

MOLECULAR HYDRODYNAMICS OF UNDERWATER EXPLOSION

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Abstract. In this contribution we report on modeling underwater explosion in the framework of molecular dynamics. We have developed a computer program which allows studying the underwater explosion in two dimensional Lennard – Jones liquid. Calculations of the dynamical structure of underwater explosion displayed the striking resemblance of the underwater-explosion evolution obtained and the real process; namely, generation of a shock wave and its expanding; formation of a cavity; disintegrating the shock wave, when reaching a surface, into two parts which begin to move in opposite direction parallel to the surface; transforming the cavity into a water crater of an arising water volcano; its activity and decay.

1. Introduction. Underwater explosion

Definition. “An explosion is a chemical reaction characterized by the extreme rapidity of the process and the release of large amounts of energy. The original material (usually solid) is converted into a gaseous mixture at a very high temperature and pressure (~ 3000 °C and ~50,000 atm). The explosion converts the inherently unstable explosive material into a more stable product” ([1], p. 288).

Explosion-generated water waves [1, 2]. When an explosion occurs, the submerged detonation almost instantaneously produces a hot gas or plasma with a limited volume at a tremendous pressure. The hot mass of gas, in turn, disturbs the surrounding medium. In underwater explosions, the medium is water. High temperatures and pressures cause two disturbances of the water:

- 1) emission of a shock wave traveling outwardly,
- 2) a radial motion of the water so that the “bubble” consisting of water vapor and explosive debris begins to expand.

Many of the fluid motions occurring in the case of small near-surface explosions have been observed through reinforced glass windows and monitored by high-speed cameras. They demonstrate the wide range of phenomena and variations of these phenomena as function of the burst depth. It is clear that near-surface underwater explosions, producing a wealth of phenomena which nature is not well understood, are very difficult object for study.

Hydrodynamics and underwater explosions. Until the present time the study of underwater explosions was a privilege of hydrodynamics. The Russian Physical Encyclopedic Dictionary [3] gives such definition: Hydrodynamics (from Greek υδωρ – water and δυναμικός – strong, powerful), part of mechanics, which studies the motion of liquids and their interaction with solids. The physical properties of liquids providing the basis for theoretical models are continuity, or continuousness, and fluidity, i.e. weak counteraction even to arbitrary small forces, which produce the relative sliding motion of liquid particles. At

the same time, the majority of liquids exhibit strong resistance to compression. In theoretical hydrodynamics, for description of the movement of an incompressible liquid, having continuity and fluidity, as well as viscosity, one uses the continuity equation and Navier-Stokes' equations. The latter are the consequence of the application of the conservation laws (mass and linear momentum) to a unit volume of a liquid. The solution of these nonlinear equations can be obtained only in a limited number of cases under some assumptions.

The hydrodynamics of explosion deals with liquid flows under shock-wave loading. Shock-loaded liquid still remains a puzzle. And it is difficult to solve these problems by simply writing a complete system of conservation laws in the form of differential equations and closing defining relations, or by developing unique computer programs and codes [2]. Families of hydrocodes have been written based on the assumption that the fluid flow is irrotational and non-dissipative. The corresponding "hydrocodes" are based on the Navier-Stokes equations for a compressible fluid, which can be treated numerically; they incorporate the appropriate equations of state and initial boundary conditions imposed by chemical or nuclear effects. However, nonlinear convective and dissipative effects are difficult to resolve or even formulate mathematically, although these effects are often too important to be neglected. Therefore, it would seem that there is little hope that such complex phenomenology can lead to well defined input boundary conditions to determine the wave field [1]. Physical models that include all main stages and features of the processes occurring in liquids must remain a key element in research [2].

First conclusion. This overview is based chiefly on the analysis of two monographs devoted to underwater explosions [1,2]. It is the authors' opinion that the little progress in the understanding of a shock-loaded liquid is connected mainly with the effort of the researchers to put such complex phenomenon as underwater explosion to Procrustean bed of the hydrodynamic phenomenology of wave generation and wave propagation. Such procedure leads to methodical errors [4]. In doing so, the researcher is compelled to divide this complex phenomenon into parts (stages, phases) and to analyze them separately. As a consequence, geometric and kinematic constraints imposed on the parts are lost, the interaction of parts disappears; and the results of study are in rather poor agreement with each other [4].

