Analitical criteria of homogeneous and heterogeneous detonation of liquid energetic materials

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Abstract. *Statistical theory of liquids is used to investigate mechanism of detonation initiation on fronts of flat shock waves in homogeneous liquid and in liquid containing spherical nanopores. We calculated thermodynamic parameters of liquid methane sufficient for shock dissociation of molecules at a front of a shock wave. Calculations of the average single-particle force potential show that at high pressures and temperatures atoms and molecules get emitted from the surface into a nanopore with hyper-thermal speeds. Implosion of spherically symmetric stream of molecules may lead to destruction of the molecules at impact. We explained existence of top and bottom bounds for pressure during detonation initiation in heterogeneous energetic materials. In terms of pair interaction potentials and correlation functions there are formulated criteria for boundary values of thermodynamic parameters which are required for initiation of homogeneous and heterogeneous detonations based on the 'hot spots' mechanism.*

Keywords*: Mechanism of detonation initiation, hot spots, nanopores, emission of atoms and molecules, shock dissociation of molecules.*

1. Introduction

Microscopic nature of detonation mechanism for condensed energetic materials (CEM) remains unknown mostly because of lack in understanding of elementary processes leading to initiation of detonation. Modern theory of detonation is based on papers of D.L. Chapman, E. Jouguet (CJ) and Y.B. Zeldovich, J. von Neuman and W. Döring (ZND) [1]. Within the framework of the CJ theory detonation is represented by a shock wave with chemical reaction at the front. The CJ theory does not take into account kinetics of chemical reactions. Width of a chemical reaction zone is considered to be equal to the thickness of shock wave front. In ZND theory structure of a detonation wave, with finite width of chemical reaction zone, was taken into account [1]. The ZND theory had explained the basic experimental facts. However some data is impossible to interpret within the framework of ZND theory, in particular, the experimental results related to detonation of heterogeneous CEM.

An extended analysis of difficulties in application of ZND theory to the CEM is given in works [2,3]. In [2] the author investigates experimental facts that do not comply with ZND, and offers a new kinetic approach for the detonation theory. According to this work, initiation of explosive reaction by a shock wave is controlled by generation of free atoms, radicals and ions at shock wave front, and by subsequent development of reactions in the 'hot spots'. High kinetic energy of particles at the shock wave front which would be sufficient for shocking rupture of molecular bonds is also a necessary condition. Majority of molecules at the front of a shock wave dissociates into atoms, radicals, molecular fragments and ions. These particles will subsequently react within the times of the order of (10^{-14} – 10^{-12}) s and will release energy required for detonation support. Some experimental observations contradicting to ZND theory are discussed in the papers [3]. Analysis of experimental data on detonation initiation in CEM shows existence in a shock wave of characteristic pressure p^* and initial charge density ρ_0^* typical for each charge, so that at large values of pressure and density in CEM there takes place the homogeneous mechanism of decomposition [4]. The 'hot spot' mechanism for different materials appears in pressure range of (30 – 200) kbar. At pressure 300 kbar there dominates the mechanism of homogeneous detonation. At intermediate values of pressure of (200 – 300) kbar the mixture of heterogeneous

and homogeneous mechanisms of CEM decomposition and detonation initiation is realized.
Direct experimental proof of rupture of all bonds in a molecule of homogeneous *BTNEA* inside the detonation wave was obtained in work [5]. There were used labeled radioactive isotopes ^{13}C and ^{18}O which were built into the *BTNEA* molecules at certain places and which formed $C^* = O^*$ pairs. The products of reaction were expected to have the isotope labels in compounds of *CO* and CO_2 since the molecules contain these groups of atoms as their fragments. The detonation products were tested on the presence of the labels. Analyses showed that ratio $^{12}C/^{13}C$ and $^{16}O/^{18}O$ were identical for all of the detonation products and were equal to the same ratio in non-detonated *BTNEA* molecules. It is possible only in case when all bonds inside the molecule have been broken and atoms are statistically mixed [2,5]. Thus, the experimental results of work [5] showed existence of the high-energetic mechanism that operates inside the detonation wave, providing the dissociation of molecules.
It is impossible to explain initiation of detonation in heterogeneous CEM, by means of rise in temperature inside the compressed substance, since the initiation occurs under conditions which are insufficient for excitation of a fast reaction inside the volume. The idea about local heating of CEM at initiation of detonation by a shock wave had been offered in [6]. The size of a local nucleation center of detonation according to [7] is about $(10^{-5} – 10^{-7})$ m.
There exists a number of models with possible mechanisms of detonation initiation in the condensed energetic materials. We will list the models that use the 'hot spots' detonation initiation mechanism:

