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On the Mechanism of Molecular Condensed EMs Transformation under the Effect of Shock and Detonation Waves

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Abstract: Considerations based on available experimental data on regularities of molecular condensed EMs decomposition under the effect of shock waves of different intensities are presented. It follows from the considerations that there exist shock wave pressures p* typical for each charge (for TNT charges p* ~ 12 GPa) and the charges' initial density $\rho_\circ$* (for TNT $\rho_\circ$* ~ 1.40 g/cm^3) such that at larger pressure and density EMs' decomposition proceeds according to the homogeneous mechanism (does not depend on the charge structure: initial density, size and structure of explosive particles, explosive state-liquid or solid, …) and at lower pressure and density – according to the hot spots mechanism (depends on the charge structure).

Keywords: detonation, decomposition regularities, homogeneous and hot spots mechanism

Introduction

It is well-known that gaseous detonation as the phenomenon of a supersonic propagation of flames in tubes was discovered by two groups of French scientists: Mallard and LeChatelier [1], and Berthelot and Vielle [2]. What physical process is responsible for flame propagation with the supersonic velocity? – it was the question of interest already to the first investigators. The supersonic detonation velocity cannot be described in terms of thermal conductivity and diffusion processes responsible for slow flame propagation. Mallard and LeChatelier [1] were the first to explain correctly the supersonic velocity phenomenon.

They suggested compression as being the principal mechanism for combustion propagation, that is, in the combustion transmission from layer to layer.

Detonation theory based on the theory of shock waves was independently proposed by Russian physicist Michelson [3, 4], Englishman Chapman [5] and Franchman Jouguet [6, 7]. Therefore, the theory should be called the MCJ theory. The thermodynamic analysis of the phenomenon carried out by Michelson, Chapman and Jouguet resulted in the generalization of the shock wave theory. The detonation wave was represented as a shock wave with explosive energy release inside the wave front (Figure 1). In this case the theory did not take into account the chemical reaction kinetics. Moreover, the followers of the theory believed that detonating gaseous mixtures were transformed into the detonation products almost instantaneously. The notion seemed to be justified, once it had been established experimentally that in all gaseous mixtures investigated the shock wave pressure initiating the chemical reaction with a vanishingly small time delay characteristic of detonation was virtually identical with the MCJ pressure, and the velocity of this shock wave was considerably smaller than the detonation velocity of the mixture (see, for example [8] and references there). It was because of this experimental finding that the MCJ theory followers thought that mixtures in detonation waves were transformed into detonation products in the course of their compression within the wave shock front leading detonation. Therefore the MCJ detonation model was sometimes called the "Zero-reaction zone" model.

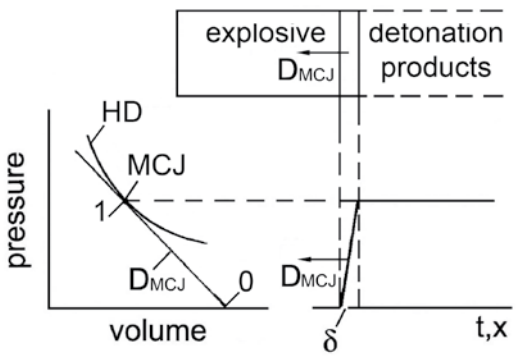

Figure 1. Michelson-Chapman-Jouguet detonation. Explosive transforms into detonation products simultaneously with its compression within the detonation wave shock front δ (zero reaction zone model). HD: Hugoniot adiabat for detonation wave. 01: Michelson straight line. D_{MCJ}: MCJ detonation velocity.

The idea that detonation wave is a shock wave with exothermic reactions in its front obtained many experimental and theoretical substantiations and is at present generally accepted. As to the notion that gaseous mixtures are transformed into detonation products in the course of their compression within the detonation wave shock front it was in obvious contradiction to the commonly adapted concept of chemical reaction progress in time with a finite rate. The matter is that the shock wave front width (shock discontinuity zone width) totals only a few molecular free path lengths (see [9] and references there) and, according to the chemical kinetics, reagents need many thousands of collisions to be converted into the final products.

