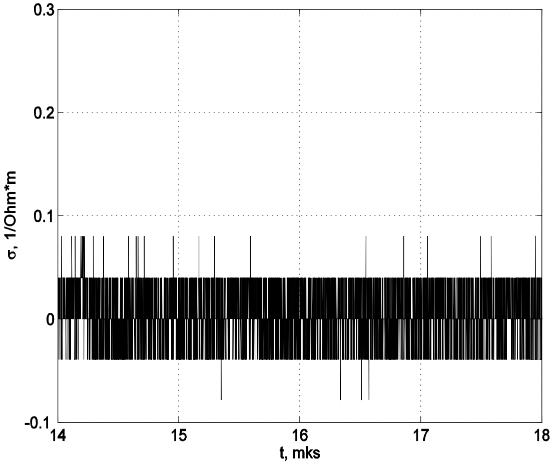


1 - Plexiglass, 2 - Al, D=0,01 mm, 3, 4 – Buffer medium, 5 - Al, D=0,05 mm, 6 – HE sample 25x4x0,75 mm^3, 7 - Al 0,05 mm, 8 – Contact screw, 9 - Reference gauge, 10 – Measuring charge shield.

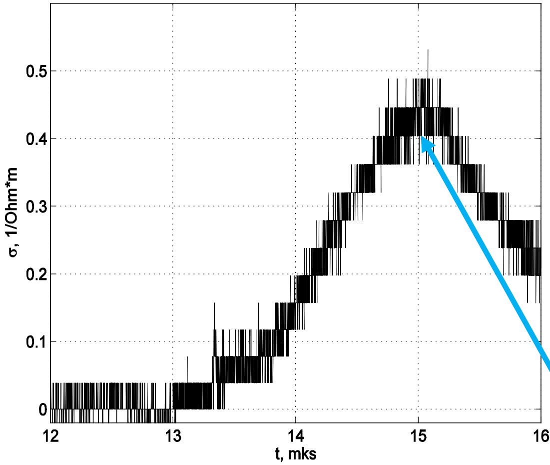
Details of the experimental setup:

1. The sample is thin – 0,75 mm.
2. Shock adiabats of the buffer medium and studied HE are comparable. (hydrodynamic homogeneity). The buffer medium volume is much larger than that of the sample.
3. Loading is produced by step pressure pulse. Constant pressure is maintained during 1 – 1.5 μs (even though the reactions take place and the energy releases).

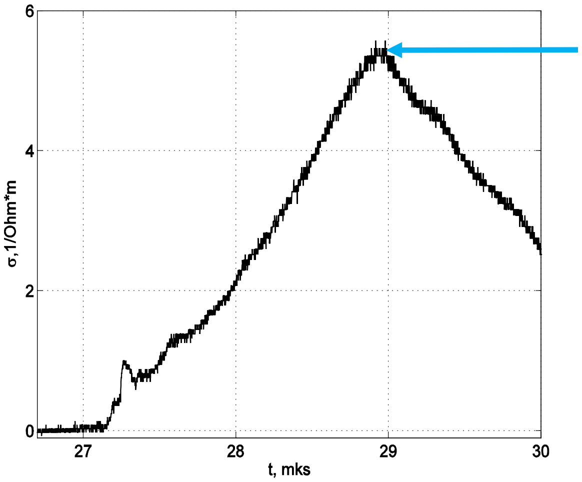
Results of shock-compressed TATB (ρ_0 = 1.865 g/cm^3) electrical conductivity measurements



6.7 GPa



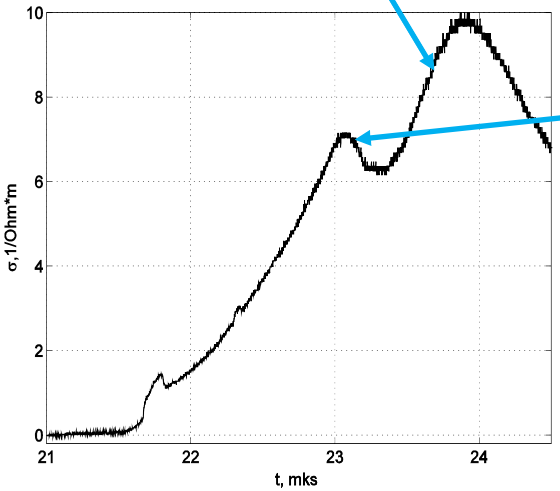
8.9 GPa



Start of sample release

11.5 GPa

Eps effect



Start of sample release

15.0 GPa

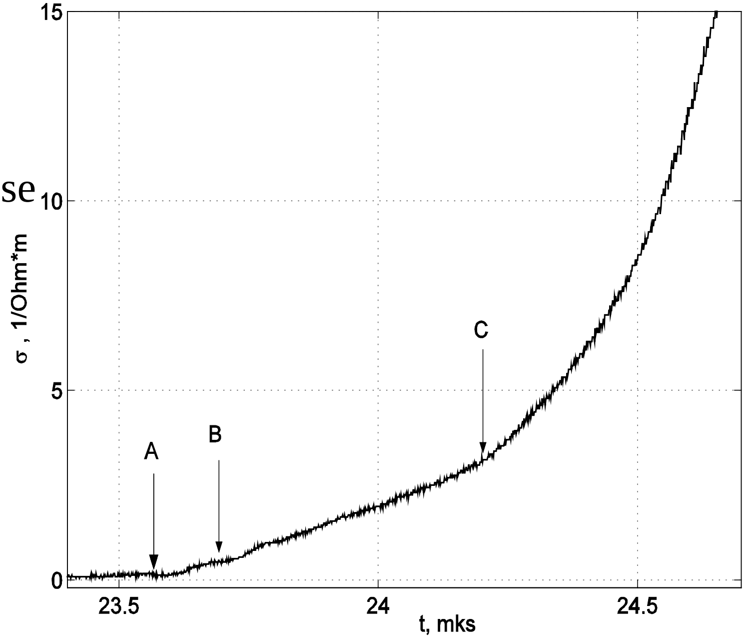
Interpretation of shock-compressed TATB electrical conductivity measurement results

