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This compendium is devoted to investigations in the fields of physics of high energy densities and thermophysics of extreme states of matter. Interaction of intense laser, x-ray and microwave radiation, powerful particle beams with matter, techniques of intense energy fluxes generation, physics of shock and detonation waves, experimental methods of diagnostics of ultrafast processes, different models and results of theoretical calculations of equations of state of matter at high pressures and temperatures, low-temperature plasma physics, issues of physics and power engineering, as well as technology projects are considered. The majority of the works has been presented at the XXVI International Conference on Interaction of Intense Energy Fluxes with Matter (March 1–6, 2011, Elbrus, Kabardino-Balkaria, Russia). The edition is intended for specialists in physical and technical problems of power engineering.

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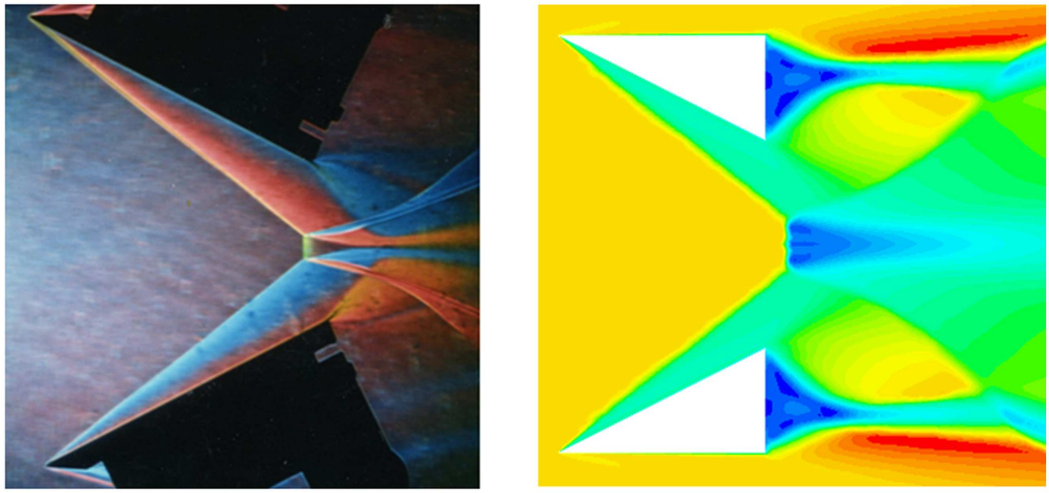

a) b)

Figure 7. Shlieren picture (a) and numerical solution (b) of three shock configuration in air, vertex angle of wedge equals 27 deg.. Mach number equals 5.

experimental data. Good agreement between numerical and experimental results gives the right to use this method for the future studies of new forms of triple shock configuration.

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NET ELECTRIC CONDUCTION OF DETONATION PRODUCTS OF CONDENSED EXPLOSIVES

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Abstract. The model of conductivity of detonation products (DP) of condensed explosives having negative oxygen balance is presented in the paper. The model is based on the formation of the space conductive net of the condensed free carbon in the DP. The molecular dynamics (MD) method was applied to the two-component mixture of DP and carbon atoms. It is shown the free carbon atoms to aggregate into the connected space net. The conductivity of DP was calculated using these data. The good enough agreement was revealed between the results of the model proposed and the well-known experimental data.

Introduction. There is no satisfactory explanation of extremely high conductivity σ of DP of many condensed explosives. The main factors influencing the value of the conductivity were indicated in one of the first russian works in this field [1]. The conductivity increases with the volume energy density of explosive. The effect of the temperature, the pressure and the mass density was studied for different explosives at various initial conditions. The attempt to distinguish the influence of each of these factors was not successful because of the complicated relations between them.

The detailed analysis of the models of the DP conductivities were made in [2]. The evaluations obtained there can hardly explain the high experimental values of σ.