a) 'Hot spots' are generated due to adiabatic compression of tiny pores, friction of solid surfaces or viscous heating [8,9].;
b) In the jet model of detonation mechanism there is postulated existence of penetration of detonation products into CEM in the form of separate streams [10,11]. Presence of pores promotes penetration of CEM and subdivision of streams.;
c) The molecular-dynamic simulations of shock wave interaction with defects inside a two-dimensional crystal showed generation of liquid-like areas [12]. Probably these areas are places of initial chemical reaction.;
d) In the work [13] there was proposed an electric mechanism of 'hot spots' formation.

During shock wave propagation inside the dielectric CEM there is generated an electric field that can lead to the local electric breakdown. The breakdown channel can be identified with 'hot spot'. Despite of the offered mechanisms of detonation initiation in heterogeneous CEM the problem as a whole remains unsolved. Difficulties in experimental investigation of the 'hot spots' mechanism are caused by the necessity to work with physical and chemical processes on the time scales of the ordered of picoseconds, nanometer spatial resolutions and mesoscopic scales. Only direct experiments can show preference of certain mechanisms or models over the others.
The method of the Bogolyubov-Born-Green-Kirkwood-Yvon kinetic equations (BBGKY) in statistical physics has no restrictions for the gradients values of thermodynamic functions and at microscopic level considers kinetics of condensed systems [14]. The BBGKY hierarchy takes into account all interparticle interactions and dynamic interparticle correlations of all ranks. Therefore, the method of the BBGKY kinetic equations can be applied to the problems of physical and chemical kinetics of detonation phenomena in homogeneous and heterogeneous CEM. Previously, to analyze the mechanism of sonoluminescence in liquids, we had used the first equation of BBGKY chain of equations for a non-uniform liquid and calculated the one-particle potential of average forces acting on separate molecules of this liquid [15]. In the present paper we use the approach developed in [15] to analyze the 'hot spots' mechanism during detonation initiation in CEM.

2. Dissociation of molecules at a front of flat shock wave inside a liquid

Let's consider the first equation of BBGKY hierarchy to analyze distribution of the one-particle potential of average force that acts on separate molecules near a shock wave front. In a solid CEM under the influence of a shock wave there occurs fluidization of substance structures at molecular level. Pair intermolecular interactions can be described by means of spherical symmetric potential. Hamiltonian of a non-uniform molecular liquid is a sum of its kinetic and potential energies

$$H = \sum_{i=1}^{N} \frac{\mathbf{P}_i^2}{2M} + \frac{1}{2} \sum_{i \neq j=1}^{N} \Phi\left(\mathbf{R}_i - \mathbf{R}_j\right), \tag{1}$$

where N is number of molecules; $\mathbf{P}_i$, M are momentum and mass of a molecule; $\Phi(\mathbf{R})$ is interaction energy of two molecules.

Taking into account flat geometry of the problem (the shock wave front is parallel to the plane $z = 0$) the first equation in a BBGKY chain of equations for the unary distribution function of molecules $F_1(z)$ in a non-uniform liquid will have the following form

$$k_B T \frac{\partial}{\partial z} F_1(z) + \frac{1}{v_0} \int d^3 R_1 F_2\left(z, z_1, \rho^{\|}\right) \frac{\partial}{\partial z} \Phi\left(z, z_1, \rho^{\|}\right) = 0, \tag{2}$$