РФЯЦ–ВНИИТФ

- The shock wave with the pressure P ≈ 10 GPa at the front converts TATB into a semiconductor having electrical conductivity on the order of 1/(O*m) which is close to a semiconductor-level electrical conductivity, for example, Ge (under normal conditions).
- What did the experiments show? Was it conductivity of unreacted crystalline HE or the conductivity of the EPs formed as a result of partial HE decomposition?
- Arguments in support of the shock-compressed unreacted crystalline TATB conductivity:
  - ✓ HS has small initial volume, and the combustion waves join together only at the final stage of the process (initial porosity is ~ 4%, the HS size is one order of magnitude less then the initial size of voids, so the initial HS volume fraction is ~ $4*10^{-3}$ %),
  - ✓ Measured electrical conductivity is 2 orders of magnitude less as compared to that of EPs.
  - ✓ The second peak at 15 GPa may result from the mode shift, when the combustion waves join together and conductivity grows even under release. A similar effect was observed at 17,3GPa.

Change of increase in the specific electrical conductivity rate at 17.3 GPa

A – the time when the shock-wave arrives at the sample
B –the time when the shock-wave goes out of the sample,
C – the time when the rate of electrical conductivity increase
changes and EPs presumably make major contribution.



- It is desirable to make experiments with single-crystalline samples. The problem is that the fabrication technology of samples with required geometry is not currently available. .
- What is the TATB molecular crystal forbidden-band width? Our calculations (ZST and Technical Physical Letters, 1998) suggested ≈ 2.0 eV.

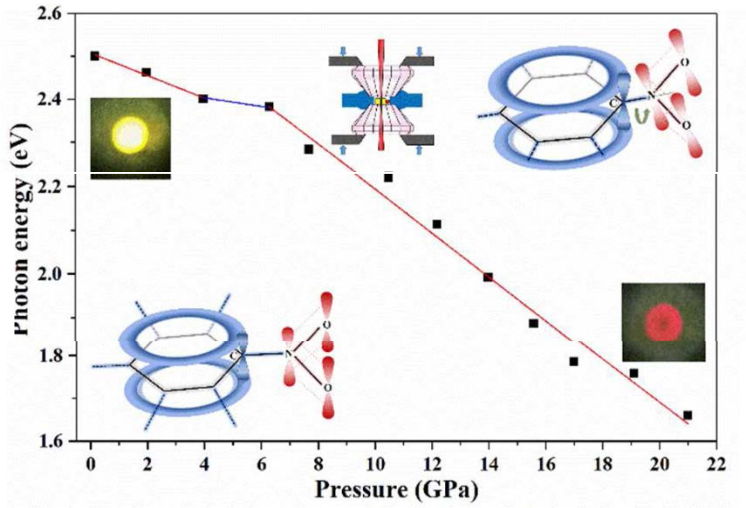
Estimates of TATB crystal band gap

РФЯЦ–ВНИИТФ

Authors	Date	E_g, eV	Comment
Kunz	PhR, 1996	≈ 11 (normal conditions/nc)	HF calculation
Grebenkin	TPL, 1998	≈ 2 (10 – 20GPa)	Estimate based on the detonation experiments' results
Kakar e.a.	PhR, 2000	6.6 (nc)	Experiment. Indirect method
Grebenkin, Kutepov	Semiconduc-tors, 2000	2 - 4 (nc) 1.5-2.0 (10-20GPa)	Estimate: DFT calculation with the systematic underestimation correction of E_g. The conclusion is that it is 11 but not 7, a << .
Wu	PhRB, 2003	2.4 (nc) 1.5 (15 GPa)	DFT calculation
Manaa	APL, 2003	2.5 (nc)	DFT calculation
Grebenkin et al.	ZST, 2003	1.5 – 2.0 (10 - 15 GPa)	Evaluation based on measured electrical conductivity behind the shock-wave front
Liu e.a.	PLA, 2006	2.6 (nc)	DFT calculation
Weihua Zhu	JMS, 2009	2.4 (nc)	DFT calculation

Estimates of TATB crystal band gap (continued)

Authors	Date	E_g, eV	Comment
Fyodorov, Zhuravlev	ChPh, 2014	2.24 (nc) 4.45 (nc)	DFT calculation G_0V_0 calculation
Appalakondaiah et al	JPhCh, 2015	2.51 (nc) 4.66 (nc)	DFT calculation G_0V_0 calculation
Yan Su et al	Chin. Ph. B, 2018	2.36 – 2.60 (nc) 1.77-1.97 (20GPa)	DFT calculation (alternatives)
Han Qin et al	Ph. B CM, 2019	2.37 (nc) 1.86 (15 GPa)	DFT calculation



