Materials Physics and Mechanics 20 (2014) 148-158 Received: April 29, 2014

MOLECULAR HYDRODYNAMICS OF SHALLOW-WATER EXPLOSIONS

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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 those of observed in the real process. For studying the structure of shock waves, a special technique was developed. It allowed observing the form of a shock wave and estimating its velocity. The most striking result of the investigation is that the form of the shock wave in a shallow water explosion has an evident wavy character similar to electromagnetic shock waves.

1. Introduction

In the previous works [1-3] we described a new approach to studying underwater explosion which is based on 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 that of observed in real process; namely, generation of a shock wave and its expanding; formation of a cavity; disintegrating the shock wave, when reaching a surface, transforming the cavity into a water crater of an arising water volcano; its activity and decay.

In [4, 5] the second step was done; a procedure was developed which allowed studying a structure of shock waves observed within the framework of molecular dynamics. In this contribution we used both procedures, one for observing a visual picture of underwater explosions under different conditions, and other for calculating a structure of shock waves arising in deep-water explosions.

2. Shallow water explosion

a) The explosive is the same as in all previous simulations. 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 Fig. 1. The calculations were begun at $t' = 0$ after the state thermodynamic equilibrium was established in the system with an inserted explosive at temperature *300 K*. After 4000 time steps, each step being $t' = 0.00025$, at $t' = 1$ one can see the explosion zone which is expanding and reaching a surface. From $t' = 2$ to $t' = 10$ water particles emission to atmosphere is observed. Simultaneously at $t' = 10$ the surface waves are forming which begun moving to both sides from the explosion epicenter. The following collapse of the crater formed leads to a new emission of particles at $t' = 10 - 28$; the process is accompanied by the appearance of more powerful surface waves at $t' = 16 - 17$.

