Dynamics of carbon nanostructures in the benzotrifuroxan detonation

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Abstract. The paper discuss the electrical conductivity in detonating benzotrifuroxan. The obtained data demonstrate that the primary carbon condensation takes less than several nanoseconds time.

1. Introduction
The mean particle size of detonation nanodiamonds (DND) extracted from condensed phase of the detonation products was found to be about 4 nm and is virtually independent of the explosive used [1–4]. One exception is DND produced by the detonation of benzotrifuroxan (BTF, C_6N_6O_6) [5], whose size may exceed 20 nm [6]. BTF is not the most carbon rich substance so this anomaly needs to be explained. Unusually high temperature corresponding to the liquid state of carbon was suggested as a factor promoting particles growth, but recent measurements [7] demonstrated detonation temperature which is by no means extraordinary. Alternative idea that the lack of hydrogen in BTF and hence in its detonation products may lead to formation of large particles was proposed in work [6].

Since the carbon released in the detonation wave is the cardinal factor affecting the electrical conductivity distribution [8, 9], the conductivity is an indicator of the carbon condensation behind the detonation front. According to work [10], the electrical conductivity profile in BTF is rather common. Nevertheless, the measurements showed certain features not observed in explosives studied before. The data allowed us to draw conclusions about the course of carbon condensation in detonating BTF.

2. Experimental
The scheme of measurements used in our experiments [11] is shown in figure 1. The measured charge resistance \( R(t) \) was shunted by the known resistance \( R_s \). The almost constant feeding current \( (I \approx 60 \, \text{A}) \) was supplied by discharge of the capacitor \( C \) (100 \, \mu\text{F} and 1 \, \text{kV}) through the ballast resistor \( r \). The shunt, which was made in the form of a folded band of constantan foil, was connected to the charge by a low-inductance, low-resistance line. The inductance of the circuit, which includes the shunt and the line, was determined in special experiments and was equal to \( L \approx 10 \, \text{nH} \). The parasitic parameters \( R_L \) and \( L \) are important in measurements of small resistances.
Figure 1. Experimental cell and the scheme of measurements.

Figure 2. (a) The record of the feeding voltage $V(t)$ at detonation of BTF with initial density $\rho = 1.09 \, \text{g/cm}^3$. (b) Experimental $V(t)$ for detonating BTF with initial density $\rho = 1.9 \, \text{g/cm}^3$ and approximation function $f(t)$.

The shunt voltage $U(t)$ was measured by a digital oscillograph. At first, the value of $U_0 = R_s I$ was recorded. After the electrodes was connected by the detonation wave, the voltage falls off.

The scheme of measuring cell is also shown in figure 1. The explosive fills the coaxial system of electrodes. An explosive charge with a diameter of $b = 8 \, \text{mm}$ was pressed into a thick copper case-electrode. The massive charge envelope was 6 cm long and its outer diameter was 4 cm. The detonation wave moves along the axis. When the wave arrives at the central electrode with diameter $a = 2 \, \text{mm}$, the conductance through the reactant appears and it changes while the wave moves with the detonation velocity $D$.

Typical records are shown in figure 2(a). Decrease of the feeding voltage $V$ is observed when the wave front reaches the central electrode. At 40 $\mu$s, detonation is over and the initial level of $V$ is restored.

3. Measurements in BTF

As stated above, the electrical conductivity profile in BTF [10] is similar to that measured in explosives of more common composition. Here we will focus on the peculiarity found for BTF, namely, the form of first change in $V(t)$ after the cell current is switched on.
Figure 3. The electric scheme of direct current \((I_0 = \text{const})\); the telegraph equation parameters have the following meanings: \(L_1 = 15 \text{ nH}, L_2 = 10 \text{ nH}\), wave impedance is \(R_W = 50 \text{ Ohm}\), specific inductance and capacitance are equal \(L_W \text{ nH/m}\) and \(C_W = 100 \text{ pF/m}\), respectively.

In all shots with dense BTF at the moment when the cell becomes conductive, i.e., when \(V(t)\) voltage should be reduced, strong high frequency oscillations were observed. An example of this behavior one can see in figure 2(b) after \(t = 31.8 \mu s\). The period of the oscillations did not depend on charge density.

The experimental \(V(t)\) record shown in figure 2(b) can be approximated by the function

\[
f(t) = \varsigma + \iota \exp\left(-\frac{t - \eta}{\zeta}\right) \cos(\kappa t),
\]

where \(\varsigma = 8.56 \text{ V}, \iota = 2.5 \text{ V}, \eta = 31.8 \mu s, \zeta = 0.03 \mu s, \kappa = 1000 \mu s^{-1}\). Function \(f(t)\) is also plotted in figure 2(b). The oscillations are produced by the parasite elements in the measuring circuit. The shunt \(R_s\) cannot be placed too close to the charge because, if the shunt were destroyed, high voltage may damage the oscilloscope input. So, the shunt was connected to the cell by either short length of coaxial cable or by flat line about 20 cm long. This connection has noticeable capacity, and the connection contours, though small, introduce parasite inductances. Thus fast oscillations may take place when the cell current starts. The frequency of oscillations \(\omega \approx 1 \text{ GHz}\) corresponds to the contour whose inductance is 50 nH and capacity is 20 pF. Such values seem to be quite reasonable estimates for the connections used in the experiments.

For effective excitation of oscillations, the characteristic time of the circuit closure must be comparable to the oscillation period or even less. Thus the presence of strong oscillations means that the rise time of the conductivity behind the detonation front in dense BTF is several nanoseconds or less (which means about 50 \(\mu m\) or lesser spacing).

Note that the oscillations fade out after first 100 ns. So they do not affect the measurements of the conductivity peak, starting about 2 \(\mu s\) later on. Since the spatial resolution was about 150 \(\mu m\), the fast rise of the conductivity could not be observed within the peak. Surprisingly, the parasite parameters usually considered as drawback of the measuring scheme revealed the steep conductivity front which is not detected by the regular procedure.

4. Modeling of the circuit

To confirm the reasoning presented above, the processes in the scheme shown in figure 3 were simulated. The circuit equations in feeding end (left side) and conductivity cell (right side) were bound by the telegraph equations in the connecting line. The cell resistance was set as

\[
R(t) = \frac{1}{1 - \exp(-t/\tau)}
\]
and the switching-on time $\tau$ was varied from 30 to 1 ns. All values are either natural or the reasonable estimates of the parasite parameters. Simulation results shown in figure 4 confirm that high amplitude of oscillations is observed at short $\tau$. Apart of main period (about 4 ns), the faster fluctuations are seen produced by the wave reflection at the ends of the transmission line. The oscillations fade out almost completely after 100 ns. The model, though quite simple, produces qualitative agreement with the experiment.

5. Conclusions
An analysis of peculiar oscillations accompanying the electrical conductivity measurements in the pressed benzotrifuroxan allowed us to estimate the rise time of the conductivity behind the detonation wave front. This time cannot exceed several ns, and the spatial distance between the wave front and high conductivity region is 50 $\mu$m or less. BTF differs from common explosives by unusually large carbon particles produced in its detonation. Since the condensed carbon is known as an important factor providing high electrical conductivity in detonation waves, these two anomalies seem to be closely related. Both can be explained by absence of hydrogen in the BTF molecule. The hydrogen atoms or molecules sticking to the surface of carbon clusters may slow down the growth of particles in the common explosives. As a result, the free carbon release should be obstructed as well as formation of the conducting net. In the reaction zone of BTF, without hydrogen, the carbon particles connect freely and grow faster, thus large particles are produced, capable to form the conducting net within shorter time.

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