Граница спектра поглощения ТАТБ
Xiaoyu Sun e.a. J. Ph. Chem., 2018

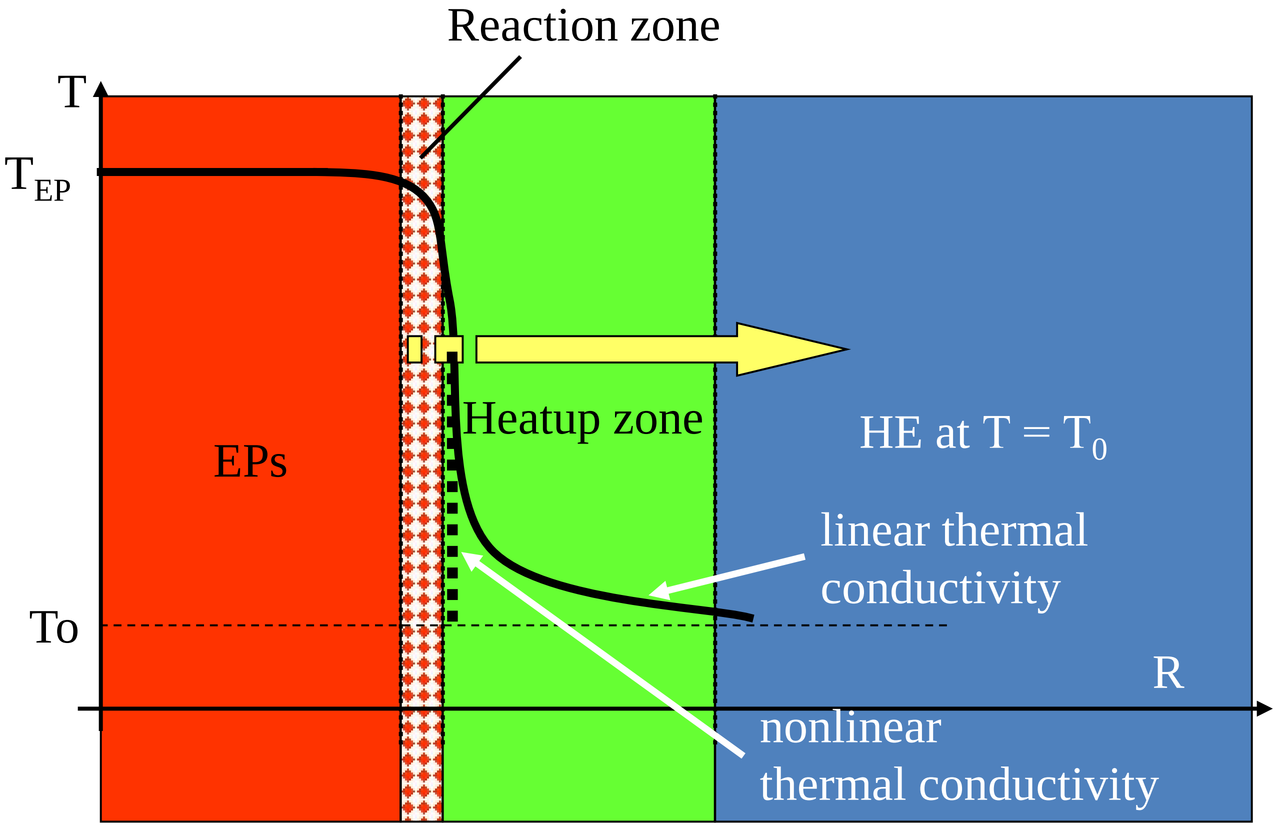
- ✓ According to the absorption spectrum measurement (2018) at P ≈ 10 - 15 Gpa, in TATB $E_g \approx 2.0$ eV.
- ✓ Why do DFT calculations show good agreement with the experiment but do not underestimate E_g just as in case of other substances? Why a more precise model of G_0V_0 does not agree closely with the experiment results?
- ✓ In addition, results of calculations with the same class models made by different authors are in good agreement (2.5eV and 4.5 eV). This indicates their correctness (within the framework of assumed approximation).

Does the shock wave convert TATB into a semiconductor? What mechanism promotes energy transfer in the combustion wave?

РФЯЦ–ВНИИТФ

- The supposition has been confirmed – yes, it does!
  - ✓ Measurements of electrical conductivity in shock-compressed TATB demonstrated that its conductivity is very similar to that of Ge (under normal conditions).
  - ✓Calculations and forbidden-band width measurements yield E_g = 2 - 3 eV and the forbidden-band width decreases at the pressure rise.
  - ✓HE heating (primary effect) and compression (forbidden-band width reduction) leads to increased electron concentration in the conduction band after shock wave passing-through.
- The driving mechanism for thermal conductivity at HSs combustion (phonon and electron thermal conductivity or both of them) remains an open question. Further research in this area is indicated.

Combustion wave velocity in the medium with nonlinear (electron) thermal conductivity



Electron thermal conductivity of semiconductors

$$\chi \sim \exp\left(-\frac{E_g}{2kT}\right)$$

Combustion wave velocity

$$D \sim \sqrt{\frac{\chi\left(T_{\text{ПВ}}\right)}{\tau\left(T_{\text{ПВ}}\right)}}$$

- ✓ χ and τ are thermal diffusivity coefficients and reaction time at temperature close to the EPs temperature. (Krishennik, Shkadinsky, Proc. of the Academy of Sciences, 2003).
- ✓ Macrokinetic velocity of reactions in TATB (and thus, the pop-plot and other detonation effects) are determined by the EPs temperature!?