The second reason of the little progress has a gnosiological origin. The basic hypothesis of hydrodynamics is continuum hypothesis. This idealization is necessary because it allows use for the analysis of movement continuous functions, differential and integral calculus [5]. Really, macroscopic properties of a physical system can be described in the framework of continuum. However, if one wants not only to describe the properties, but understand their nature, one should establish their origin turning to the particles which constituent the system [6]. In the latter case one is able to express observed physical values not only through the constants and parameters which characterize continuum, but through the characteristics of the particles [7].

2. New approach to underwater explosion. Statement of the problem

Molecular hydrodynamics. Contrary to the customary approach, briefly considered above, we will use molecular dynamics [8] for studying underwater explosions. The main motive is such: since the accepted methods of studying "a wealth of phenomena which nature is not well understood" seem to be ineffective, it is reasonable to try other methods. The other reasons are as follows [4]. Firstly, molecular dynamics is an integral method of investigation; it plays the role of a synthesizer of all initial fundamental events, which were incorporated into the model of a process studied. Secondly, molecular dynamics allows obtain an exhaustive account of all the interactions of the initial fundamental events. Thirdly, and it is more important, in doing so, molecular dynamics operates very prudently without disturbing the liaisons existing in a system.

In addition to this assertion, it should be noted that molecular dynamics has shown its effectiveness in studies of a great variety of phenomena, e.g. radiation damage of solids, deformation and fracture of various materials, nucleation, evolution and self-organization of biological structures and so on [8]. In particular, this investigation was motivated by the fact that molecular dynamics has proved its effectiveness in modeling the action of shock waves on phospholipids in water [9].

The problem of modeling underwater explosion, formation and propagation of explosion-generated water waves, their interaction with a target can be divided into three parts: how to model water, how to model an explosive, and how to model the interaction of explosion-generated water waves with a target. In this contribution we consider mainly the first and the second parts.

Modeling water. “The importance of water in a wide range of scientific disciplines needs no emphasis. The investigation of water properties has a long history which can be possibly be extended back to the ancient Greeks when water constituted one of the four elemental forms of the universe (the others being earth, air and fire)! In a more modern context, water consists of an apparently simple molecule (H_2O) containing only two atomic species and is present in large quantities on the Earth’s surface and in the atmosphere above it. The almost universal presence of water in our everyday lives and the very ‘common’ nature of its presence and properties possibly deflects attention from the fact that it has a number of very unusual characteristics. It is at the molecular level that our scientific understanding must begin and it is here that many of the intriguing questions need to be posed. We learn quickly that the nature of the interaction between water molecules is complex and, even now, is not fully defined. The essential structures and microdynamical features are found to be extremely sensitive to physical parameters (such as temperature and pressure) chemical environment (such as ions, macromolecules) and other influences (interfaces, confined geometry, biomolecular function). In order to properly understand the sensitivity of water behavior, it becomes essential to study the ‘water substance’ in a wide range of conditions” [10].

After such pre-statement taken from the preface to the NATO Advanced Research Workshop on Hydrogen Bond Networks, we pass on to the modeling of water. In the previous 3D molecular dynamics simulations of phospholipids in water, both phospholipids and surrounding water were taken in the form of real molecules [9]. The interactions between atoms were given by the Morse potential, the parameters being dependent on an atom species and its position in a molecule [11]. The investigations had come to conclusion that the structure of a water molecule is not as simple as it is usually deemed. Further investigations have shown that for its correct description it is necessary to use the bond-charge theory in which in addition to interatomic interaction one should take into account electronic interaction of covalent bond charges [12]. However such global approach could come to big difficulties of both computational character and understanding. For this reason, it was decided to take a simpler model for water changing a real molecule by one particle.

The basis for this decision is the following. Many phenomena are connected with cooperative motions of atoms, e.g. phase transition. Modeling such phenomena does not require knowing all the details of atomic structure; it is enough to be aware how many atoms act as a whole forming a cluster. In water such cluster consists of three atoms and, we suppose, for our problem can be replaced by a fictitious particle. Transition to fictitious particles simplifies the matter considerably. The interaction of the particles can be described with the help of potentials considered in [7]. Besides at this stage of study, we restrict ourselves to 2D computer simulations.

Modeling explosive. Generally, modeling an explosive is a separate problem of computer simulation. There is no difficulty in modeling a plane shock wave in water; in fact,

here an explosive is excluded from computer simulation [9]. As a consequence, we have only two systems: a target and surrounding water. In the case of underwater explosion, there is necessary to model also an explosive.