where k_B, T are the Boltzman constant and temperature; v_0 is volume per one molecule; $F_2(z, z_1, \rho^{\|})$ is a pair distribution function of molecules in a non-uniform liquid; $\rho^{\|} = |\mathbf{R} - \mathbf{R}_1|$ is the component of vector difference, parallel to the plane $z = 0$. We represent the pair distribution function $F_2(z, z_1, \rho^{\|})$ using the pair correlation function $g(z, z_1, \rho^{\|})$

$$F_2(z, z_1, \rho^{\|}) = F_1(z)\, F_1(z_1)\, g(z, z_1, \rho^{\|}) \tag{3}$$

and the equation (2) can be rewritten now in the equivalent integral form

$$F_1(z) = \exp[-U(z)/k_B T], \tag{4}$$

$$U(z) = -\frac{1}{v_0} \int_{-\infty}^{z} dz_1 \int d^3 R_2 F_1(z_2) g\left(z_1, z_2, \rho_{12}^{\|}\right) \frac{\partial \Phi(R_{12})}{\partial R_{12}} \frac{z_2 - z_1}{R_{12}}. \tag{5}$$

Thus, the potential $U(z)$ has meaning of an one-particle self-consistent potential of average force in Boltzman distribution.

We can use the expression for the one-particle potential of average force (5) to model this potential in a near-surface layer of the shock-compressed liquid. To be able to do this, we need to know analytical expressions for the unary distribution function and for the pair correlation function. Thus we will use Fowler's approximation of the unary distribution function and the pair correlation function in a semi-bounded liquid [15,16]

$$F_1(z) = \Theta(z), \;\; g\left(z_1, z_2, \rho_{12}^{\|}\right) = g_0\left(|\mathbf{R}_{12}|\right), \;\; \Theta(z) = \begin{cases} 1, z \geq 0, \\ 0, z < 0, \end{cases} \tag{6}$$

where $g_0(R_{12})$ is the pair correlation function of homogeneous liquid; $\Theta(z)$ is Heaviside step function. Using this approximation we can derive the work function of molecules from a semi-bounded liquid in vacuum [15]

$$A_{l-v} = \frac{4\pi}{3 v_0} \int_0^{\infty} dR \frac{\partial \Phi}{\partial R} g_0(R) R^3. \tag{7}$$

Using the expression for the work function from liquid into vacuum we can rewrite the generalized equation of state for homogeneous liquid with interaction of molecular central forces in terms of this work function

$$p = n(k_B T - A_{l-v}/2), \tag{8}$$

here p, n, T are pressure, density of number of molecules and temperature of the liquid, correspondingly.

Numerical calculations of one-particle average force potential in the shock-compressed methane were performed using the Lennard-Jones potential

$$\Phi(R) = 4\varepsilon[(\sigma/R)^{12} - (\sigma/R)^{6})], \tag{9}$$

with parametres ε = 144 K and σ = 3.796Å [17] and the pair distribution function in the form of Weeks-

Chandler-Andersen (WCA) approximation [18]. Fig.1 shows distribution of the one-particle potential of average force $U(z)$ near the surface of methane with the Fowler's step function density profile. Width of the layer where we observe sudden jump of potential $U(z)$ is of the order of 5Å. As we can see from the Fig.1 the one-particle potential of average force is repulsive and, as a result, the surface is unstable with respect to emission of separate molecules. The near-surface layer, where we observe the jump of potential $U(z)$ plays a role of 'accelerator' for the emitted molecules.

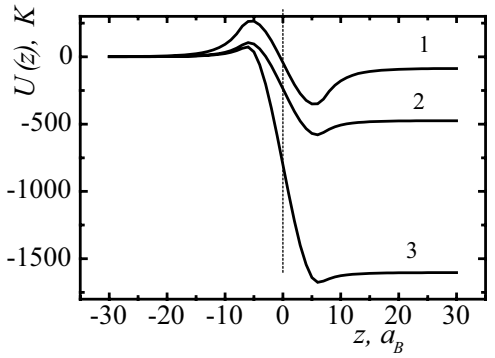

Fig. 1. Results of calculations for the one-particle potential $U(z)$ for methane in Fowler's approximation: – for the curve 1: $T = 108.28$ K, $v = 2.208$ dm^3kg^{-1}, – for the curve 2: $T = 687.68$ K, $v = 6.161$ dm^3kg^{-1}, – for the curve 3: $T = 2404$ K, $v = 8.6$ dm^3kg^{-1}