Returning to the issue of V.G. Morozov's paradox

- For the combustion wave velocity evaluation, we need to evaluate the values of two parameters χ and τ at the temperature on the order of T_{EP} in HSs.
- In 2001, MD-calculations were used to evaluate the reaction time. (J. of Technical Physics, 2001):
  - ✓ for TATB ~ 30 ps,
  - ✓ for HMX ~ 1 ps,
- Independent calculations by other authors subsequently confirmed this evaluation for HMX (Manaa et al, 2002) and TATB (Manaa et al, 2010) .
- If energy transfer in the combustion wave is assumed to follow the phonon mechanism ($\chi \sim 10^{-7}$ m ^{2}/s), then we obtain the combustion wave velocity estimate ~ 300 m/s for HMX and ~ 60 m/s for TATB. Just what we needed!
- Possible explanation of the paradox – the reaction time but not the energy transfer mechanism has been refined. Calculations of the combustion wave velocity used the combustion kinetics model obtained from the HE ignition experiments at low temperatures and during large times of ignition (≥1s). This model is useless during short reaction times. Molecular dynamics (MD) is highly successful at picosecond times.

Why is TATB so low-sensitive?

- This question is discussed in details in our publication in Combustion, Explosion and Shock Waves, 2009, #1.
- Two main parameters characterize external effect on HE:
  1. P_f – pressure at the first shock wave front which determines the HSs density,
  2. T_{EP} – EPs temperature in the reaction HSs which determines the combustion wave velocity.
- The PTATB shock-wave initiated detonation pressure is ≥10GPa, the HS density attains the saturation and the HSs are almost immediately ignited.
- The primary (in fact, the only one) factor of the PTATB detonation kinetics is the combustion wave velocity determined by the EPs temperature in the HSs.

$$D \sim \sqrt{\frac{\chi\left(T_{ПВ}\right)}{\tau\left(T_{ПВ}\right)}} \sim \exp\left(-\frac{T_{ef}}{T_{ПВ}}\right) \qquad T_{ef} = \frac{E_g}{4} + \frac{E_a}{2}$$

E_a - activation energy of chemical reactions
(nitrogroup binding energy)
~ 60 kcal/mol – TATB
~ 40 kcal/mol – HMX, RDX

- For TATB $E_g \approx 40$ kcal/mol and the second summand T_{ef} makes the main contribution.
- **Such low-sensitivity of TATB is due to its abnormal low temperature ~2000K, smaller by a factor of 2 as compared to conventional explosives and its molecule is more resistant.**

In what way does the EPs temperature-based microkinetics produce its effect (Combustion, Explosion and Shock Waves)?

РФЯЦ–ВНИИТФ

- TATB decomposition microkinetic velocity is thus dependent on T_{EP}:
  $\sim exp(F(T_{EP}))$, where $F = - T_{ef} / T_{EP}$
- **The question:** How can we obtain the relationship between the reactions’ velocity and the initiation effect degree, i.e. the pressure?
- **The answer is surprising:** after the shock wave passing-through, the HE effective caloricity rises as the shock wave contributes extra energy to the medium. The EPs temperature in the reaction HSs is consequently dependent on the initiation shock wave intensity – the stronger the shock wave, the higher the temperature in the EPs hotspots is.
- The HE and EPs equations of state can be used to calculate $T_{EP}(P)$ and present $F(T_{EP})$ in terms of $F(T_{EP}) \approx T_1 + \alpha \cdot P$. ($T_1$ and α are calculated constants).
- It is possible to use linear approximation as T_{EP} rise due to shock-wave extra energy is not very high. Yet, due to the fact that $T_{ef} >> T_{EP}$, the reaction velocity is heavily dependent on pressure.
- Finally, we arrive at a fairly common dependence of the reactions’ velocity on pressure $\sim exp(\alpha \cdot P)$. It can be further approximated by a more common dependence $\sim P^{m}$.

The conclusions drawn regarding the TATB decomposition kinetics

$$-\frac{d\xi}{dt} = F(\xi)\cdot N^{1/3}(P_f)\cdot D(P) = Z\cdot\xi\cdot(1-\xi)^{2/3}\cdot exp(\alpha\cdot P)$$

- $F(\xi)$ is obtained from the model problem solution $F(\xi)\approx 4.5\cdot\xi\cdot(1-\xi)^{2/3}$
- $N^{1/3}(P_f) = const$ at $P_f \geq 10$ GPa.
- $D(P) \sim exp(\alpha\cdot P)$, where $\alpha \approx \frac{T_{ef}}{T_*^2}\cdot\frac{1}{C_{EP}}\cdot\frac{dE_f(P_f)}{dP_f}$ is obtained using an approximate solution of the combustion wave propagation velocity.