In the preliminary trials [137] we have investigated the explosion of two types of polymeric explosives. Their structures were not specified in advance but were obtained automatically as a result of folding in [14]. After that they were subjected to uniform compression. As a result, the structures accumulated a large amount of elastic energy. Decompression simulated an explosion [14]. However, in this case the bubble consists of water vapor and explosive debris. To gain a more penetrating insight into the explosion phenomenon, we excluded explosive debris from further research [15]. For this purpose, we developed a simpler explosive model (Fig. 1). A certain number of water particles were placed in a circular area of a given size at a predetermined distance. Thereafter the particles, as in the previous case, were subjected to radial compression. As a result of changing the distance between particles, the compressed structure accumulates a large amount of elastic energy. During decompression the particles acquire enormous velocities, producing an explosion.

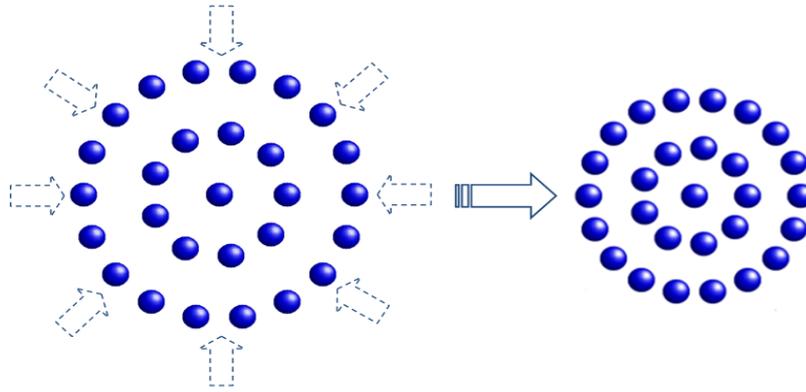


Fig. 1. Model of self-explosive.

3. Computational procedure

Molecular dynamics. In classical molecular dynamics [8], the motion of a system of N particles is described with the help of Newton equations

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{f}_i = \mathbf{f}_i^F + \sum_{j=1, j \neq i}^N \mathbf{f}_{ij}.$$

Here t is the time, \mathbf{r}_i is the radius-vector of particle i , m_i is its mass. The force \mathbf{f}_i acting on a particle is the sum of an external-field force \mathbf{f}_i^F and the interaction forces between particles. Write down the equations in Cartesian coordinates

$$m_i \frac{d^2 x_{ia}}{dt^2} = f_{ia}^F + \sum_{j=1, j \neq i}^N f_{ij} \frac{x_{ia} - x_{ja}}{r_{ij}},$$

where $a = 1, 2, 3$; $f_{ij} = |\mathbf{f}_{ij}|$, $r_{ij} = |\mathbf{r}_{ij}|$.

The equations can be written as the system of differential first-order equations

$$\left. \begin{aligned} \frac{d x_i(t)}{d t} &= v_i \\ \frac{d v_i(t)}{d t} &= \frac{1}{m_i} f_i \{x_1(t), x_2(t), \dots, x_{3N}(t), F\} \end{aligned} \right\}.$$

Here v is the velocity and the symbol F means that the force f_i takes into consideration the action of an external field. In our case f_i^F is the force of the gravitational field. Notice that index i is changing from 1 to $3N$. Now it is not the number of a particle, but the counter of the number of freedom degrees. Usually it is supposed that each particle has three degrees of freedom.

Any computer works with discrete values which are obtained by counting out the values of a continued function in fixed time intervals

$$t_k = k \Delta t, \quad k = 0, 1, 2, \dots$$

Then the computer integrates the motion equations for each degree of freedom.

$$x_{k+1} = x_k + \int_{t_k}^{t_{k+1}} v(t) dt, \quad v_{k+1} = v_k + \frac{1}{m} \int_{t_k}^{t_{k+1}} f(t) dt.$$

With all this going on, the integrand is presented as the Taylor series with a finite number of terms

$$f(t) \cong f(0) + f'(0)t + f''(0)\frac{t^2}{2} + \dots = \sum_{s=0}^{n-1} \left(\frac{d^s f}{dt^s} \right)_0 \frac{t^s}{s!}.$$

The derivatives are replaced by the finite differences using various schemes.

There are various numerical schemes for solving the classical equations of motion, from the simplest first order Euler's methods to the predictor – corrector scheme of high order accuracy. One of the most common and, at the same time, stable and efficient approach to the time discretization of Newton's equations is the Velocity–Verlet algorithm [16]. This algorithm was used in the present study as a compromise between speed and accuracy.