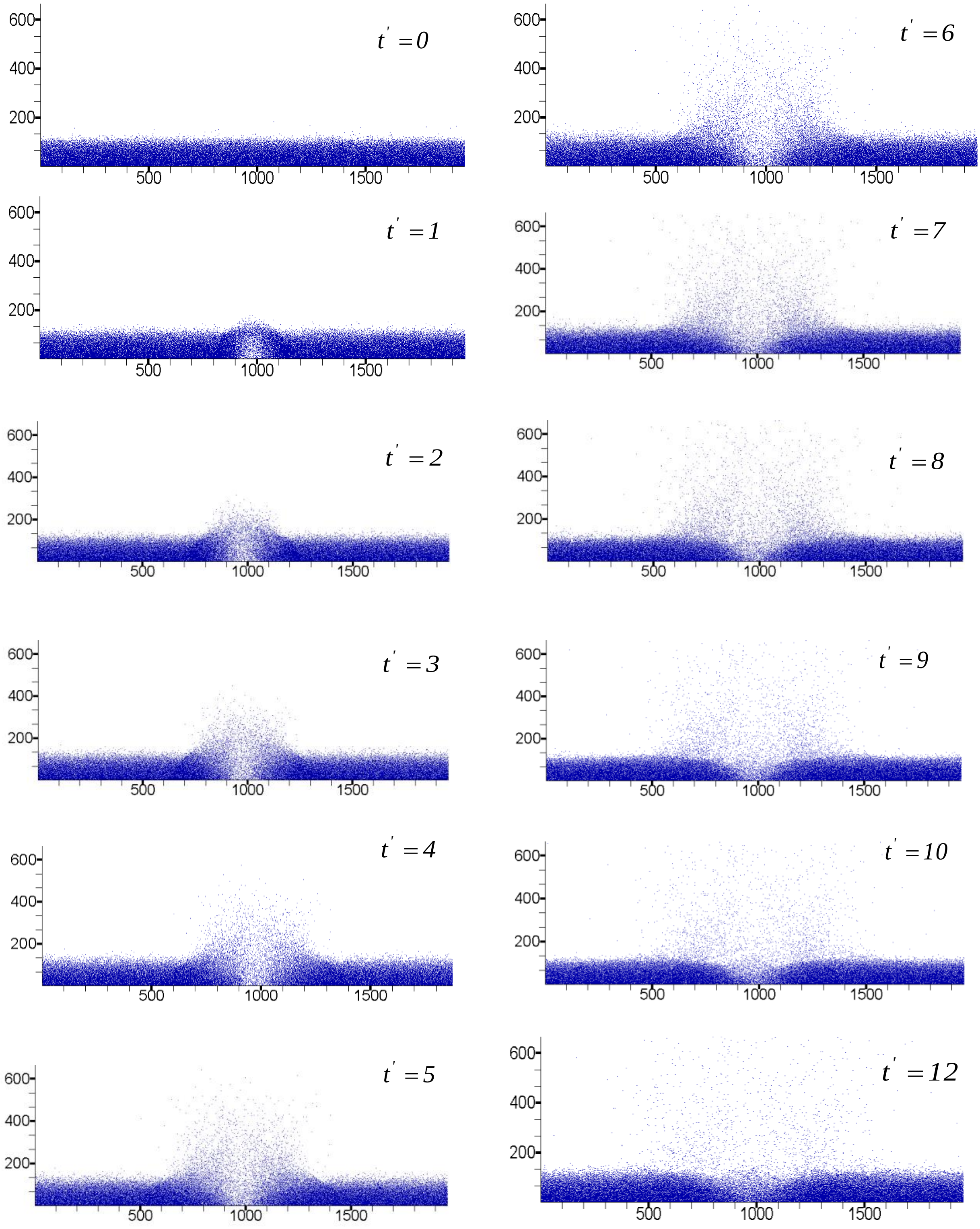

Fig. 1a. Time evolution of a shallow water explosion.