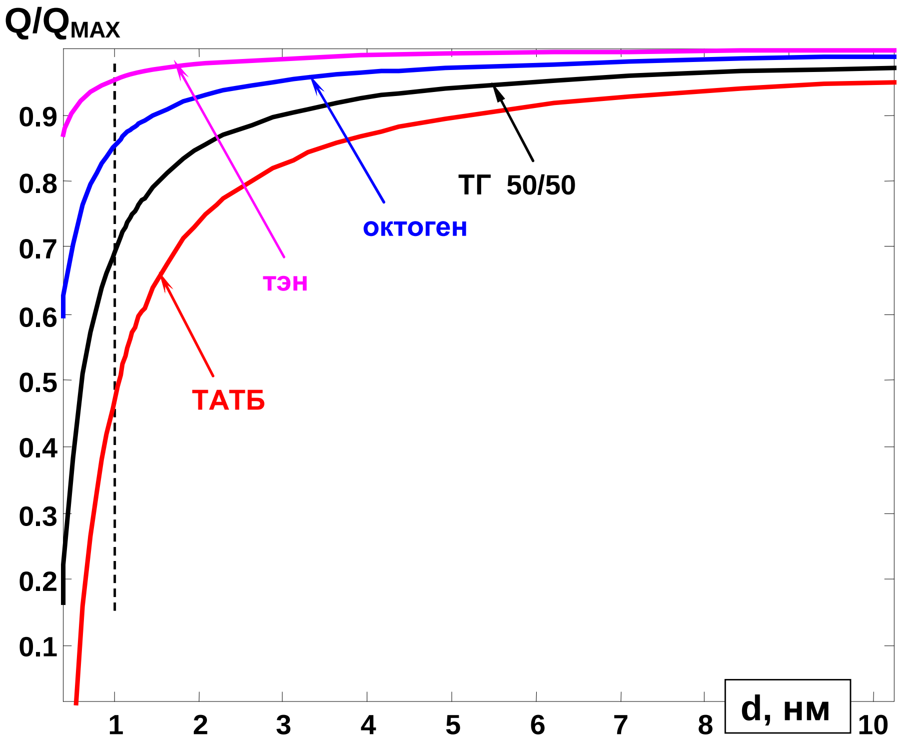
- The estimates give the value α = 0.2 – 0.3 1/GPA (Combustion, Explosion and Shock Wave, #1, 2009),
- The fit by the detonation experiments’ simulation yields the value α = 0.32 1/GPa (KhST 2007

Semiempirical model – simulated processes are analyzed on a microlevel and this makes possible to plot physically based, though approximate, dependencies of the three co-factors on the medium parameters Then the detonation experiments’ results are used to correct constants Z and α (there are only two of them!).

Features of the negative oxygen-balance HE detonation

РФЯЦ–ВНИИТФ

- The negative oxygen-balance HE detonation is accompanied by exothermal process, that is ultra-dispersed diamond (UDD) growth.
- HE caloricity depends on the extent of the process completion, i.e. the UDD average size (see Fig.).
- TATB EPs contain extremely high content of carbon and its caloricity is determined by the UDD condensation contribution.

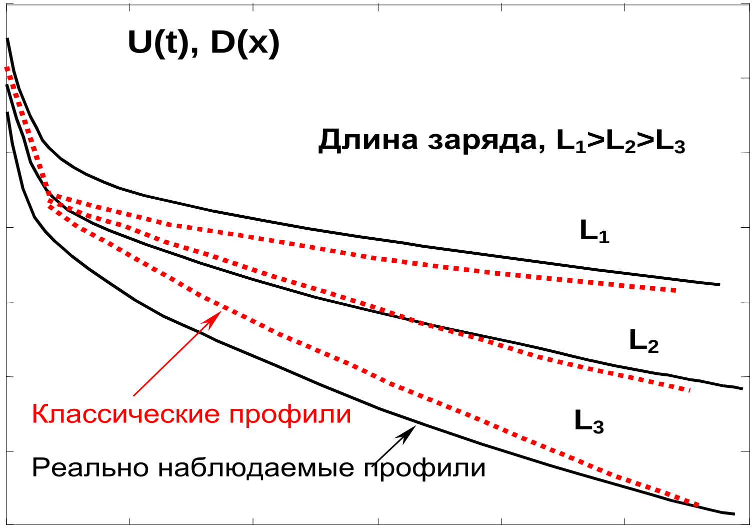


Predicted caloricity of several HEs versus the UDD average size in the EPs (Zherebtsov et al, 2005)

Slow long-term energy release takes place in the EPs beyond the chemical reaction zone and the detonation model should consider this

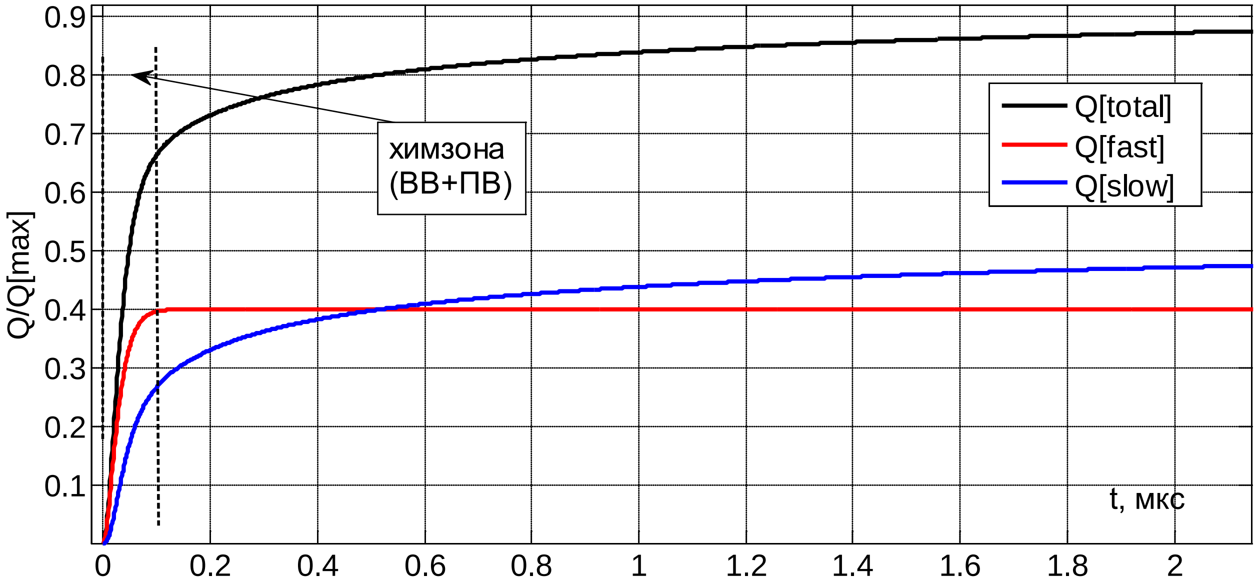
Experimentally confirmed UDD growth and slow energy release beyond the chemical reaction zone