Interparticle potential. Integration of the motion equations allows us to find the trajectories of particles. The force acting on a particle is defined as the negative derivative of the particle potential energy. If the initial positions and velocities of the particles are given, the evolution of the system in time depends only on the potential, which determines the interaction between the particles. There are many of potentials which are used in molecular dynamics calculations [7]. We have chosen the Lennard–Jones potential for the following reasons.

The simplest substances are composed of inert gas atoms with closed electron shells. Even when their atoms approach to a minimal distance, the electron wave functions of neighboring atoms do not overlap and the atom attractions remains of van-der-Waals nature. In the thirtieth years of the twentieth century, numerous calculations of kinetic properties of inert gases were done by Lennard-Jones with the help of the Mie potential [4, 7]

$$U(R) = \frac{A}{R^n} - \frac{B}{R^m},$$

where $A, B > 0$, $n > m > 0$. By then, with the help of quantum mechanics it was found that for van-der-Waals attraction $m = 6$, so that Lennard-Jones used this value. As for repulsion, the value n was unknown, and up to now has no theoretical grounds. Lennard-Jones tried different values. It turned out that experimental data can be equally well described, if one chose n in the interval from 9 to 12. For convenience of calculations it was accepted that $n = 12$. The 6–12 potential is called the Lennard-Jones potential and is written in the canonical form as

$$U(R) = 4\varepsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^6 \right].$$

Here $\sigma = (A/B)^{1/6}$; $\varepsilon = B^2/4A$; A and B are the constants of Mie potential. The parameter ε gives the depth of the potential well, the parameter σ defines the radius of repulsion and can be found from the condition $U(\sigma) = 0$.

We suppose that the rather simple Lennard-Jones potential is the most suitable, in the first approximation, for describing the interaction between the fictitious particles modeling the molecules of water. Besides, with its parameters $\sigma = 0.317$ nm, $\varepsilon = 0.651$ kJ/mol, it is possible to obtain agreement between calculated and experimental properties of water taken from [17]. Nevertheless, it should be remembered that strictly speaking the object of study is the Lennard–Jones liquid.

Interaction region. The Lennard–Jones liquid was considered in two–dimensional space with periodic boundary conditions on the side walls and rigid boundary at the bottom of basin. The external gravitational field was acting on the particles of liquid only in the direction normal to the bottom. For setting the liquid in motion, the iterative process has to start with some initial distribution of particles in the computational domain; the particles having their predetermined positions and velocities at a certain temperature. The initial velocity components were obtained with the help of the Maxwell-Boltzmann distribution.

Modeling systems consisting of several thousands of particles, it is necessary to achieve calculation optimization, in order to reduce computing costs. For this purpose, in the present study we used the linked cell method [16]. The method allows evaluating approximately the forces and energies and is very effective for rapidly decreasing potentials. At the same time, it can be relatively easily implemented. The idea of the cell method consists in splitting the physical simulation domain into uniform cells. If the cutoff radius is less or equal to the length of a cell side, then the interparticle interactions are limited to the particles within a cell or within and in adjacent cells. In our case the cutoff radius was equal to two interparticle distances; one interparticle distance $2^{1/6}\sigma$ corresponds to the minimum of the Lennard-Jones potential.

Until the moment of explosion, within a certain period of time, we let gravity act on the particles in the bottom of the computational domain in order to bring the system in the state of stable equilibrium. Then the particle velocities were scaled every thousand iterations over time, to avoid too large values.

In the beginning of calculations, the liquid completely fills the lower part of the computational domain having the size of $0 < x < Lx$, $0 < y < Ly$ (Fig. 2). The particles are ordered at the distance $2^{1/6}\sigma$ from each other what corresponds to the energy minimum. After

a certain time, which is necessary for setting thermodynamic equilibrium, a compressed explosive of radius R was placed into the system at a depth H from the bottom. Then an underwater explosion came into play as a result of explosive decompression.

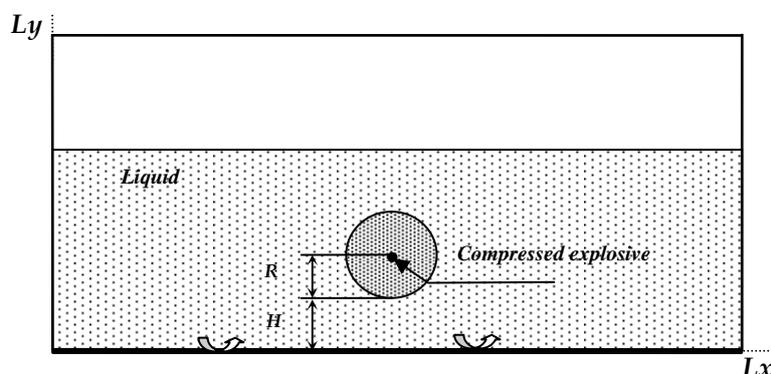


Fig. 2. Computational domain.