It should be mentioned that the erroneous notion that gaseous mixtures are transformed into detonation products in the course of their compression within the detonation wave shock front came into being on account of an incorrect interpretation of the foregoing experimental finding. The latter took place through ignorance at that time that detonation front for all gaseous mixtures is kinetically unstable, pulsating [10]. And the transformation of mixtures into detonation products within the kinetically unstable detonation front proceeds through local adiabatic explosions of the shock-compressed mixtures created within the wave front under the effect of detonation products of MCJ pressure [11, 12]. In this case the transformation time turnes out to be naturally some orders of value larger than the wave shock discontinuity zone time.

The MCJ detonation theory was established at the close of the ninetieth and the early twentieth centuries and a notion of a finite chemical reaction zone in gaseous detonation was formulated only in 1936. Bone, Fraser, and Wheeler [13] as well as Rivin and Sokolik [14] were the first to suggest the approach. In 1940, Rosing and Chariton published their interpretation of the condensed explosive detonation failure diameter phenomenon on the basis of a chemical reaction zone of finite length in the detonation [15].

A physical model of detonation wave with finite chemical reaction zone was developed by Grib [16], Zeldovich [17], von Neuman [18], and Dőring [19]. Therefore the theory should be named the GZND theory. According to the GZND detonation theory, the wave front is more complicated. In the MCJ detonation wave, the explosive mixture is converted into the detonation products in the process of its compression within the wave shock front, and in the GZND detonation wave, on the contrary, explosive does not change chemically at all within the wave shock front, it is only compressed within the front and its decomposition in the explosive's selfignition form starts under the effect of a high temperature of the shocked material behind the front in some induction time proper for the state (Figure 2). In essence the detonation changed to

deflagration spreading behind the shock front with the shock front velocity. The zone containing the shock-compressed mixture is characterized by an increased pressure and is called the chemical spike. The spike time t_{CS} is a time needed for the explosive material to be converted into the detonation products.

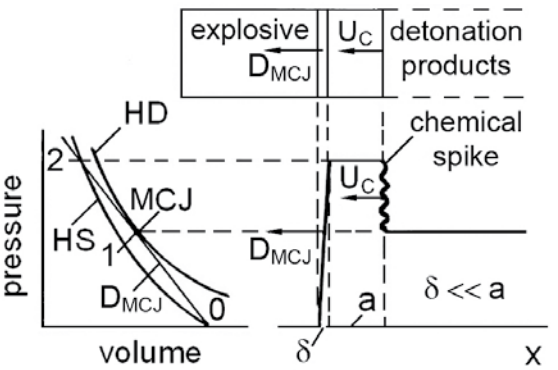

Figure 2. Grib-Zeldovich-vonNeuman-Döring detonation. Explosive is compressed without chemical change within the detonation wave shock discontinuity zone δ, and its decomposition in selfignition form of the shock-compressed explosive sets in behind the front under the effect of high temperature due to shock compression. After the selfignition the shock-compressed explosive burns with the velocity U_C exactly equals in magnitude to the velocity of the wave front D_{MCJ}. HS: Hugoniot adiabat for shock wave without chemical reaction. HD: Hugoniot adiabat for detonation wave. Lines 01: Michelson straight line. Point 2 corresponds to a normal detonation chemical spike. D_{MCJ}: MCJ detonation velocity.

Molecular Condensed EMs

It follows from the foregoing that both the MCJ and the GZND detonation models were developed for gaseous systems. And pioneering investigations of condensed explosives detonation made their appearance in the thirties-forties of the previous century. At that time the possibility to transfer the stationary one-dimensional complex of the GZND detonation theory to detonation process in condensed explosives was not obvious. First, it was not clear whether the shock heating of condensed explosives was sufficient to ensure a rapid course of their chemical reactions. The doubts in the possibility of the shock mechanism

forced scientists to introduce other conceptions on the detonation transformation mechanism in condensed explosives. For solid heterogeneous explosives the most widely used were conceptions about "explosion combustion" according to which explosive particles first are ignited over their surface within the detonation wave front and then are consumed through combustion [20, 21]. There existed also an assumption that the condensed heterogeneous explosive detonation was led by explosion products [22]. According to the assumption the velocity of jets of explosion products was just the velocity of the detonation propagation. In essence, this was another model of a detonation wave, different from the hydrodynamic model.