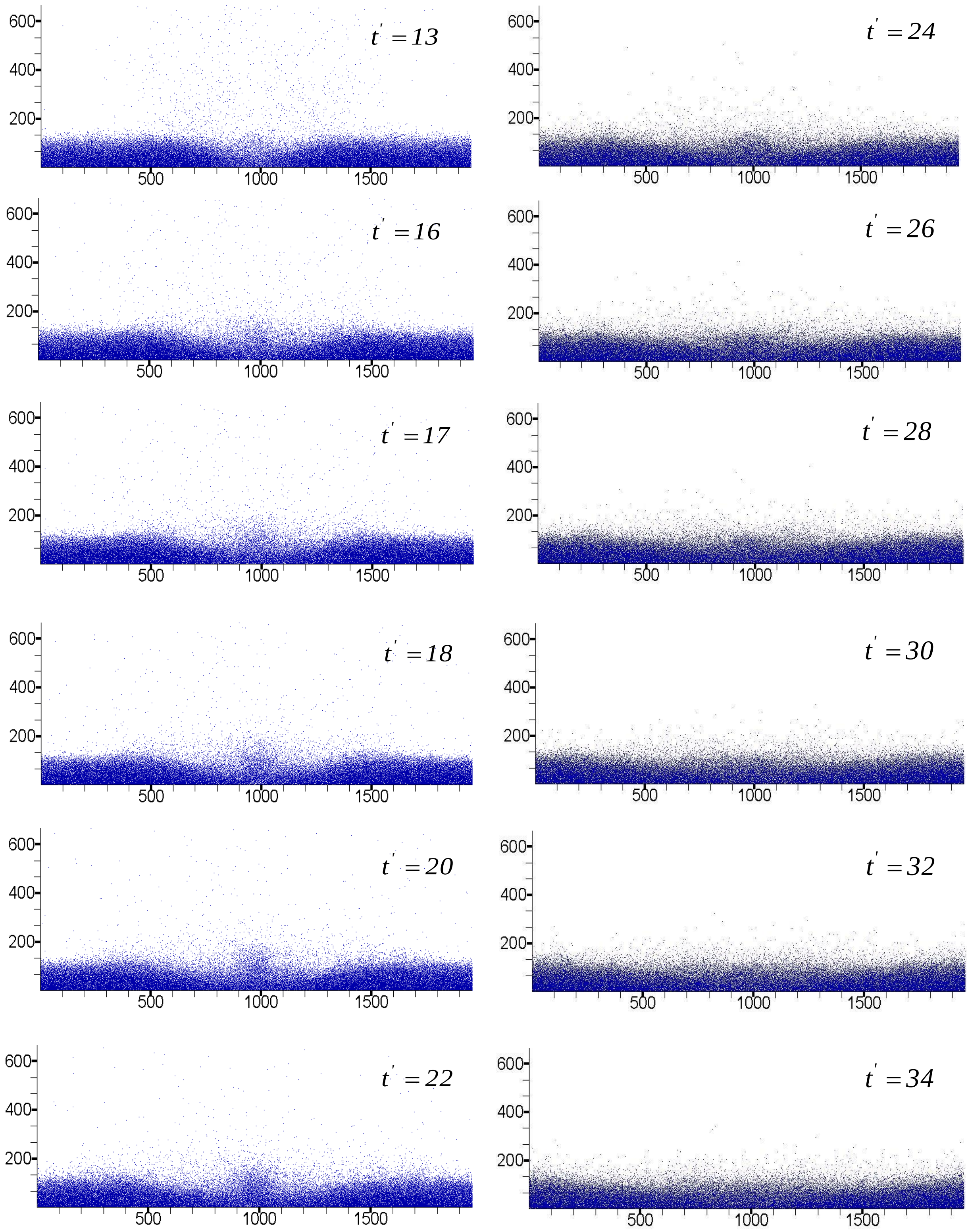

Fig. 1b. Time evolution of a shallow water explosion.

Using the procedure developed in [4, 5], one can calculate the radial density of the shock wave. Figure 2 shows the evolution of shock-wave shape in different sectors (counter-clockwise from x-axis) in an orderly sequence. The wave is moving from left to right. The temporal dependencies were approximated with polynomials of the seventh degree. The approximation allows calculating the velocity of the shock wave.

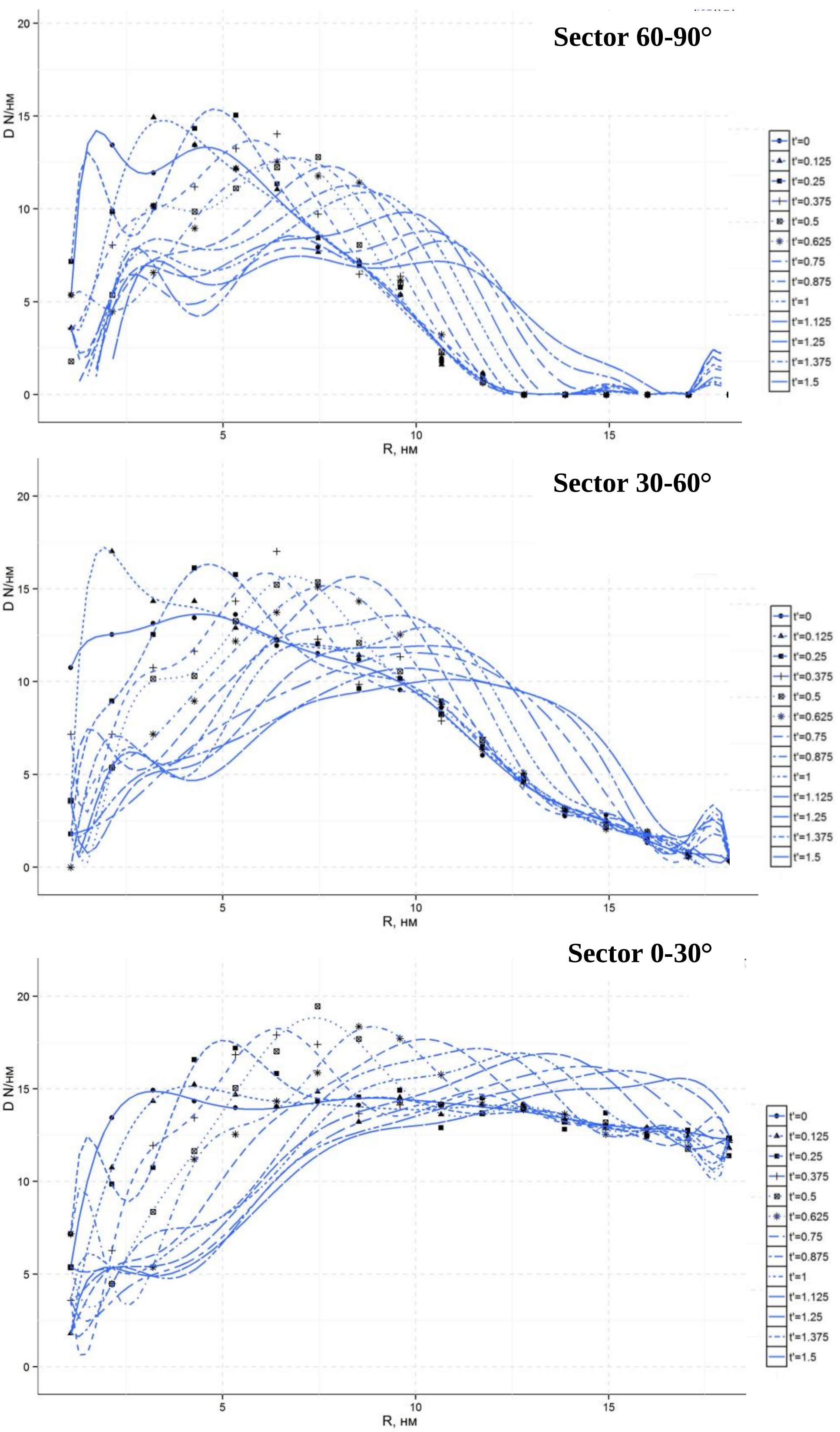

Fig. 2. Time evolution of shock-wave shape, t’ = 0 – 1.5.