- Small-angular scattering of synchrotron radiation in the EPs (Titov et al, 2001 +).
- Stage of slow growth of polymer-bonded TATB (PTATB) EPs electrical conductivity (Combustion, Explosion and Shock Wave, 2007, # 1). P=34 and 27 GPa.
- Splitting of curves of the shock-wave attenuation in the barrier. The shock wave contacts with the detonating high explosives «Comp. B» (Bdzil, 1975) and PTATB (Loboiko et al, 2005). “The detonation pressure depends on the charge size”.



Unified model of PTATB detonation

- Energy release in detonating negative oxygen-balance HE consists of two components (13-th Int. Det. Symp., 2006):
  1. Fast – destruction of initial HE molecules, formation of stable two-, three-atom TATB molecules and small carbon clusters (10-100 atoms less than 1 nm). Characteristic time of this process is ~ 10 - 100 ns in stationary detonation modes.
  2. Slow – residual energy release in the EPs due to carbon clusters’ growth. Characteristic time is ~ 1 μs.



$$E(t) = E_f(t) + E_s(t)$$

$$E_f(t) = q_0 \cdot \alpha \cdot \left[1 - \xi(t)\right]$$

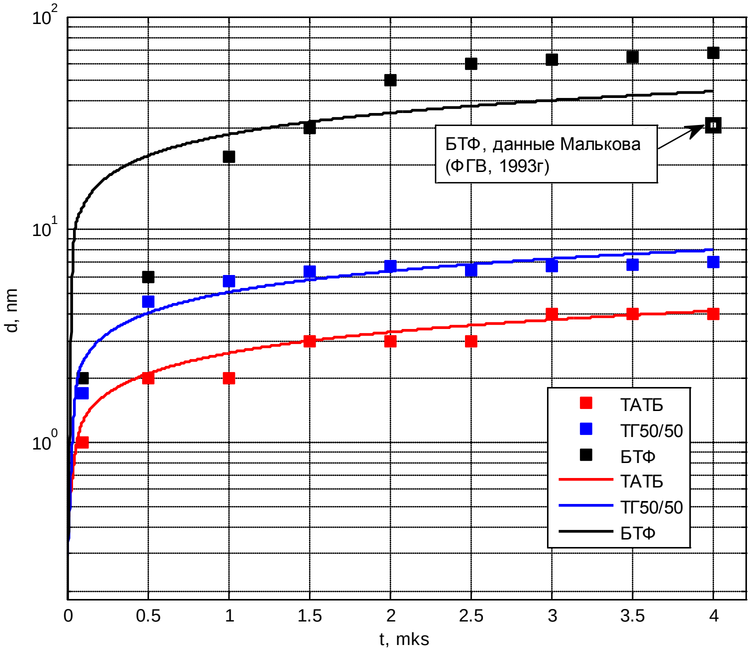
Selection of slow kinetics constants

$$E_s(t) = q_0 \cdot [1 - \xi(t)] \cdot (1 - \alpha) \cdot [1 - f(t)]$$

$$f(t) = \begin{cases} 1, & npu \quad t < t_f, \\ \dfrac{1}{\left(1 + \dfrac{t - t_f}{\tau_s}\right)^{\frac{1}{n}}}, & npu \quad t \geq t_f \end{cases}$$

q_0 is HE total caloricity, α is its fraction corresponding to the phase of HE transformation into EPs.

1. Power dependence on time with **n≈3** corresponds to the theoretical model (Show, Johnson, 1987)
2. Let us assume that formation of UDDs sized ~ 1 nm (~ 100 atoms) is part of the fast kinetics phase HE→EPs (formed during the same characteristic times as the final gas components), then we can estimate the energy release fraction in the fast phase α by the predicted dependence $Q(d_{UDD})$.
3. Parameter $\boldsymbol{\tau_s}$ can be estimated based on the experiments aimed at studying of the condensed carbon nanoparticles' growth dynamics with synchrotron radiation.



