

Correlation of Electrical Conductivity in the Detonation of Condensed Explosives with Their Carbon Content

N. P. Satonkina^a

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Abstract: This paper presents the comparative analysis of the results of more than fifty experiments on measuring the electrical conductivity of detonation products of RDX, HMX, PETN, TNT, and TATB-based explosives. It is revealed that there is a correlation between the electrical conductivity and the mass fraction of carbon both in the chemical spike and at the Chapman–Jouguet point.

Keywords: detonation, condensed explosives, chemical reaction zone, chemical spike, electrical conductivity, carbon nanostructures, conductivity grid.

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INTRODUCTION

Despite more than half a century of research, the nature of high electrical conductivity in the detonation of condensed explosives is not sufficiently clear, and there is still no universally accepted predictive hypothesis.

Hayes [1, 2] suggested that there was a correlation between the electrical maximum conductivity in the detonation and the free carbon content in the detonation products of explosives and proposed a contact conduction mechanism in carbon grids. The free carbon content at the Chapman–Jouguet (CJ) point was obtained numerically from the Becker–Kistiakowsky–Wilsion (BKW) equation, and the electrical conductivity was taken as maximum, though the question of a correlation between the electrical conductivity and detonation waves is still open.

The analysis of the experimental data carried out in this paper shows that the maximum electrical conductivity depends on the mass fraction of the total carbon and the free (condensed) carbon is related with the electrical conductivity at the CJ point.

EXPERIMENTAL RESULTS

The detonation wave comprises the shock front, the chemical spike region adjacent to it (the Neumann peak) where chemical reactions occur, and the Taylor unloading wave separated from the chemical spike by the CJ point, where the mass velocity of products is equal to the local speed of sound. According to the Zel’dovich–Neumann–Döring theory, the chemical reactions at the CJ point are completed.

A typical profile of electrical conductivity in the detonation of condensed explosives is shown in Fig. 1: it takes a few tens of nanoseconds for the electrical conductivity to reach the maximum value σ_{\max} , then it rapidly drops (σ_{CJ}) to the CJ point, which is followed by the region of smooth changes in the electrical conductivity in the Taylor wave. The comparison of the data from the literature shows that, in the presence of a peak extremely prominent in the electrical conductivity distribution, the duration of this peak is close to the length of the chemical reaction zone [3]. Much like in pressure profiles, the end of the chemical reaction zone is defined in Fig. 1 as an inflection point (the point of σ_{CJ}).

^aLavrentyev Institute of Hydrodynamics, Siberian Branch, Russian Academy of Sciences, Novosibirsk, 630090 Russia; snp@hydro.nsc.ru. Novosibirsk State University, Novosibirsk, 630090 Russia.

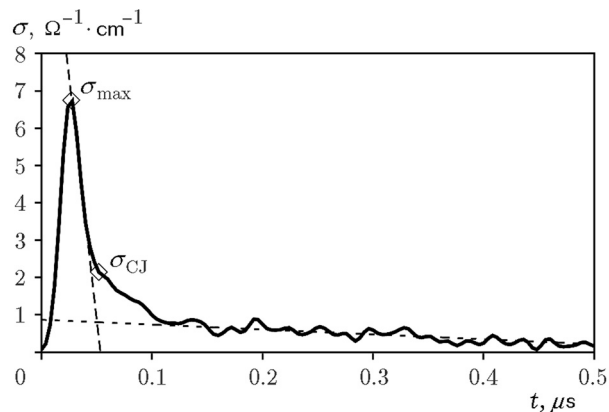


Fig. 1. Electrical conductivity profile of the HMX detonation products whose density is $\rho = 1.8 \text{ g/cm}^3$.