At the time when the above-mentioned notions were put forward, there were no direct experimental data available. Therefore, explanations of isolated experimental findings based on these or others conceptions, were considered as some demonstration of their validity. For example, from the position of the explosion combustion conception it was easy to explain the increase in the failure diameter value with the increase in the initial size of the explosive's particles. According to the explosion combustion's model the reaction time $t \sim \delta_p/u_c$, where δ_p is the initial particle size, and u_c is the combustion velocity under detonation pressure. Using the relationship of the reaction time with the failure diameter $d_f \sim 2ct$ [23], where c is the velocity of sound within the reaction zone, partisans of the explosion combustion's theory reasoned that an increase in the failure diameter value with the δ_p's rise was connected with the increase in the reaction time.

Soon after the Second World War experimental methods were developed which allowed to determine directly both the parameters of shock and detonation waves (particle velocity, pressure,…), as well as the chemical reaction time (see [24] and references in). The data obtained provided the basis for more detailed analysis of the mechanism of detonation transformation of condensed explosives.

It has been established by many investigators that the response of heterogeneous solid explosives (cast, pressed, poured) in the majority of cases have significantly greater susceptibility to detonation in comparison with that of homogeneous liquid explosives. It is manifested in a substantially smaller value of an initiating shock wave intensity required to make detonation in heterogeneous solid explosives in comparison with that to make detonation in liquid explosives (see Proceedings of Detonation Symposia which contain many papers pertaining to the "Shock-to-Detonation" topic). The difference between shock sensitivities of heterogeneous and homogeneous explosives stems from the marked difference between initial rates of their energy release immediately behind the front of

initiating shock waves. In homogeneous liquid explosives the initial rate of their energy release behind the front of initiating shock waves of near critical intensity is normally very slow, so that the bulk of their energy is released at some distance downstream of the shock wave front. For the reason first the shock-compressed explosive detonation appears at the distance behind the initiating shock wave front, the detonation overcoming the initiating shock wave front and generating in the initial explosive a strong detonation which transits gradually to the MCJ detonation. On the contrary, in heterogeneous explosives the initial rate of their energy release behind the front of initiating shock waves is normally fast and leads to a gradual transition of the reactive shock wave to the MCJ detonation, provided the shock intensity exceeds its critical value. Therefore, it was assumed that a decisive role in the release of heterogeneous explosives energy behind the front of shock waves of any intensity till up to their detonation pressure was played by the hot spots mechanism [11, 25, 26].

Two lines of experimental research were used at the Institute to gain data on the kinetics of energy release in condensed explosive materials: first, the investigation of shock-to-detonation transition (SDT) processes and, second, studies of the chemical reaction zone (chemical spike) in detonation waves, both in their dependences on various parameters of the explosive charges structure [initial density, particle size and their structure (single crystals or fragments of cast charges), the explosive's state (liquid or solid), …]. It was demonstrated that SDT processes depended on the structure. One should mention specially that it has been found out comparatively recently that heterogeneous condensed explosives are characterized by some density $\rho_\circ^*$ (for example, TNT's $\rho_\circ^* \approx 1.40\ g/cm^3$) such that the explosive's energy release proceeds with the maximum rate directly in the front of shock waves of arbitrary intensity up to detonation pressure if the explosive density $\rho_\circ < \rho_\circ^*$ [27]. It means that the transformation of heterogeneous condensed explosives at detonation in charges with $\rho_\circ < \rho_\circ^*$ proceeds mainly through the hot spots mechanism. For charges of the explosive density $\rho_\circ > \rho_\circ^*$ the maximum rate of energy release under the action of shock wave of critical intensity is reached at a certain distance behind the front. In this case the so-called "hump" profile of the wave is formed. With increasing the initiating shock wave intensity as well as with the increase of the reactive shock wave intensity during its transition to detonation, the "hump" enhances and shifts to the front. The "hump" profile resembles that for homogeneous liquid explosives [11] and means that the transformation of heterogeneous condensed explosives at detonation in charges with $\rho_\circ \geq \rho_\circ^*$ proceeds mainly through the homogeneous mechanism.