Comparison of the predicted dependence d(t) (Zherebtsov et al, 2015) to the experimental one (Titov et al, 2011)

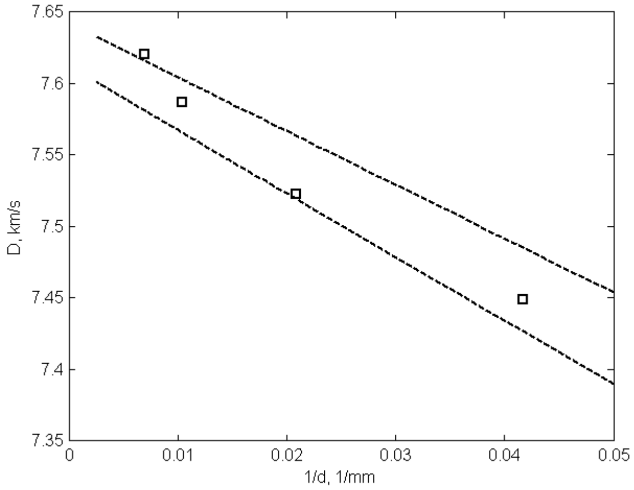
$$\left.\begin{matrix} Q^{РАСЧ}\left(d_{УДА}\right) \\ Q^{РАСЧ}\left(t\right) \end{matrix}\right\} \Rightarrow d_{УДА}^{РАСЧ}(t) \Longleftrightarrow d_{УДА}^{ЭКСП}(t)$$

Weakly nonideal detonation model

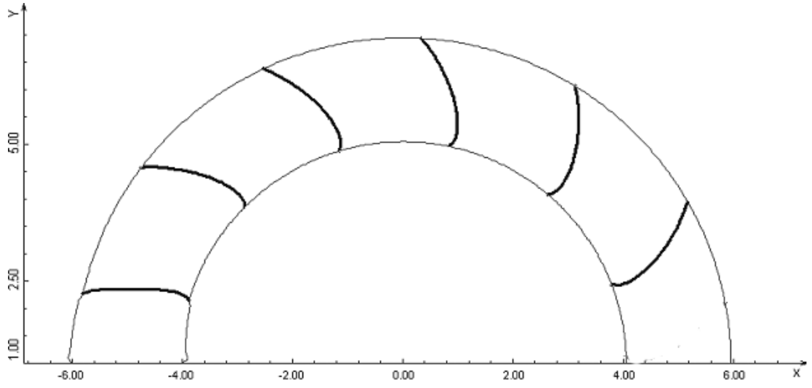
- Under high-level initiation conditions and with over-critical sized system, the weakly nonideal detonation model can be used (Combustion, Explosion and Shock Waves, 2008, # 2):
    - ✓ Immediate HEs-to-EPs transformation and release of the caloricity part corresponding to the first stage.
    - ✓ Slow energy release of the remaining caloricity part in completely reacted EPs.
- The weakly nonideal detonation model describes the experimental results, as well as the diameter-effect and the detonation propagation in curvilinear channels. This further confirms the existence of slow-phase kinetics and correctness of the selected parameters.

Weakly nonideal detonation model used to describe results of some experiments

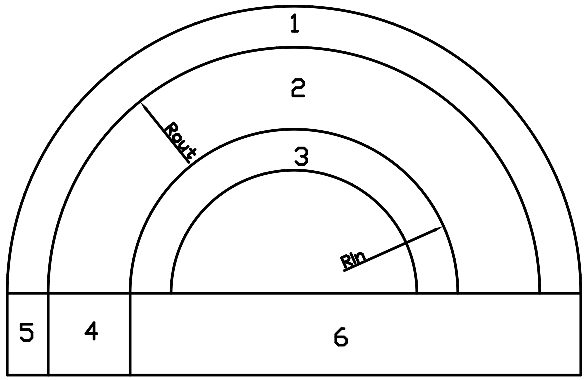
РФЯЦ–ВНИИТФ



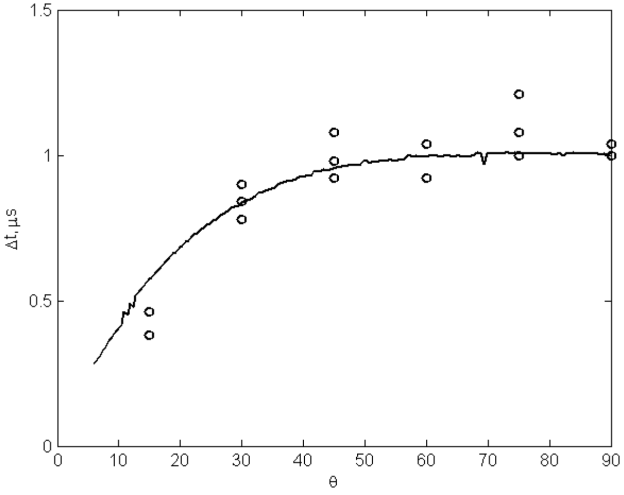
1. Diameter-effect. Square shows WND calculation, lines show the experimental data measurement limits (Campbell, 1976)