The structure of a detonation wave is investigated experimentally [9]. The front of a detonation wave has a zone of heightened pressure and density, the so-called 'chemical spike'. Behind the 'chemical spike' is a chemical reactions zone, where intensive chemical reactions take place and detonation products are produced. At the front of the detonation wave there takes place dissociation of CEM molecules, which is a necessary condition of the subsequent chemical reactions. The dissociation process has physical nature. At the front of the detonation wave the molecules accelerate to the velocities sufficient for shock-dissociation and movement of the front itself. Values of the molecules dissociation energy are much higher than values of their thermal energy. In our model, forces that accelerate the molecules at the front of a detonation wave, are defined by the potential of average force which has a one-particle and short-range nature, however it originates from the pair intermolecular interactions and correlations.

To establish the compression conditions required to accelerate the molecules at the front of a shock wave up to the values of impact dissociation initiation, we calculated the work function A_{l-v} for semi-bounded liquid methane along the maximum compression line (see Fig. 2.).

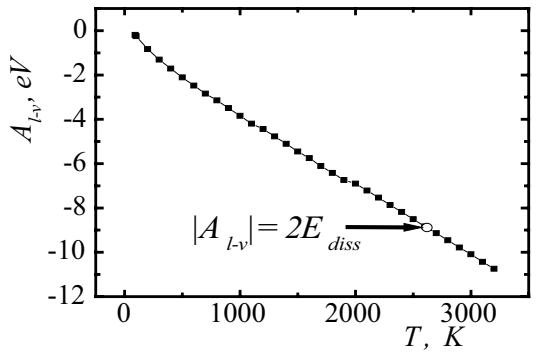

Fig. 2. The work function A_{l-v} along the maximum compression line. Temperature varies within the range of [91; 3200] K

As we can see in the near-surface layer due to the field $U(z)$ the molecules have possibility to accelerate and as a result potential energy will be transformed into kinetic one. The minimal kinetic energy required for dissociation during collision of the two molecules will be twice the value of dissociation energy. The arrow on Fig.2 shows the point where the equality $|A_{l-v}| = 2E_{diss}$ holds true, and E_{diss} is the dissociation energy of methane molecules in the $CH_4 \rightarrow CH_3 + H$ bond rupture scheme (4,4 *eV*). Thermodynamic parameters at this point have the following values: temperature $T = 2620$ *K*, specific volume $v = 1.165$ dm^3kg^{-1}, pressure $p = 241024$ *bar* and the speed of emitted molecules $V = 10336$ $m{\cdot}s^{-1}$.

The performed estimations for the parameters of semi-bounded liquid methane correspond to a process of homogeneous dissociation initiation of molecules. According to the experiment, accounting for the temperature effects at the front of 'initiating' shock wave in CEM is not sufficient for initiation of detonation. Our calculations show high sensitivity to density and to potential energy of the system at initiation of chemical reactions during detonation. The liquid CEM fits the best for the mechanism of homogeneous detonation. For example, detonation initiation in nitromethane is accompanied with appearance of a 'superfast' wave. Pressure at the front of this wave reaches up to 250000 *bar* [9]. Width of the chemical reaction zone at the front is so thin, that it is hardly detected experimentally.

Fig. 3 exhibits calculation results for the one-particle potential of average force $U(z)$ near the surface of a semi-bound liquid whose parameters satisfy the initial conditions for dissociation of methane molecules. Thickness of the layer where we observe the drop of potential $U(z)$ is about 5Å. This thickness corresponds to width of shock wave front with a step density profile.