As in the case of a deep water explosion, the height of the shock wave decreases with time whereas the width increases. The form of the shock wave is asymmetric too, and its asymmetry is increasing with time too, but contrary to the case of the deep water explosion the form of the shock wave in the shallow water explosion has an evident wavy character.

b) The explosive is doubled. The temporal evolution of underwater explosion is demonstrated in Fig. 3. The temporal variation of shock wave in different sectors (counter-clockwise from x-axis) is given in Fig. 4. The wave is moving from left to right.

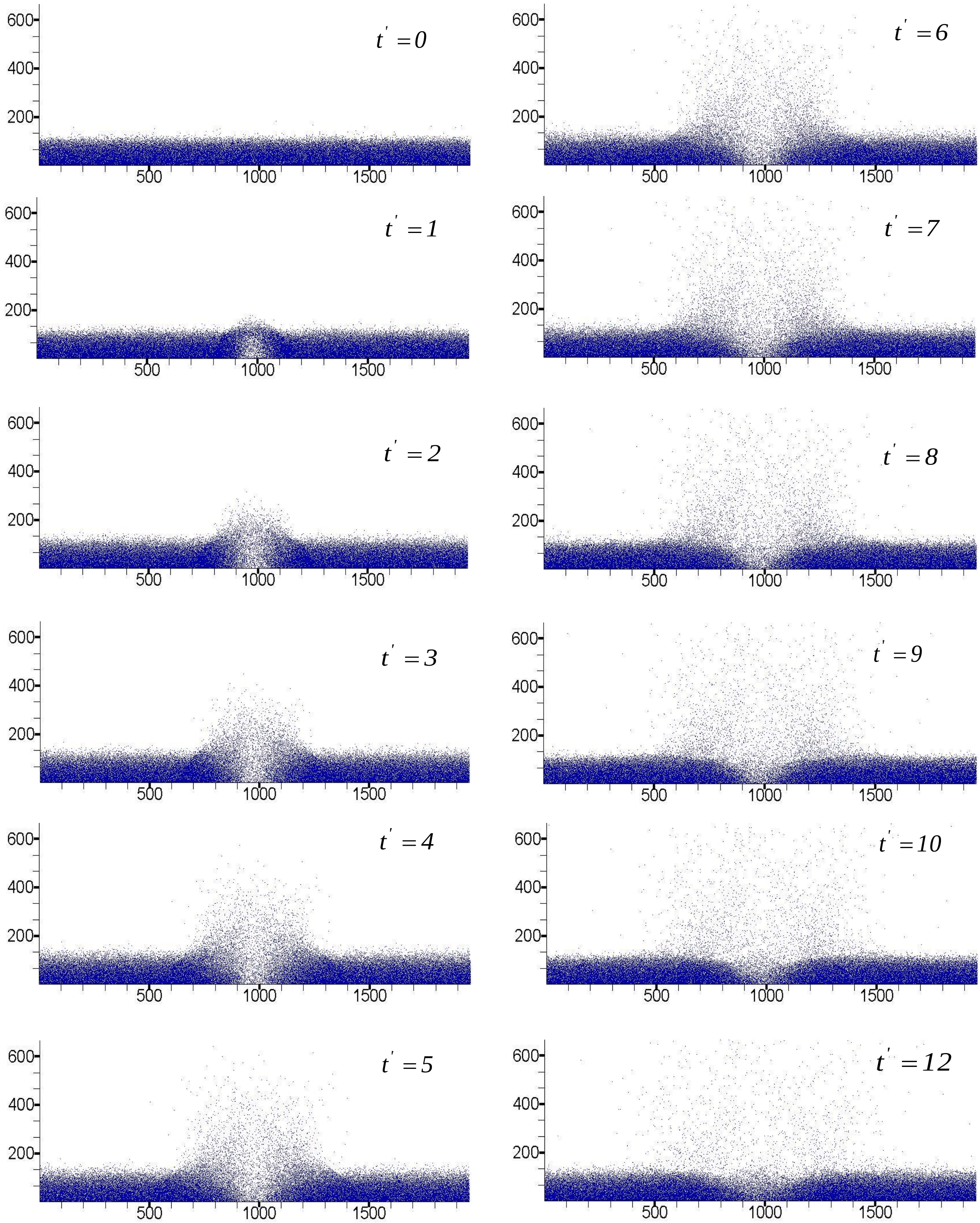

Fig. 3a. Time evolution of a shallow water explosion.