Test calculations before explosion. The test calculations were done with a system consisting of 12,500 particles that was brought into the state of thermodynamic equilibrium. A process of setting a prearranged temperature is shown in Fig. 3. One can see that to the time $t = 9$ ps (18,000 iterations) large oscillations disappeared, and the temperature begins to fluctuate about the given temperature $T = 300$ K. It means that the system came to the state of thermodynamical equilibrium.

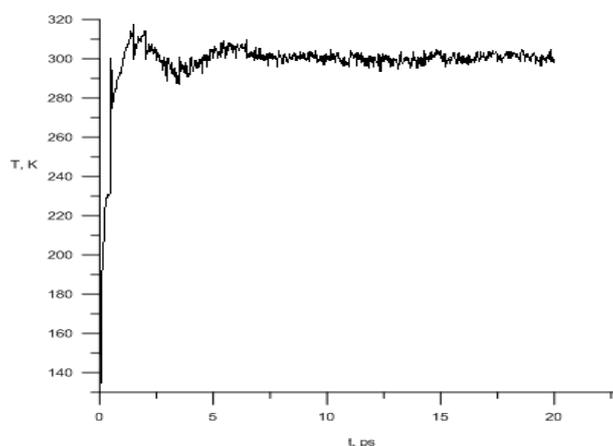


Fig. 3. Convergence to a given temperature.

In Fig. 4 one can see the evolution of liquid structure during the establishment of equilibrium. Initially the particles were located in the lower part of computational domain (Fig. 4a). The zoom area gives a more detailed view of particles arrangement. Further the system was brought to the state of thermodynamic equilibrium at the temperature $T = 300$ K. For this purpose, from the beginning (time $t = 0$) up to $t = 20$ ps the calculations were done with a time step $\delta t = 0.0005$ ps. After the start, the particles begin to move; the most of agitation being located near the surface of liquid (Figs. 4b, c). As a consequence, the upper layer becomes more rarefied (Fig. 4c); but the establishment of equilibrium leads to decreasing of rarefaction (Fig. 4d).

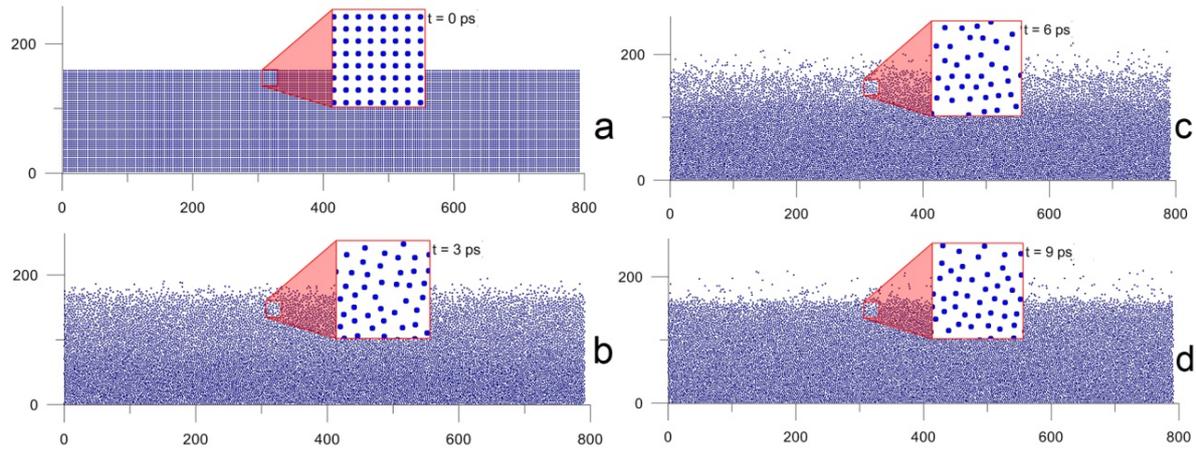


Fig. 4. Establishment of equilibrium at $T = 300$ K. Units are in nm^{-1} .