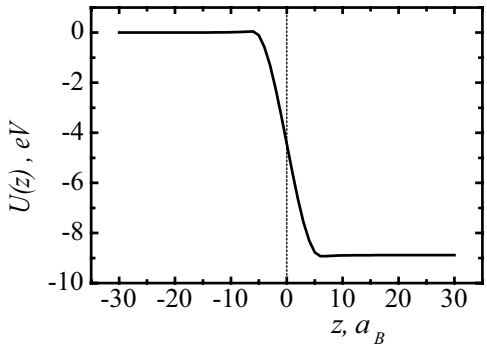

Fig. 3. Coordinate dependence of potential of average force near the flat open surface of methane with the following set of thermodynamic parameters $T = 2620$ *K*, $v = 1.165$ dm^3kg^{-1}, $p = 241024$ *bar*

3. Potential of Average Force in a spherical nanopore

Let's consider the potential of average force for a case of a spherical pore in a simple liquid with the frame of reference placed at the centre of the pore. We assume that the atom unary distribution function depends only on distance to the centre. The pair distribution function will be approximated by means of the pair correlation function of a non-uniform liquid $g(R_1, R_2, |\mathbf{R}_1 - \mathbf{R}_2|)$

$$F_2(\mathbf{R}_1 - \mathbf{R}_2) = F_1(R_1)F_1(R_2)g(R_1, R_2, |\mathbf{R}_1 - \mathbf{R}_2|). \tag{10}$$

Then the unary distribution function $F_1(R)$ can be expressed in terms of the potential of average force $U(R)$

$$F_1(R) = \exp[-\mathrm{U}(R)/k_BT], \tag{11}$$

$$U(R) = -\frac{1}{v_0}\int_R^\infty dR_1 \int d^3R_2 F_1(R_2)g(R_1, R_2, |\mathbf{R}_1 - \mathbf{R}_2|)\frac{\partial\Phi(|\mathbf{R}_1 - \mathbf{R}_2|)}{\partial R_1}. \tag{12}$$

Relation (11) for the unary distribution function $F_1(R)$ depending on the potential of average force $U(R)$, corresponds to Boltzmann distribution for particles in an average force field. The expression (12) for the potential of average forces contains a quadruple integral, however, using the Fowler's approximation it is possible to reduce it to a unitary integral.

The molecule work function from liquid into the centre of a pore can be calculated as difference of potential of average force values at the centre of the pore and far away inside the liquid $A = U(0) - U(\infty)$. Since $U(\infty) = 0$, then the work function $A = U(0)$, and the average force potential at the centre of the pore of radius a has form

$$U(0) = \frac{4\pi}{3v_0}\int_0^{\infty} dRR^3F_2(R)\frac{\partial\Phi(R)}{\partial R} + \frac{4\pi}{3v_0}\int_a^{\infty} dRF_2(R)\frac{\partial\Phi(R)}{\partial R}\left(a^3 - R^3\right). \tag{13}$$

The emission stability boundary of the surface of a pore is defined by the equality of the work function from liquid into the pore interior, and by characteristic thermal energy of molecules $A = k_BT$.

The provided estimations of influence of geometry allow us to track size dependence of the average force potential. Fig.4 shows calculation results of the potential of average force in methane for different pore radii $a = 10a_B$, $15a_B$, $20a_B$ (a_B is Bohr radius). Line 4 corresponds to molecule work function from a flat surface of methane $A_{l\text{-}v} = -2.2$ *eV*.

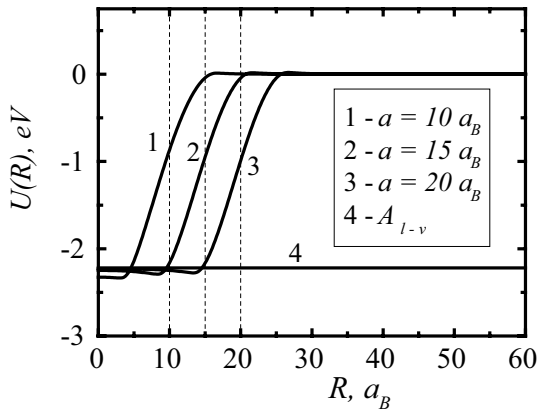

Fig. 4. Distribution of the potential of average force for the pores with different radii in methane (thermodynamic parameters correspond to the condition of dissociation initiation)

We can observe a relatively fast decrease of curvature influence of the pore surface with the growth of radius. For the radius values $a < 20a_B$ contribution of curvature is less than 5% from the values of $U(0)$.