As for the detonation processes it was found out, opposite to the SDT

processes, that the structure of heterogeneous condensed explosive charges (experiments were performed with charges of TNT, RDX, PETN, Tetril) had practically no effect on the time t_{CS} of their detonation transformation [28, 29]. As an illustration the data for the most extensively studied TNT are shown in Figure 3. One can see from Figure 3 that data for t_{CS} corresponding to charges of different structure lie within the experimental precision (10÷20%) on one the same t_{CS} dependence on detonation pressure.

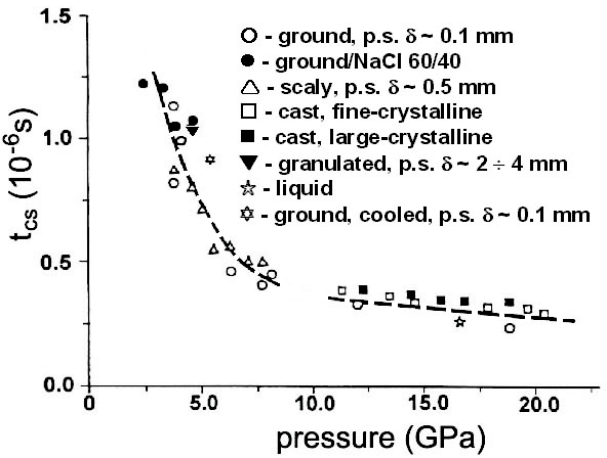

Figure 3. The dependence of chemical spike time t_{CS} on the pressure P of TNT charges detonation. p.s. δ: explosive particle size δ.

The evident difference in the influence of the structure of heterogeneous condensed explosives on the regularities of their transformation under their SDT process, on the one hand, and their detonation process, on the other, testifies that the hot spots mechanism of their transformation worked under the effect of shock waves of not any pressure. It was revealed that there was for each charge rather narrow range of shock pressures (it can be characterized by an average value P^*) such that the structure affected the rate of the explosive energy release at lower pressures and, vice versa, practically did not affect it at higher pressures [30]. It turned out that the P^*'s value for charges of any structure is always smaller than the chemical spike pressure of their detonation waves [11].

It follows from the foregoing that the transformation of molecular condensed explosives proceeds through the hot spots mechanism under the effect of initiating shock waves of any intensity till up to their detonation pressure if the density of their charges is smaller than their $\rho_\circ{}^*$ density. And as for charges of $\rho_\circ > \rho_\circ{}^*$ densities the mechanism of the explosives transformation is governed by the

level of the intensity of initiating shock waves. It is the hot spots mechanism if the intensity is smaller than the explosive's P^*. And it is the homogeneous mechanism if the intensity is larger than the explosive's P^*.

In this connection it should be mentioned that it was also revealed experimentally that the nature and pressure of gases as well as the nature of fillers in pores of heterogeneous charges of molecular explosives did not affect the regularities of the explosives' energy release within the range of shock intensities from the critical intensity of the initiating shock wave and till up the detonation pressure [11, 30]. It means that the transformation process takes place always within the body of the explosives' particles. In this case the transformation proceeds under the effect of shock or detonation waves propagating within the body of particles. The matter is that it has been observed that the stable (without any perturbations) front of shock and detonation waves in transparent homogeneous liquid media reflects visible light like a mirror [11]. It means that the width of the front's shock discontinuity zone is much smaller than the light wavelength (which corresponds to the shock discontinuity zone width of the order of some tens of A°). And it spells that particles of even a micron size (that is in some orders of value larger than the shock discontinuity zone width) are in essence considerable space for the propagation of waves.