4. Preliminary results

The calculations were done with a system consisting of 27,500 particles. An explosive was inserted into the water after reaching the equilibrium. The temporal evolution of underwater explosion is demonstrated in Figs. 5–8. Fig. 5a shows the system before explosion; the zoom area specifies the location and structure of explosive. Decompression of the explosive creates a shock wave and a cavity Fig. 5b. It should be emphasized that the cavity is not empty and resembles fog (rarefied water). The expanding shock wave produces a dense compression shock in a narrow region (Fig. 5c). Simultaneously, at this moment the shock-wave front reaches the free surface. It takes some time for the shock wave to break up into two parts, which begin to move in opposite directions parallel to the surface (Fig. 6). Simultaneously the cavity reaches the surface transforming into a water crater. The following picture resembles a volcanic eruption. At first the volcano is very active (Figs. 7-8) and then becomes extinct (Figs. 9-10).

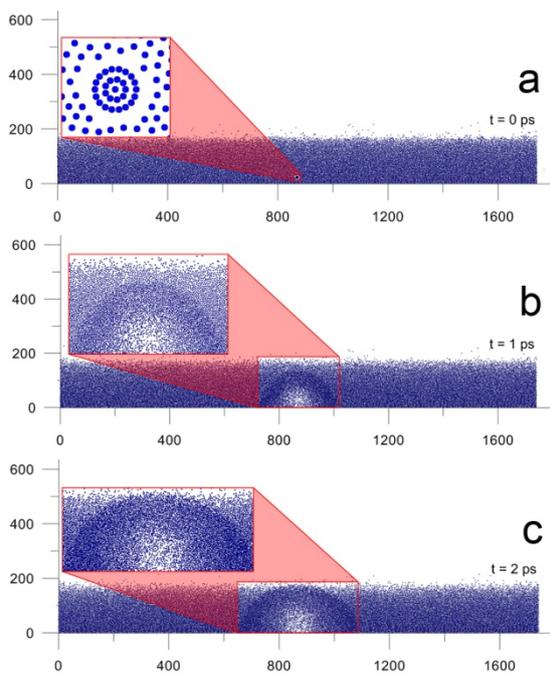


Fig. 5. Time evolution of underwater explosion, $t = 0 - 2$ ps. Units are in nm^{-1}

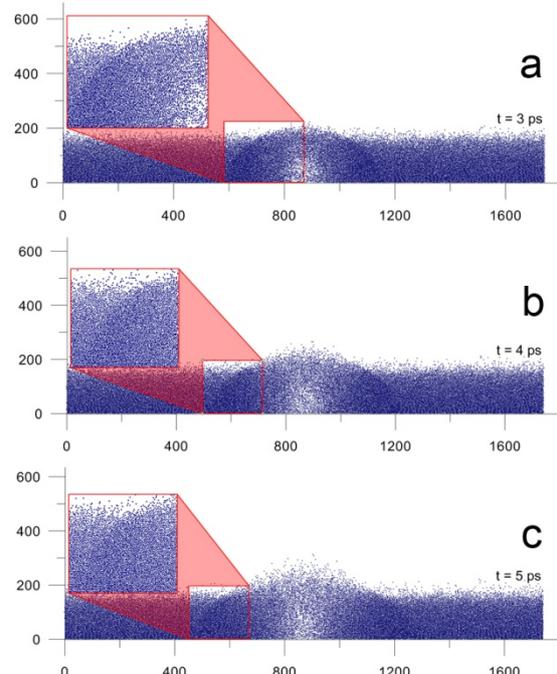


Fig. 6. Time evolution of underwater explosion, $t = 3 - 5$ ps. Units are in nm^{-1}

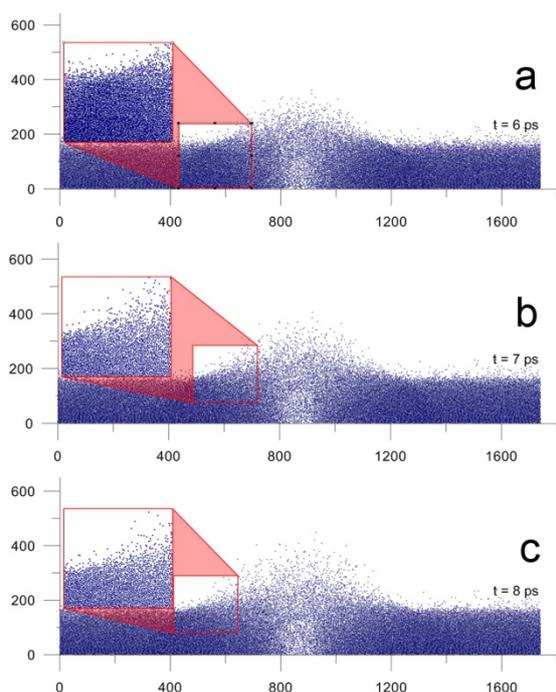


Fig. 7. Time evolution of underwater explosion, $t = 6 - 8$ ps. Units are in nm^{-1} .