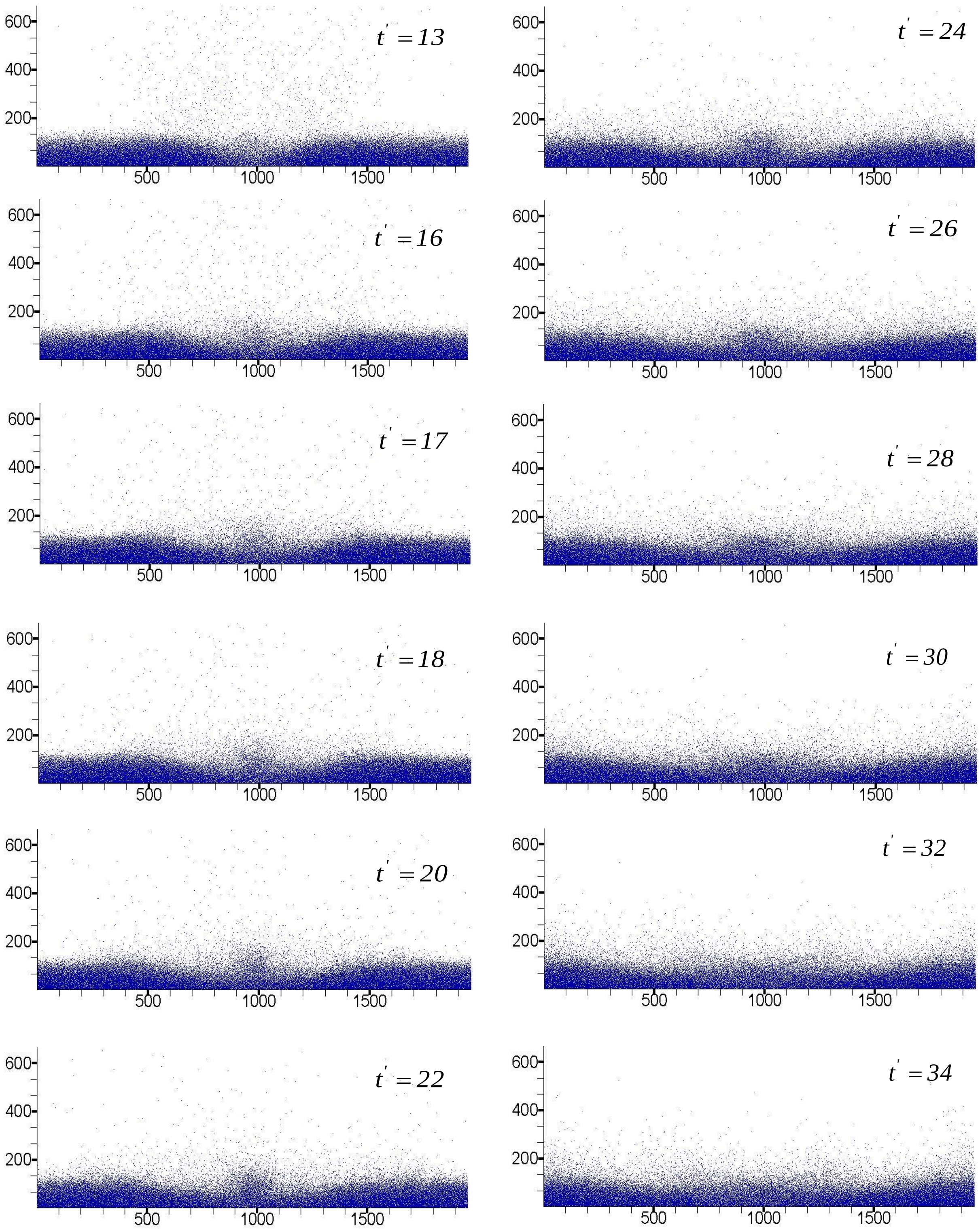

Fig. 3b. Time evolution of a shallow water explosion.