The explosives having the carbon-rich DP are of special interest. The relation between detonation wave parameters and the conductivity value for them is not so clear as for other explosives. For example, the DP of TNT that has middle detonation parameters have the conductivity $\sigma \sim 100$ Ohm^{-1}cm^{-1}.

The authors of [2–4] have proposed earlier that charge transfer is possible in connected structures formed by aggregated carbon particles in the DP of carbon-rich solid explosives. There were neither theoretical nor experimental proofs of this idea.

The authors of [5] studied the DP retained after explosion. They revealed not only the separated particles of the condensed carbon of sizes from 2 to 6 nm but the clusters of low density of the size of several tens of nanometers consisting of these particles. The clusters have non compact porous structure with fractal dimension of about 2.

The method of molecular dynamics was first applied to study the condensation of the carbon to particles and structures in [6, 7]. The authors of this work simulated the formation of separated carbon particles and formulated a simple and good enough model. But they

could not simulate the growth of connected space net of carbon because of lack of the available computational capabilities.

Thus, the model of net conductivity of DP was proposed and discussed earlier by several author but there were neither numerical nor experimental confirmation does the concentration of free carbon be enough to form conductive nets in DP.

In the present work, we used high-end computational capabilities [8] and demonstrated the possibility of formation of carbon nets in DP for the first time. We calculated also the electric conductivity of these nets for the first time. The model of DP conductivity proposed allows to explain the large values of σ for the low concentrations of free carbon in contrast with the percolation model proposed earlier by other authors.

Molecular dynamics simulation. The dynamics of the ensemble consisting of the two sorts of the particles (atoms) was studied. The particles of the sort C represented the atoms of the free carbon whereas the P-sort particles were the detonation products. Pair interactions between particles of the same sort and between particles of different sorts were simulated with Lennard-Jones potential

$$U(r) = 4\varepsilon \left(\left(\frac{b}{r}\right)^{12} - \left(\frac{b}{r}\right)^{6} \right).$$

All the "atoms" had the same mass of 20 u. that corresponded to the average weight of DP molecule approximately. The parameters of Lennard-Jones potential for different pairs of atoms were $\varepsilon_{CC} = 2$ eV, $\varepsilon_{PP} = 0.01\varepsilon_{CC}$, and $\varepsilon_{CP} = 0.1\varepsilon_{CC}$. The value of b characterizing the atom size was considered to be equal to $2.7 \cdot 10^{-10}$ m

The value of the parameter ε_{CC} was taken so that obtain the reasonable agreement between parameters of the melting point for the MD-ensemble in the calculations and the carbon in experiments. The phase composition of the condensed carbon was not taken into account in the model. The condensed carbon was considered to be the graphite.

All the other parameters that characterize mainly the DP were chosen so as to fit the calculated pressure, the temperature and the density to the reasonable parameters behind the detonation wave $\rho = 2.5$ g/cc, $p = 20$ GPa, $T = 3000$ K.

MD-calculations were performed in the region of sizes 20 nm × 20 nm × 20 nm. The total number of particles was 512000.

The simulations started from the initial state with the fixed temperature and pressure and the approximately homogeneous distribution of the atoms in the region.

The simulations were carried out for the values of the volume fraction of the carbon atoms from 2 to 40 percents. The carbon atoms aggregated to the dense particles with linear sizes of the several atomic diameters in all the cases. The characteristic size of the particles changes with the parameters of the phase equilibrium of liquid carbon – solid graphite at the significant contribution of the surface energy of the particle into its total energy. At such a condition small particles coalesce into a big particle and lose their individuality. The small particles can be considered liquid drops. The big particles are also combined together but without loss of the individuality. We can consider the big particles of size of $d \approx 3$ nm and more to be mechanically strong. They are found in the DP retained after explosion.