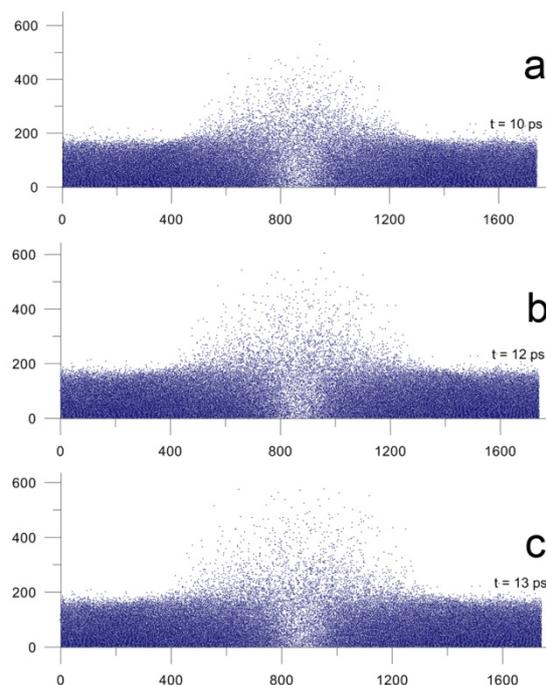


Fig. 8. Time evolution of underwater explosion, $t = 10 - 13$ ps. Units are in nm^{-1} .

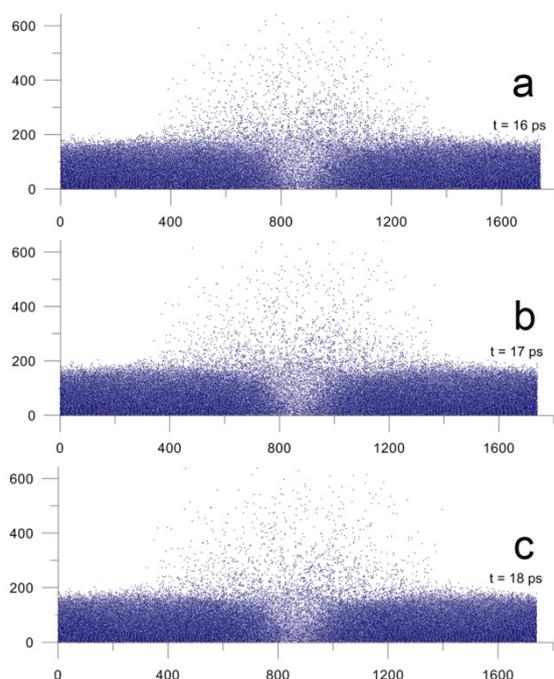


Fig. 9. Time evolution of underwater explosion, $t = 16 - 18$ ps. Units are in nm^{-1} .

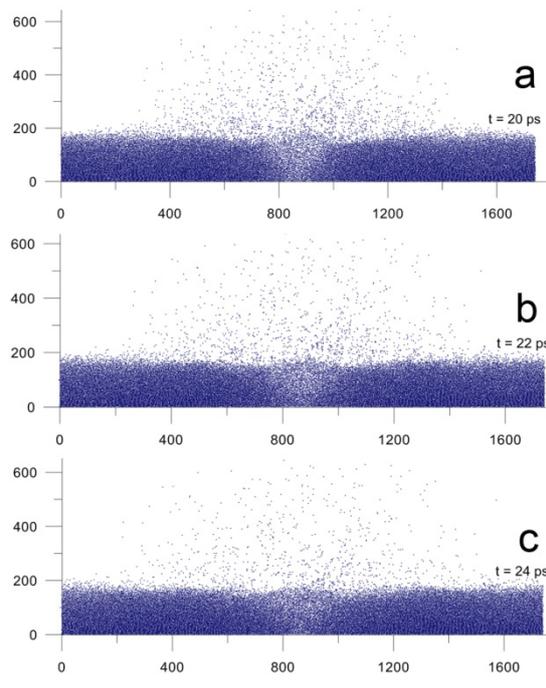


Fig. 10. Time evolution of underwater explosion, $t = 20 - 24$ ps. Units are in nm^{-1} .