4. Criteria of homogeneous and heterogeneous detonation

At certain thermodynamic conditions from the surface of a pore there will be emitted streams of particles which have hyper-thermal velocities and are directed to the centre of the pore. These streams will collide at the center of a spherically symmetric pore. Dissociation process for the pair-collided molecules will take place when total kinetic energy of this pair will be higher than doubled dissociation energy. During emission a molecule may possess kinetic energy (if it reaches the center of the pore) equal to $MV^2/2 = |U(0)|$, where V is velocity of the molecule at the center of the pore. Relative velocity of two molecules at central collision reaches value of $2V$ and the molecule dissociation condition can be written as

$$MV^2/2 = |U(0)| \geq E_{diss}/2. \tag{14}$$

Taking into account (13) we can rewrite it as

$$\left|\frac{4\pi}{3v_0}\int_0^{\infty} dRR^3F_2(R)\frac{\partial\Phi(R)}{\partial R}+\frac{4\pi}{3v_0}\int_a^{\infty} dRF_2(R)\frac{\partial\Phi(R)}{\partial R}\left(a^3-R^3\right)\right|\geq E_{diss}/2. \tag{15}$$

We can also write the condition of molecule dissociation at the front of a flat shock wave as

$$\left|\frac{4\pi}{3v_0}\int_0^{\infty} dRR^3F_2(R)\frac{\partial\Phi(R)}{\partial R}\right|\geq 2E_{diss}. \tag{16}$$

Comparison of the molecule dissociation condition (16) at the front of a flat shock-wave with the dissociation condition at the center of the pore (15) shows much easier detonation initiation at presence of pores inside liquid. There is a difference of the factor of four between the right sides of expressions (16) and (15). Besides that, due to curvature of the pore surface, the left side of the expression (15) has an additional term that simplifies satisfaction of this inequality. Since dissociation of molecules promotes chemical reactions the conditions (15) and (16) can be qualified as necessary conditions for detonation initiation in homogeneous and heterogeneous CEM.

As we can see, there are two major factors facilitating dissociation of molecules inside a pore. The first factor related to possibility of head-on collisions of molecular streams having the opposite directed velocities. The second one is curvature of the pore surface. To clarify relative contribution of these two effects into dissociation of molecules we have investigated conditions at which holds true the equality which was derived from (15) by neglecting the second term in the left part.

$$\left|\frac{4\pi}{3v_0}\int_0^{\infty} dRR^3F_2(R)\frac{\partial\Phi(R)}{\partial R}\right|=E_{diss}/2, \tag{17}$$

Using (17) we can calculate the thermodynamic parameters at the front of a flat shock wave in methane under the condition of its maximum compression: temperature $T = 520\ K$, specific volume $v = 1.45\ dm^3kg^{-1}$, pressure $p = 47923\ bar$ and speed of emitted molecules $V = 5167.8\ m{\cdot}s^{-1}$. These results correspond to the geometry where we have a head-on collision of two streams of molecules emitted by the fronts of two flat shock waves propagating towards each other.

When parameters of a the flat shock wave satisfy the initiation condition of homogeneous dissociation of molecules in methane ($T = 2620\ K$, $v = 1.165\ dm^3kg^{-1}$, $p = 241024\ bar$, $V = 10336\ m{\cdot}s^{-1}$), the relative speed of molecules emitted into the interior of the pore at head-on collision will be twice higher $V = 20672\ m{\cdot}s^{-1}$. Relative energy of molecules at collision will be four times larger then the minimal energy required for dissociation, and will reach a value of 35.52 *eV*. This is enough energy for complete dissociation of methane molecules or for partial dissociation and ionization of produced atoms. As a result, at the center of the nanopore there will appear the 'hot spot' of plasmic nature. According to the shock-wave experiments the decomposition initiation of methane (decomposition into carbon and hydrogen) occurs at pressure values of 23 *GPa* [19]. However the experiments on electric conductivity by means of a two-stage light gas gun track methane decomposition at 30 *GPa* [20]. Boundary lines of shock dissociation at the front of a flat shock wave can be calculated by means of the formula (8). Results of calculations for methane and nitromethane are shown in Fig. 5 (α is degree of dissociation).