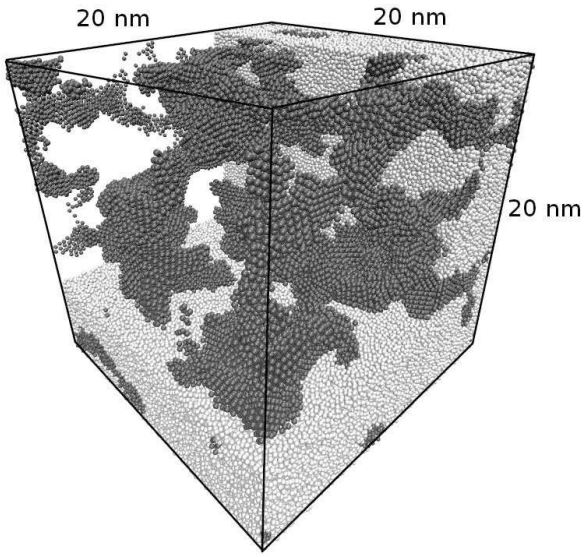

Figure 1. Simulation of the carbon condensation in DP. The light balls are the DP molecules, the dark balls are the carbon atoms. The volume fraction of the carbon atoms was 10 percents. Only the carbon component is shown in the part of the simulation region for clarity.

The formed carbon particles continue coalescing and are combined into branched clusters if the carbon volume fraction is not less than 7 percents. The concentration of the particles is low in the clusters. The cluster spatial structure is rarefied and has large sizes at the small mass. The clusters aggregate forming the spatial nets that can conduct electric current (fig. 1).

The carbon particles moving slowly are also combined into clusters with the linear size of about ~ 10 atomic diameters if the carbon volume fraction is less than 7 percents. The further growth gets slower and takes from tens to hundreds nanoseconds. The separate clusters that have no contact each other are observed in the MD simulations. They give no contributions to the conductivity of the DP.

The model of formation of conducting nets and conductivity. The carbon particles arising in the DP aggregate to sparse clusters with the large volume of pores between particles. Combining with their neighbors, a cluster grows in the sizes with the branches form retaining approximately the same. The process is completed in one of the two possible states depending on the cluster size. If the size of the cluster is large enough the fluctuating forces of the DP bend and break the branches of the cluster that restricts its final size. In the other case, the clusters make contact and form the conducting net.

The clusters have the geometry of fractals that is the total quantity of the particles in a cluster (N) increases

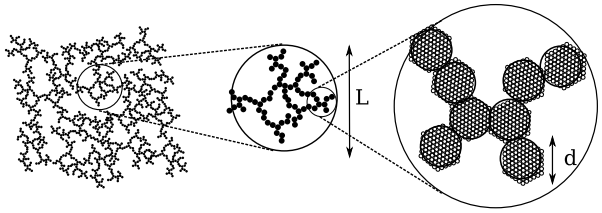

Figure 2. The pattern of a conducting carbon net at various scales.

slowly than its maximal size (L^3) 2. One can estimate the number of the particles as follows $N \sim (L/d)^n$, here n is the fractal dimension of the cluster. The value of n seems to be close to 2.

If the mechanical strength of the clusters is high enough they grow until reach their neighbors and form the net penetrating the DP. The average density of the carbon atoms is low because of the high porosity of the clusters.

The characteristic size of the clusters forming the conductive net is a significant parameter of the model. One can evaluate this parameter taking the value of volume fraction of free carbon and the relation

$$\frac{V_C}{V_0} = \frac{d^3 N}{L^3} = \left(\frac{d}{L}\right)^3 \left(\frac{L}{d}\right)^n = \left(\frac{d}{L}\right)^{3-n}. \quad (1)$$

The volume fraction of free carbon in the DP is $V_C/V_0 \sim 10\%$ and the power $3 - n \approx 1$. Then, the characteristic size of the clusters is of the order of 10 atomic sizes. This is in agreement with the our results of the MD simulation.