Currently, there is no theoretical justification for the correlation of electrical conductivity and pressure profiles, so let us discuss that relationship in more detail within the framework of the given hypothesis. For the explosives under consideration, the maximum value of the electrical conductivity in the region of the chemical spike σ_{\max} is always greater than the electrical conductivity at the CJ point σ_{CJ} [3], so we assume that σ_{\max} depends on the total carbon present in the chemical spike, which, by that time, forms carbon grids, and the value of σ_{CJ} may be correlated with the free carbon remaining after the chemical reactions. Thus, the formation of conductive carbon structures proceeds to the point σ_{\max} , and the main carbon oxidation reactions occur between σ_{\max} and σ_{CJ} . The reactions complete at the CJ point, the carbon grids become thinner and partially rupture, and the electrical conductivity $\sigma_{\text{CJ}} < \sigma_{\max}$ is provided by the remaining structures. A further decrease in the electrical conductivity is due to the fracture of part of the conductive branches in the dense medium of detonation products and to the possible transfer of some carbon to the nonconductive phase (diamond) in the unloading wave [4].

Table 1 shows the experimental data [3, 5–8] for a number of secondary explosives: RDX, HMX, PETN, TNT, and TATB-based explosives. The values were obtained in the experiments where steady detonation was implemented, with the bulk and maximum densities of the charge, and the values of σ_{\max} and σ_{CJ} were averaged according to the results of 2–5 experiments. The mass fraction of the condensed carbon r_{CJ} at the CJ point was calculated by means of interpolation of the data from [9] over the initial density.

Table 1 shows that, as the initial density of each explosive and, consequently, the carbon density increase,

Table 1

ρ , g/cm^3	σ_{\max} , $\Omega^{-1} \cdot \text{cm}^{-1}$	r_{CJ}	σ_{CJ} , $\Omega^{-1} \cdot \text{cm}^{-1}$	Source
RDX, $\text{C}_3\text{H}_6\text{N}_6\text{O}_6$				
1.15	1.8	0.040	0.4	[7]
1.72	5.0	0.078	1.65	[3]
HMX, $\text{C}_4\text{H}_8\text{N}_8\text{O}_8$				
1.30	2.8	0.058	0.7	[7]
1.79	6.7	0.079	2.0	[3]
PETN, $\text{C}_5\text{H}_8\text{N}_4\text{O}_{12}$				
1.05	0.6	0.0	0.2	[7]
1.73	9.4	0.033	1.6	[3]
TATB, $\text{C}_6\text{H}_6\text{N}_6\text{O}_6$				
1.78	19.1	0.208	10.0	[8]
TNT, $\text{C}_7\text{H}_5\text{N}_3\text{O}_6$				
1.04	15.0	0.217	8.9	[10]
1.57	95.2	0.267	26.8	[6]

Table 2

Explosive	ρ_c , g/cm^3	r_c	σ_c , $\Omega^{-1} \cdot \text{cm}^{-1}$
RDX	1.82	0.162	6.50
HMX	1.96	0.162	8.33
PETN	1.77	0.190	10.37
TATB	1.93	0.279	29.85
TNT	1.66	0.370	108.66

so do the values of σ_{\max} and σ_{CJ} . With an increase in the fraction of the condensed carbon r_{CJ} , the electrical conductivity at the CJ point σ_{CJ} increases.

As the initial density becomes more different from the maximum density, the related phenomena that complicate the interpretation of experimental data become more significant. The maximum conductivity (σ_c) was obtained in the detonation of samples of crystal density (ρ_c) by extrapolating the values σ_{\max} from [2, 3, 5–8, 10] over the maximum density. The results are shown in Table 2. With increasing mass fraction of carbon in the molecule r_c , the maximum electrical conductivity σ_c becomes greater.

It can be concluded from Tables 1 and 2 that there is a correlation between the mass fraction of carbon and electrical conductivity both in the chemical spike and at the CJ point.

The analysis of mixed explosives in the presence of a correlation between the fraction of carbon and electrical conductivity is much more complicated: the dispersion of mixed explosives plays a role at the molecular level without mixing. The effect of dispersion of the TNT–RDX mixture is discussed in detail in [11]. The same paper also touches upon the TNT–ammonium nitrate, but the results of that study were never published. Let us share one of these unpublished results. The TNT–ammonium nitrate explosive with a certain ratio of components has a zero oxygen balance, and it was possible to obtain a record-breaking minimum value of electrical conductivity of about $0.01 \Omega^{-1} \cdot \text{cm}^{-1}$ with the bulk density of the charge, which confirms the conclusion that carbon plays the key role.