Experimental data shown in Figure 3 on the dependence of TNT's detonation wave chemical spike time t_{CS} on the wave's MCJ pressure for charges of different structure are definitely divided into two groups. In this case the first group's data correspond to charges which detonation wave chemical spike pressures are smaller than their P^*. It means that the explosive transformation within the front of the detonation waves proceeds through the hot spots mechanism. It is well-known that the initial rate of explosives' energy release according to the mechanism is fast. The fast rate is governed by the heterogeneous centering character of the reaction origin. For the slow kinetics of the explosive's reaction within the hot spots [$dN/dt \sim Nexp(-E/RT)$ with a large activation energy and at relatively small temperature] it leads also to the decrease of the dependence of the overall transformation rate on the explosive's initial conditions. It follow from that the total number of molecules reacting per time unit dN/dt is increased if some portion of molecules is cooled and the released heat is transferred to the remaining molecules. The temperature of the latter will thus rise. The explosive overall transformation will be accelerated since the increment of the exponential with increasing temperature (about inverse-proportional to the number of "hot" molecules at a fixed total energy) will completely compensate the diminishing of N before the exponential. It follows that the given volume of the explosive will react faster if the amount of the heat released by the reacted molecules and

sustaining the reaction is imparted to a smaller volume of the explosive. It should be emphasized once more that the reaction in the case can proceed within the hot spots in accordance with the normal kinetic laws (large activation energy) but the overall transformation rate will correspond to regularities of the so called degenerated thermal explosion (lowered activation energy). Just for the reason the group's data give evidence of their rather weak dependence on explosives' initial condition.

The data of the second group (see Figure 3) correspond to charges which detonation wave chemical spike pressures are larger than their P^*. The conclusion has been drawn above that the explosive's transformation within the front of the detonation waves proceeds through a homogeneous mechanism. The mechanism are governed by the structure of explosive's molecules rather than by the structure of its charges. In this connection one can recall that the GZND theory of detonation implies actually that all degrees of freedom of explosive molecules relax in the process of their compression within the shock front of detonation waves. However, it is impossible as the time of excitation of vibrational degrees of freedom, for example, in molecules of aromatic compounds (many condensed molecular explosives are aromatic compounds) varies within wide limits: from fraction of picoseconds to *0.1 – 1.0 nsec*. It follows that many molecules do not have enough time to be excited in the shock front.

Because of the great difference between the time of explosive loading within the shock discontinuity zone and the time the explosive's molecules need for excitation of their bonds the kinetic energy of molecules, which should be uniformly distributed between all degrees of freedom behind the wave front is absorbed inside the front mainly by their translational degrees of freedom. It leads inevitably to a tremendous overheat of the translational temperature. The statement was justified by numerical experiments [31, 32]. (The maximum value of the translational temperature overheat is $T_{oh} = 2(n - 1)(T - T_{\circ})$, where n is the number of atoms in a molecule, and $T_{\circ}$ and T are equilibrium temperatures in front and behind the front of shock waves [12]).

The overequilibrium translational energy is distributed between the remaining degrees of freedom behind the front of shock waves. The total time of the redistribution process of the molecules' kinetic energy over all internal degrees of freedom, obviously, will be equal to the time of excitation of the most slowly excited bonds. If during this time the flux of the translational energy to some vibrational bonds exceeds the outflow of their energy due to vibrational-vibrational relaxation the bonds will be oversaturated by energy and destroyed. The destruction mechanism was named the accumulation mechanism [33].

The origin of the translational temperature overheat is of great significance

for understanding the mechanism of the detonation transformation of molecular condensed explosives consisting of complex polyatomic molecules. The translational temperature overheat for molecules consisting of tens of atoms can be tens of thousands of degrees for shock wave intensities characteristic of detonation of powerful explosives. At such temperatures the processes electronic excitation [34] (activation energy 2-5 eV [35]) and even the thermal ionization process (activation energy 6-10 eV [36]) become possible within the over-heat zone.