The model of the connected carbon nets in the DP gives the dependence of the DP conductivity on the volume fraction of the carbon atoms in the form $\sigma = \sigma_0 (V_C/V_0)^\gamma$, where σ_0 is the conductivity of compact graphite and the γ value is close to 2.

Calculation of conductivity of carbon nets. The conductivity of the carbon nets obtained in the MD simulations was calculated using the following model. Let's consider a cubic lattice consisting of M^3 nodes. The bonds of the lattice that connect neighbor nodes can be conductors or isolators. The region of MD simulation of carbon condensation was projected onto this spatial lattice. The distance between the lattice nodes was chosen so that the size of the lattice matches the size of the region of the MD simulations. The each atom of a carbon cluster is considered to occupy a spherical region of the diameter of b. Those nodes that are covered by one of the atom of the carbon cluster are considered to be the part of a conducting structure. The six lattice bonds connected with this node get conductive with conductivity of compact graphite σ_0.

The accuracy of this approximation influences significantly on the calculated values of the cluster conductivity. If the lattice is rough (distance between its nodes is much more than the atomic size) we will obtain overestimated values of the conductivity. If the lattice step is too small the calculations becomes impossible for lack of the computational capabilities. Thus, we took the lattice step not more than 2-3 times larger than the atomic diameter.

Table 1. Calculated values of carbon net conductivity.

V_C/V_0%	10	12	15	20	30	40
$<\sigma>/\sigma_0$	0.0093	0.020	0.037	0.059	0.119	0.198

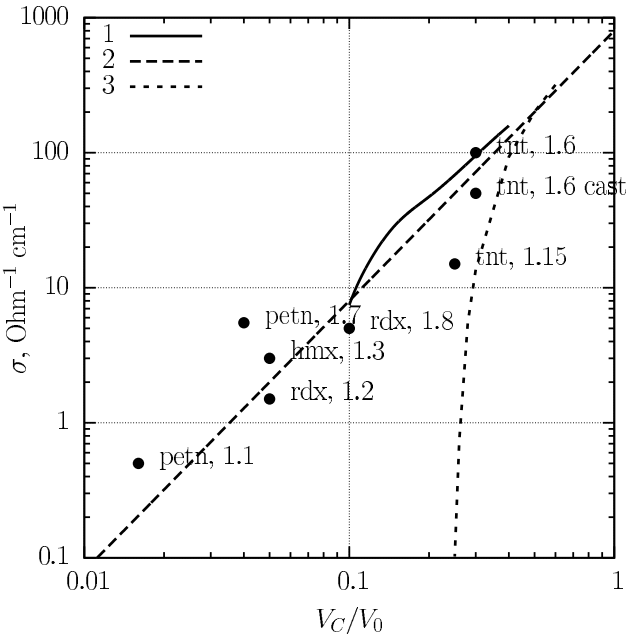

Figure 3. Electrical conductivity of detonation products. 1—electrical conductivity of carbon nets simulated usind MD, 2—$\sigma_0(V_C/V_0)^2$, 3—percolation model, points are the experimental data for different HE.

The equations of electrodynamics in the stationary case was used for calculating electric current in the carbon cluster. The Ohm's law was used to obtain the value of the DP conductivity. One of the side of the cubic lattice was considered to be an anode with the electric potential $\varphi = 1$, the opposite side was the cathode with $\varphi = 0$. Periodic boundary condition was applied on the other sides. A system of finite-difference equations with respect to the electric potential was solved using the method of simple iterations. The accuracy of the calculations of the total current was better than 10^{-5}.

The conducting nets obtained with the MD simulations are irregular since they grew under non-equilibrium conditions. The conductivity of a net depends on the direction of current flowing through the net. We calculated the values of the conductivity in x, y, and z directions and took the average value as estimation of the net conductivity. The calculated data of the conductivity are shown in the table 1.