DISCUSSION

The only paper discussing electrical conductivity as an indicator of the growth of carbon nanoparticles [12] was written with the use of plastic-bonded TATB, and an increase in the electrical conductivity was attributed to thermal ionization, which becomes greater with a temperature rise occurring due to merging of individual carbon particles. The presence of carbon structures was not considered in the paper.

The correlation of the maximum electrical conductivity and the content of total carbon is described in [13, 14] on the example of TNT. The estimates of the electrical conductivity of the heterogeneous medium on the percolation model showed that the carbon content is not sufficient to explain the maximum electrical conductivity $\sigma_{\max} = 250 \Omega^{-1} \cdot \text{cm}^{-1}$ obtained in these studies. It is suggested there are grids with almost metallic conductivity. This conductor could be carbon, whose mass fraction in TNT is 0.37, but the presence of spatial carbon structures in the reaction zone is also necessary.

Figure 2 taken from [14] shows summarized data [2, 3, 13–15] on the correlation of electrical conductivity and carbon density; the maximum electrical conductivity of detonation products (σ_1) in the chemical spike and the electrical conductivity outside the chemical reaction zone (σ_2) are given with the same density of the carbon condensed at the CJ point, which was calculated from the BKW equation [9]. There are two approximately parallel lines, each showing the effect of the initial density of explosives. The electrical conductivity of each explosive increases with growing density. But it is very difficult to find a universal law for all the given explosives in the chemical reaction zone and in the Taylor wave in Fig. 2. Meanwhile, the calculation of the carbon density in the detonation wave is associated with

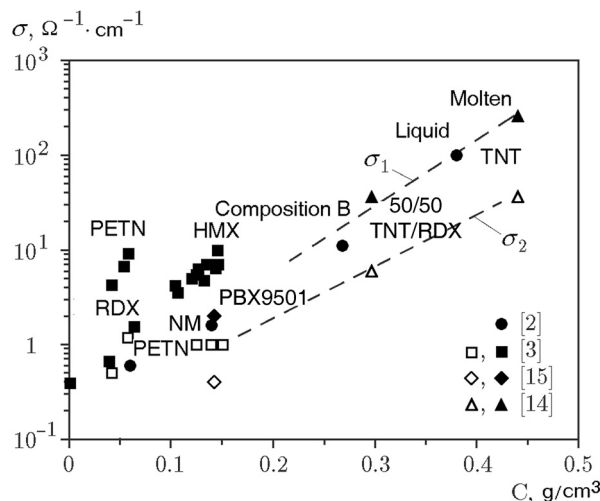


Fig. 2. Electrical conductivity in the chemical reaction zone (filled points and the line σ_1) and outside of it (open points and the line σ_2) depending on the solid carbon content in the detonation products calculated by the BKW equation (the figure is taken from [14]).

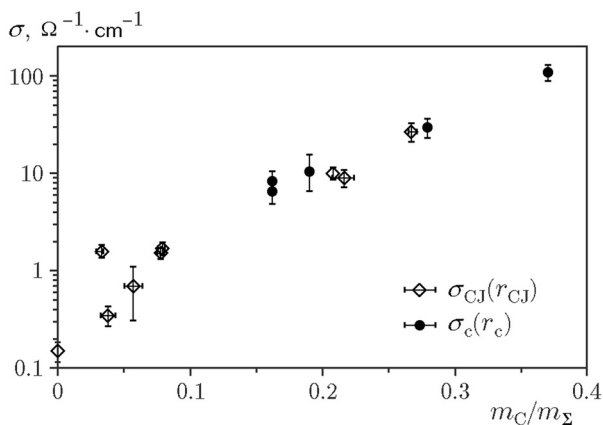


Fig. 3. Electrical conductivity at the CJ point (see Table 1) versus the mass fraction of condensed carbon and the maximum electrical conductivity versus (see Table 2) the mass fraction of carbon in the molecule with crystal density.

difficulties in the varying degrees of compression, which depends on the distance to the front, on the initial density, and the type of explosive.