Thus condensed explosives consisting of complex polyatomic molecules can experience nonequilibrium destruction within their detonation wave shock front. At first the statement was introduced hypothetically [37] as a surmise on the possible destruction of explosive molecules in the course of their compression within the detonation wave shock front. Later on the surmise was justified experimentally [38] and by numerical experiments [32]. At the experimental substantiation of the statement it was found out that aromatic compounds, such as benzene, naphthalene, and anthracene experience decomposition under the effect of shock waves of rather weak intensities (*1.1 – 1.5 GPa* and *100 ÷ 200 °C*), the decomposition corresponding to the rupture of strong bonds of the benzene ring [38]. Under static conditions with the same pressure and temperature the benzene does not experience any chemical transformation at all [39].

The fact that complex polyatomic molecules are destructed within the front of shock waves has other experimental verification [38]. It was shown that trioxane shock wave polymerization process proceeds without any catalyst during the time of shock wave pulse. In this case under the action of shock waves of the same pressure but different pulse duration the same number of polymer chains forms but the chain's length becomes longer with increasing pulse duration. It means, first, that active particles originate within the front of shock waves due to the destruction of some trioxane molecules, and second, the active particles serve as nuclei of the polymerization process.

The above-mentioned surmise on the possible partial destruction of complex polyatomic explosive molecules within the detonation wave shock front was introduced to interpret the weak dependence of the detonation wave chemical spike time t_{CS} on the wave's pressure (Figure 3). In this case it was assumed after the GZND detonation theory founders that detonation reactions proceed in a similar way to thermal explosion. It is known that during the explosion induction period (activation stage time), which is the main part of the entire reaction time, only a small portion of the explosive decomposes but the reaction later becomes of an explosive nature. It follows from the theory that the activation-stage time of the explosion is a strong (exponential) function of the explosive state, and conversely,

the time for the final stages depends only weakly on the initial explosive state [40]. Taking into account the foregoing regularities and complex polyatomic molecules possible destruction within the front of shock waves an idea was introduced that the final stages of the explosive transformation process at detonation is only registered [12, 37]. If this is so, it means that the process activation stage does take place during the explosive's compression within the shock front. In other words it means the following: events that occur at normal pressure during the induction period of a thermal explosion at detonation proceed some orders of magnitude faster within the extremely narrow shock front zone.

Conclusion

It follows from the foregoing that according to available experimental data on the effect of shock waves of different intensities on organic molecular condensed explosives consisting of complex polyatomic molecules there exist such shock wave intensity P^* and the initial density $\rho_\circ^*$ typical for each explosive charge that at larger pressure and density explosives' decomposition proceeds through the homogeneous mechanism. In this case the experimental data on the time of explosives' transformation into detonation products (chemical spike time t_{CS}) does not depend on the structure of charges (initial density, size and structure of explosive particles, explosive state – liquid or solid, …) and they are scarcely affected by the pressure of their detonation waves. Nonequilibrium athermal destruction of some part of explosive molecules within the shock front of detonation waves was suggested to be responsible for the weak dependence of t_{CS} on detonation pressure. The destruction takes place for translational and vibrational degrees of freedom overheat within the shock front of detonation waves for a tremendous rate of explosive loading inside the shock discontinuity zone of the front. The overheat of translational and vibrational degrees of freedom of complex polyatomic molecules were substantiated by some experiments and computer simulations. As activation energy for the interaction of active particles, originated through the destruction, with explosive molecules is low ($5 \div 15$ kcal/mol [41]) the following transformation process proceeds extremely fast and is almost independent on the variation of explosive's state.

For the explosive charges of initial density smaller than their $\rho_\circ^*$ the transformation proceeds through the hot spots mechanism under the effect of shock waves of any intensity till up to their detonation pressure. The transformation process is fast and depends appreciably on the pressure of their detonation waves, although the dependence being not so strong as well.

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