Predicted shape of the detonation front

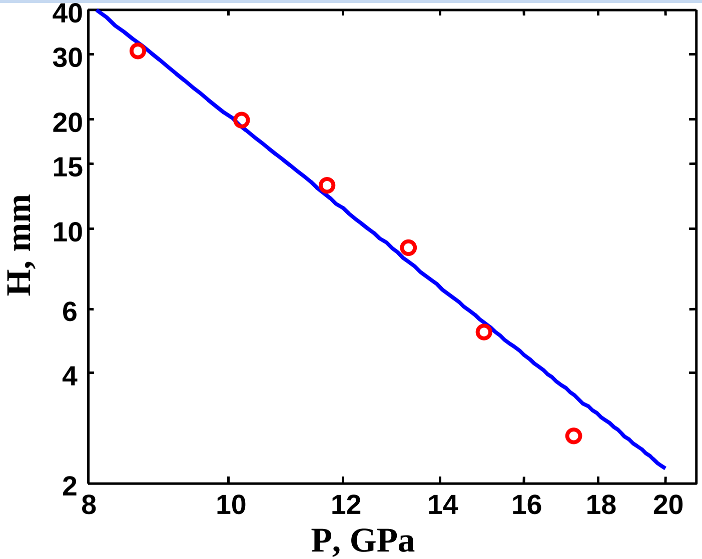


2. Experiment to study PTATB detonation propagation in a semiannular clearance sized 40/60 mm (Loboiko et al, 2004)

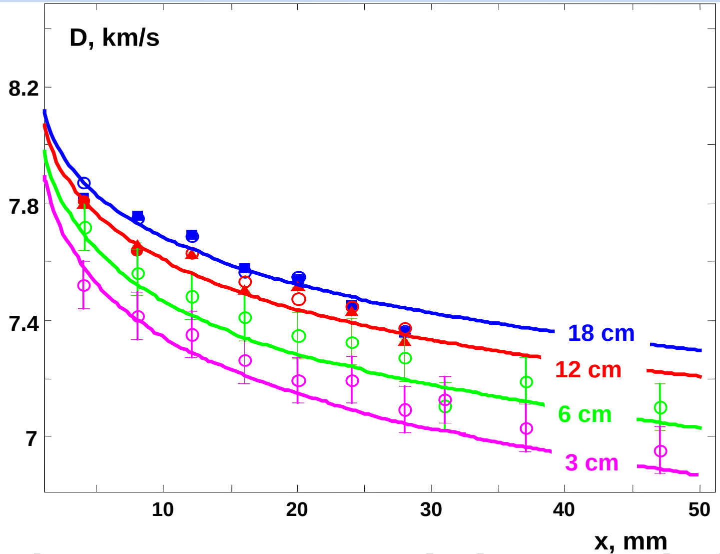


Time difference of the detonation wave (DW) arrival at the external and internal HE surface versus the DW rotation angle

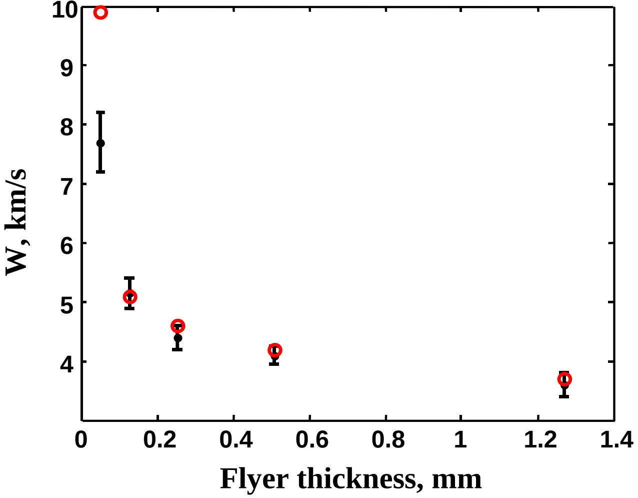
Combined overall model compared to results of some experiment



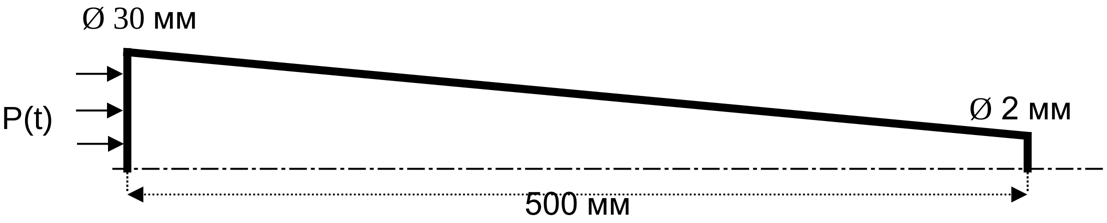
Pop-plot (R.L. Gustavsen, 2001)



Shock-wave attenuation in the barrier (Loboiko et al, 2005)



Thin-film initiation
(Honodel et al, 1981)



Critical diameter
Prediction L= 31,5 cm and Ø ~ 12 mm,
Experiment (Dobratz , 1995) Ø ~ 12 mm.

Collection of papers

The collection of papers describes in details the results that has been demonstrated in the presentation and gives consideration to the following:

- Cooperative effects in the EPs.
- Low-velocity detonation model,
- Undercompressed detonation model of the phlegmatized HE, etc.

Физические модели детонации
гетерогенных кристаллических
взрывчатых веществ

Coauthors of papers mentioned in the presentation

РФЯЦ–ВНИИТФ

- **Development of physical models**

  A.L. Zherebtsov, M.V. Tarannik, D.V. Kochutin,

  A.L. Kutepov.

- **Mathematical simulation**

  A.S. Shnitko, S.K. Tsarenkova, G.V. Kovalenko, D.A. Varfolomeev, V.V. Popova, M.A. Vorobieva

- **TATB electrical conductivity measurements**

  M.M. Gorshkov, V.T. Zaikin, V.M. Slobodenyukov, O.V. Tkachev.

Conclusion

- Ab initio calculations of the heterogeneous crystalline HE decomposition macrokinetics cannot be performed yet, but a more or less clear general idea of how this can be done is now available.
- A semiempirical approach, transient between empirical and ab initio, seems to be productive. With this approach, the simulated processes are being analyzed on micro- and mesolevels to construct a physically-based, though approximate, dependence of the chemical-reaction energy release rate on the medium parameters. The detonation experiments' results will be further used in the "fine tuning" of this dependence.
- Hopefully, some questions posed by Boris G. Loboiko have been answered and we have come closer to understanding of the relationship between HE microstructure and its detonation properties.