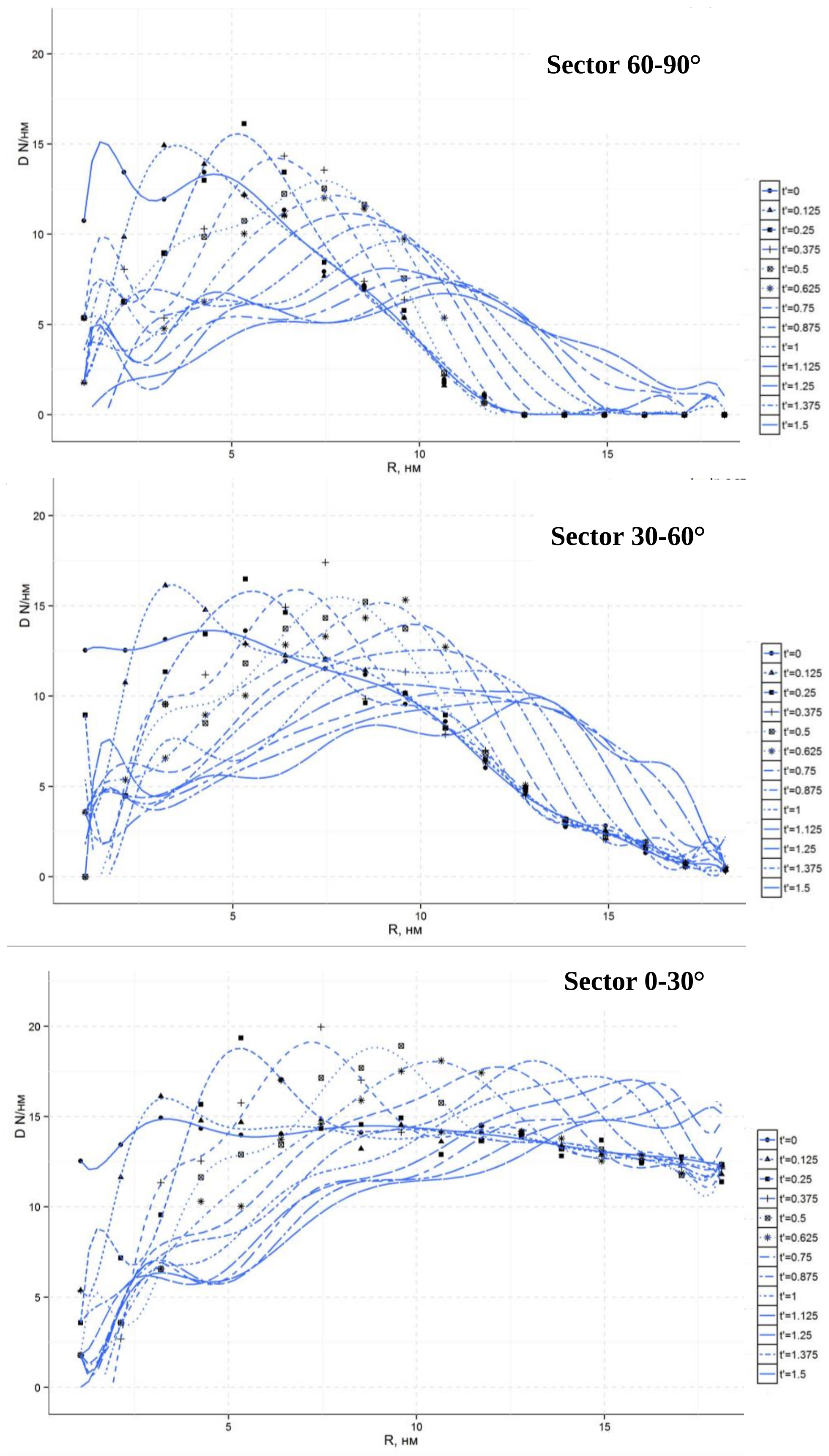

Fig. 4. Time evolution of shock-wave shape, t = 0 – 1.5.

The arrangement of particles in a standard circular explosive and in a double circular explosive is shown in Fig. 5.