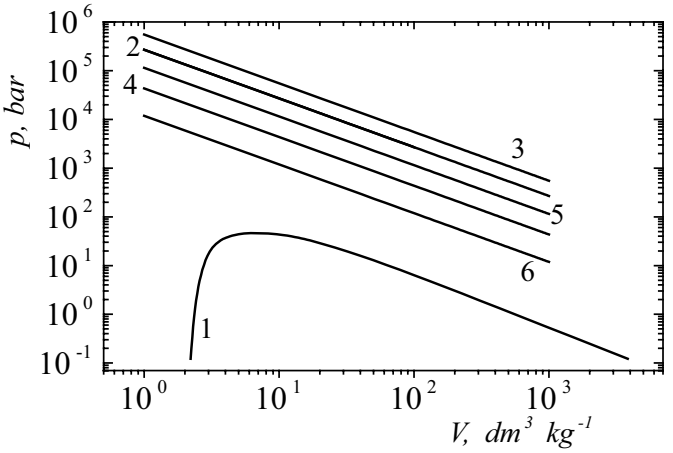

Fig. 5. Boundary lines of dissociation at the front of a flat shock wave in methane and nitromethane: 1 - Liquid-gas equilibrium line CH_4; 2 - $CH_4 = CH_3 + H(\alpha = 0.5)$; 3 - $CH_4 = CH_2 + 2H(\alpha = 0.5)$; 4 - $CH_3NO_2 = CH_3 + NO_2(\alpha = 0.5)$; 5 - $CH_3NO_2 = CH_3 + N + O_2(\alpha = 0.5)$; 6 - Pore $CH_3NO_2 = CH_3 + NO_2(\alpha = 0.5)$.

5. Discussion of results

Current work develops a new approach that allows explaining detonation initiation in homogeneous and heterogeneous CEM's. This approach accounts for the average force field that acts on separate atoms and molecules in a non-uniform fluidized medium. The physical source of this one-particle average force field is the pair inter-particle interactions and correlations. The energy range of detonation phenomena is of order of tens of *eV*, which considerably exceeds thermal energy of atoms and molecules or binding energy of crystal lattice. Significant role in the heterogeneous CEM initiation and detonation propagation is played by the defects of material structure, such as pores, which are the basis of 'hot spots'. Inside the porous CEM the detonation initiation threshold is considerably lower. High sensitivity of the heterogeneous CEM to initiation of detonation by the shock waves in comparison to the homogeneous materials acquires transparent physical meaning within the framework of the approach developed in the current work. During propagation of the shock waves of sufficient intensity through the CEM with pores inside, the emission of molecules and atoms from the surface occurs with hyper-thermal velocities. The head-on collision of particles, emitted from the opposite walls of a pore is much more efficient in comparison to the collision of particles emitted from the front of a flat shock wave and particles of non-perturbed material. As it is shown, this simple geometrical fact makes the heterogeneous CEM more sensitive at detonation initiation.

The present work elucidates the microscopic criteria of detonation initiation at the front of a flat shock wave in homogeneous and heterogeneous CEM with spherical nanopores. The criteria are expressed in terms of pair interparticle interaction potentials and pair correlation functions. As a result the existing correlation theory of liquids can be applied to the shock-wave phenomena and to the phenomena of CEM detonation. Initiation of heterogeneous detonation occurs when the criterion (15) holds true. The transition from heterogeneous detonation initiation mode into the homogeneous one occurs when values of thermodynamic parameters satisfy the criterion (16). It is clear that if the thermodynamic parameters satisfy both criteria, (15) and (16), there will be observed coexistence of homogeneous and heterogeneous detonation mechanisms.

Experimental data that point to presence of cumulative flows at the fronts of detonation waves co-directed to the propagation direction of a normal detonation front was obtained in [21]. It was shown that presence of voids inside the explosive media leads to formation of cumulative jets and as a result, of mass and energy transfer from the chemical reaction regions into an unperturbed region. Velocity of the main part of the jet is two times faster than propagation speed of the normal detonation front. This experimental data fits absolutely accurately into the 'hot-spot' generation mechanism proposed in the current work.

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