Figure 3 shows the dependence of electrical conductivity at the CJ point (see Table 1) on the mass fraction of condensed carbon $\sigma_{\text{CJ}}(r_{\text{CJ}})$ and the dependence of the maximum electrical conductivity with crystal density (see Table 2) on the mass fraction of carbon in the molecule $\sigma_c(r_c)$. The values of both σ_c and σ_{CJ} have a

pronounced dependence on the fraction of carbon. The lines $\sigma_c(r_c)$ and $\sigma_{CJ}(r_{CJ})$ are arranged close to each other. The transition to the mass fraction of carbon, which is easy to calculate, helped finding the key role of this factor. A hypothesis about the dependence of the maximum value of σ_c on the total carbon shifted the line σ_1 shown in Fig. 2 along the horizontal axis, thereby making the dependence $\sigma(r)$ unique.

With a small fraction of carbon, the formation of related nanostructures becomes impossible due to the lack of a sufficient amount of conductive substance. For example, in [10], the numerical experiment revealed the limiting volume fraction of carbon equal to 0.07 at which the construction of holey grids in the detonation products is theoretically allowed. Given these data, it is possible to assume that, even if the fraction of carbon is lower than 0.07, the effect of carbon is still strong, and its mechanism may be related with, for example, highly conductive inclusions in a weakly conducting medium. In the detonation of PETN of bulk density, there is no condensed carbon. In this case, the electrical conductivity does not vanish, which makes it possible to determine its nature in the carbon-free products.

The problem of electrical conductivity is a multiparameter problem, and there is correlation between the electrical conductivity σ_{\max} and the pressure for HMX, RDX, and PETN, where density and temperature affect the situation as well. In the mass fraction of carbon–electrical conductivity coordinates, their effect vanishes.

When considering the impact of all the chemical elements contained in the explosive and all components of the detonation products on the maximum electrical conductivity and the electrical conductivity at the CJ point, we could only find the uniform correlation between the five explosives and carbon.

There are indirect data confirming the model proposed in this paper. Thus, Breusov [16] showed that the formation of ultrafine diamonds has nothing to do with the intermediate formation of free carbon and proposed the mechanism of the formation of nanodiamonds caused by partial rupture in the molecular bonds and the occurrence and growth of a carbon frame. In [17, 18], the data from the experiments with isotopes were used to conclude that carbon oxidation occurs after the formation of carbon particles and that carbon atoms quickly unite after the arrival of the detonation front.

Another argument in favor of the proposed model may be different detonation characteristics of the considered explosives, which does not prevent the dependence $\sigma(r)$ from being universal. It can be assumed that carbon is in the same conductive phase in the chemical spike and at the CJ point for all explosives considered.

It is stated in [4] that, for TNT, RDX, TNT–RDX alloy, and TATB, with the characteristic size of the ultrafine diamond, the parameters at the CJ point shift to the region of liquid nanocarbon and diamonds are formed from the liquid phase in the unloading wave by means of crystallization. In [19], the electrical conductivity of liquid carbon was obtained experimentally at detonation temperatures. Its value $\sigma \approx 10^3 \Omega^{-1} \cdot \text{cm}^{-1}$ explains the high values of σ_{\max} and σ_{CJ} observed in the experiment in the contact conductivity through carbon structures penetrating the inter-electrode space.

CONCLUSIONS

This paper describes the analysis of the results of experiments with condensed explosives over a wide range of mass fraction of carbon; from zero (at the CJ point for PETN of bulk density) to 0.37 (the fraction of carbon in the TNT molecule). There was found a correlation between the carbon content and electrical conductivity both in the chemical spike and at the CJ point. The high values of electrical conductivity are ensured by the contact conduction mechanism, which is carried out through current-conductive carbon nanostructures.

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