5. Conclusion

We have developed a molecular dynamic approach for studying underwater explosion. Contrary to the customary approach based on different equations of hydrodynamics, which in their turn are based on some postulates, molecular dynamics has evident advantages. Firstly, molecular dynamics is based in fact on the ‘first principles’ because it uses only two fundamental laws: the second Newton’s law of and the Coulomb law. All the potentials of

interatomic, intermolecular, interparticle and so on interactions are deduced in reality from the Coulomb law. Secondly, molecular dynamics is an integral method of investigation; it plays the role of a synthesizer of all initial fundamental events, which were incorporated into the model of a process studied. Thirdly, molecular dynamics allows obtain an exhaustive account of all the interactions of the initial fundamental events; in doing so, molecular dynamics operates very prudently without disturbing the liaisons existing in a system.

In the framework of molecular dynamics we developed a model that simulates underwater explosion. It allows studying the underwater explosion in two dimensional Lennard – Jones liquid. Calculations of the dynamical structure of underwater explosion displayed the striking resemblance of the underwater-explosion evolution obtained and the real process; namely, generation of a shock wave and its expanding; formation of a cavity; disintegrating the shock wave, when reaching a surface, into two parts which begin to move in opposite direction parallel to the surface; transforming the cavity into a water crater of an arising water volcano; its activity and decay. However, it is necessary to do the next step, namely, to use one more advantage of molecular dynamics: to study simultaneously both dynamical structure of a system, observing the motion of separated particle, and to calculate averaged characteristics of the system, such as energy, pressure, temperature, etc., especially their distribution in the system and their changing in time. This work is in progress.

References

- [1] Bernard Le Méhauté, Shen Wang, *Water Waves Generated by Underwater Explosion* (World Scientific Publishing Co. Singapore, 1996).
- [2] Valery K. Kedrinskii, *Hydrodynamics of Explosion: Experiments and Models* (Springer, 2005).
- [3] *Physical Encyclopedic Dictionary* (Large Russian Encyclopedia, Moscow, 1995), in Russian.
- [4] A.I. Melker // *Modeling Experiment*, Ser. Physics, No. 10 (Znanie, Moscow, 1991), in Russian.
- [5] L.I. Sedov // *Mechanics of Continuum, vol. 1* (Nauka, Moscow, 1973), in Russian.
- [6] A.I. Melker // *Dynamics of Condensed Matter, vol. 1, Vibrations and Waves* (St. Petersburg Academy of Sciences on Strength Problems, 2004), in Russian.
- [7] A.I. Melker // *Reviews on Advanced Materials Science* **20** (2009) 1.
- [8] A.I. Melker. // *Proceedings of SPIE* **6597** (2007) 659702.
- [9] A.V. Fedin, *MSc Thesis* (St. Petersburg State Polytechn. Univ. 2001), in Russian.
- [10] M-C. Bellissent-Funel, J.C. Dore, In: *Hydrogen Bond Networks*, ed. M-C. Bellissent-Funel, J.C. Dore, (Kluwer Acad. Publishers, Dordrecht/Boston/London, 1994), p. XIX.
- [11] M. Pokhilenko, D. Soloviev, A. Melker, In: *Int. Workshop on New Approaches to Hi-Tech Materials: Nondestructive Testing and Computer Simulations in Materials Science and Engineering; NDTCS-97* (St. Petersburg Academy of Sciences on Strength Problems, 1997) p. C3-9.
- [12] A.I. Melker, M.A. Vorobyeva // *Proceedings of SPIE* **6253** (2006) 625305.
- [13] S. Igolkin, A.I. Melker // *Proceedings of the Junior Scientist Conf. 2010* (Technische Universität Wien, 2010) p. 83.
- [14] T.V. Vorobyeva, *PhD Thesis* (St. Petersburg State Technical Univ. 1994), in Russian.
- [15] S.I. Igolkin, A.I. Melker, In: *14th Int. Workshop on New Approaches to High-Tech: Nano-Design, Technology, Computer Simulations; NDTCS-2011* (Aalto University publication series SCIENCE+TECHNOLOGY 17/2011) p. 37.
- [16] M. P. Allen, D. J. Tildesley, *Computer simulation of liquids* (Clarendon Press, 1989).
- [17] Y. Wu, H. L. Tepper, G. A. Voth // *J. Chem. Phys.* **124** (2006) 024503.