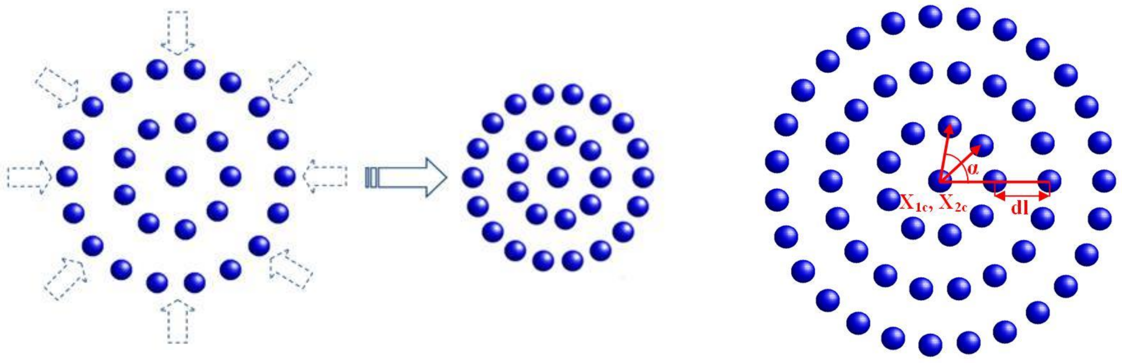

Fig. 5. Standard circular explosive (on the left) and double circular explosive (on the right).

As for the case of the standard explosive, the shock wave height decreases with time whereas the width increases; the form of the shock wave is also asymmetric, the asymmetry increases with time too, and the form of the shock wave is obtaining with time an evidently wavy character. The overall picture of explosion with a double explosive resembles that of with a standard explosive, but the process intensity, in particular, water particles emission to atmosphere is larger. The shock wave velocity for standard and doubled explosive is shown in Fig. 6. Time $t' = 1$ corresponds to real time $t = 7.072\,ps$. On this interval the velocity gradually decreases from 3014 m/s to 1808 m/s for the standard explosive and from 3617 m/s to 1959 m/s for the doubled explosive.

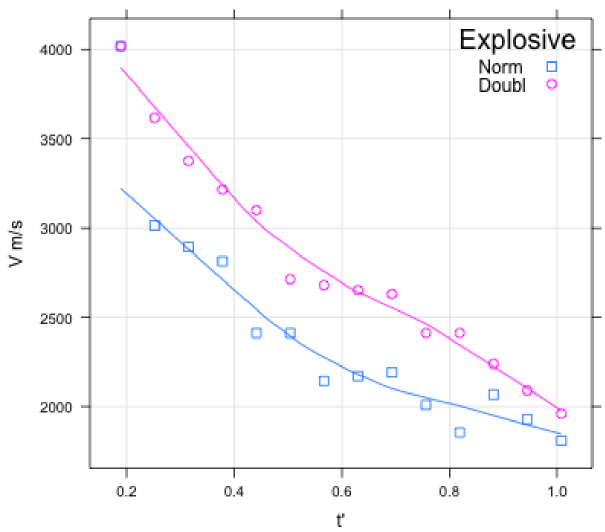

Fig. 6. Shock wave velocity on the time interval t' = 0 – 1.

4. Kadomtsev approach

In the previous works [4, 5] an asymmetric form of a shock wave arising in a deep water explosion was discovered. The impression is such as if the shock wave disintegrated, at least, into two parts. It should be emphasized that the disintegration started from the very beginning of forming the shock wave. We have suggested that such waves could be described with the Korteweg-de Vries-Burgers equation [6]:

$$u_t + u u_x + \beta u_{xxx} = \alpha u_{xx},$$

which is a combination of the Korteweg-de Vries (KdV) equation

$$u_t + u u_x + \beta u_{xxx} = 0,$$

and the Burgers equation

$$u_t + u u_x = \alpha u_{xx}.$$

Here α defines the dynamical viscosity, and β characterizes the dispersion in a system.

The most striking result of this investigation is that the form of the shock wave in the shallow water explosion has an evidently wavy character. This phenomenon is analyzed briefly in [6] for electromagnetic shock waves. Consider it in detail.