Let's accept the value of the electrical conductivity of carbon $\sigma_0 = 800$ Ohm^{-1} cm^{-1} (compact graphite) and compare the results of the calculations of the electrical conductivity of the conductive nets with the electrical conductivity of DP of condensed explosives measured in the experiment. Figure 3 gives the experimental and theoretical values of conductivity for all the cases, depending on the volume fraction of carbon.

Resume. Condensation of carbon in the detonation products to clusters and spatial nets was simulated using molecular dynamics method.

The electrical conductivity of the resulting carbon nets was calculated for different volume carbon concentrations.

It is shown that the formation of the carbon nets is a mechanism that can really explain the high values of conductivity in the zone of the detonation of condensed explosives.

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INVESTIGATION OF DETONATION WAVE STRUCTURE IN EMULSION HIGH EXPLOSIVES

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Emulsion high explosives (emulsion HE, EHE) are widely used in practice, but the process of EHE detonation is still not sufficiently studied. In particular, the influence of macrokinetics of chemical reaction in EHE on its critical diameter of detonation and other detonation properties is not clarified yet. At the same time, radiographic study of matter using high energy charged particle beams provides a unique opportunity for obtaining absolute information about spatial distribution of density in optically non-transparent objects in ultra-fast dynamic experiments. Also one of the important features of this method is its multi-frame imaging capability in a pulse mode, which gives an opportunity to measure in the same experiment the dynamic and macrokinetic parameters of shock and detonation waves, such as their spatial structure, wave and particle velocities.

Therefore the investigation of detonation waves in EHE charges of different diameters was conducted at proton radiography facility at ITEP-TWAC accelerator [1].

The energy of the proton beam at the facility was 800 MeV, its intensity was about 10^{10} particles per pulse that consisted of 3-4 consequent 70±5 ns long bunches with 250±15 ns intervals between them. The images were taken by CCD cameras, where each of them was synchronized with a single consecutive proton beam bunch. It allowed to register up to three proton radiographic images of a dynamic target in a single experiment. The spatial resolution of the facility that was measured in static conditions was about 50 to 100 μm in different experiments.

Investigated EHE was made from the emulsion matrix that consisted of 92.2% of ammonium nitrate as an oxidant, 6.6% of diesel oil as a fuel and 1.2% of emulgator. It was then sensitized by 3 wt.% of hollow glass microballoons. Density of prepared EHE was 1.07 g/cc. Charges in polyethylene shells with internal diameter of 15 mm and 20 mm were used. The length of charges was about 75-80 mm. Detonation in all the experiments was initiated by a small active HE charge.

Preliminary investigation of detonation wave structure in EHE was held with the VISAR laser interferometer. Experimental results are presented in Fig. 1 in the form of particle velocity profiles of thin aluminum foil that borders with detonation products.

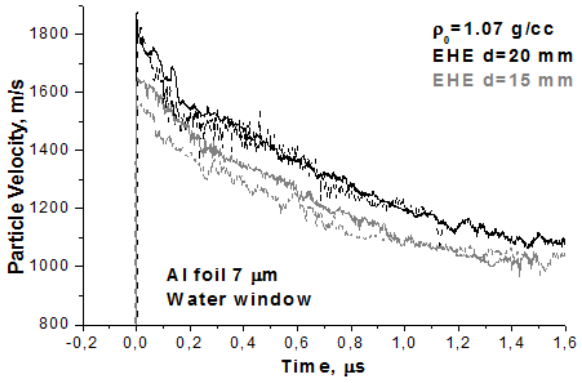

Figure 1. Particle velocity profiles of 7 μm Al foil situated between an explosive charge and a water window obtained in VISAR experiments with EHE. Grey profiles are for 15 mm diameter charges; black profiles are for 20 mm diameter charges.

Particle velocity profiles for 20 mm charges showed good reproducibility. They have similar reaction zone structure: behind a shock wave front there is a region of a rapid decline of particle velocity that lasts about 0.2 μs. It is then followed by a long zone of slower de-