Following to the Kadomtsev approach [7] let us seek the solution of the Korteweg-de Vries-Burgers equation in the form of a stationary wave

$$u(x,t) = u(x - Vt),$$

traveling with the constant velocity V. In this case

$$du = \frac{\partial u}{\partial t} dt + \frac{\partial u}{\partial x} dx = 0.$$

Dividing by dt, one obtains

$$\frac{\partial u}{\partial t} = -V \frac{\partial u}{\partial x}, \qquad V = \frac{dx}{dt}.$$

Therefore one can rewrite the Korteweg-de Vries-Burgers equation as follows

$$(u - V)\frac{du}{dx} + \beta \frac{d^3 u}{dx^3} - \alpha \frac{d^2 u}{dx^2} = 0$$

or in a simpler form

$$(u - V)u' + \beta u''' - \alpha u'' = 0.$$

Upon integrating the equation with respect to x, we have

$$\beta u'' - \alpha u' - V u + \frac{u^2}{2} + f = 0,$$

where f is a constant.

Let us take up the coordinate x as time, and u as a coordinate of a certain fictitious particle having the mass β, which is oscillating in the field of the effective potential energy

$$U(u;V) = -V\frac{u^2}{2} + \frac{u^3}{6} + f u = const.$$

In such notation the last equation expresses the conservation law of the total energy $E = const$; the velocity V playing a role of a parameter.

Consider the form of the function $U(u;V)$. The constant f is an external force which displaces the equilibrium position around which the oscillations occur. If there is no an external force, we have

$$U(u;V) = -V\frac{u^2}{2} + \frac{u^3}{6}.$$

The extremum condition gives

$$-Vu + \frac{u^2}{2} = 0.$$

This equation has two roots

$$u_1 = 0, \qquad u_2 = 2V,$$

so the potential energy has the form (Fig. 7a). It is equal to zero at $u = 0$ and $u = 3V$. The points where $U(u) = E$ define the boundaries of motion area. They are turning points where the velocity of a fictitious particle is equal to zero. If the vibrations of the particle are small, they are almost harmonic and are localized near the minimum at $u_2 = 2V$.

The equation

$$\beta\frac{d^2u}{dx^2} - \alpha\frac{du}{dx} = -\frac{\partial U(u;V)}{\partial u} = Vu - \frac{u^2}{2}$$

may be interpreted as the equation of a nonlinear oscillator with damping.

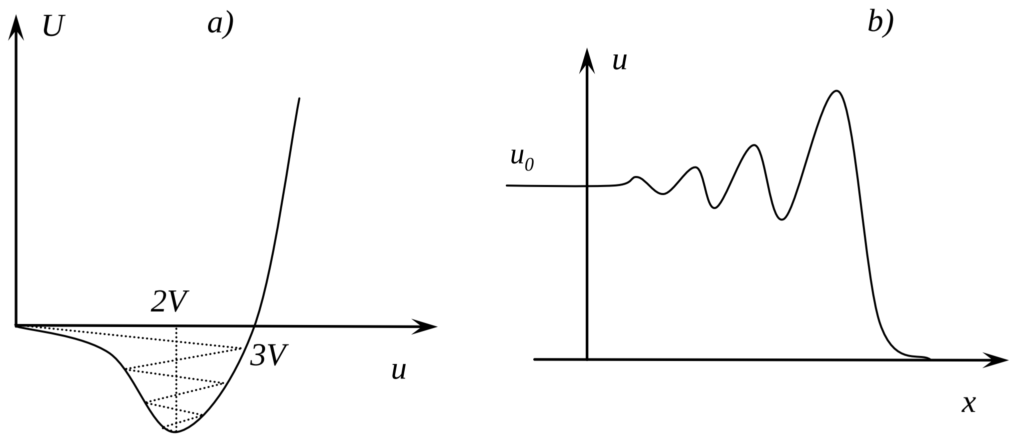

Fig. 7. Potential energy of a nonlinear oscillator (*a*) and a shock wave (*b*).
[B.B. Kadomtsev, *Collective Phenomena in Plasma* (1976)]

Considering the coordinate x as time, Kadomtsev writes that it is not difficult to construct the solution on the whole axis x [7]. According to Kadomtsev, it begins at the point $x = +\infty$ located at the origin of coordinates $u = 0$, then this point slides down into the potential well $U(u)$ where it performs damping vibrations, obtaining the value $u_0 = 2V$ at $x = -\infty$ (Fig. 7a). As a consequence, one obtains a shock wave having an oscillating structure (Fig. 7b). This semi-quantitative approach explains well the form of the shock waves observed in our computer simulations.

5. Conclusion

We have developed a method for studying the structure of shock waves arising in underwater explosions which were observed in molecular dynamics computer experiments. The most striking result of this investigation is that the form of the shock wave in the shallow water explosion has an evidently wavy character. This phenomenon is analyzed similar to the Kadomtsev approach [7] for electromagnetic shock waves.

References

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