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# APPLICATION OF PARTICULAR SOLUTIONS OF THE BURGERS EQUATION TO DESCRIBE THE EVOLUTION OF SHOCK WAVES OF DENSITY OF ELEMENTARY STEPS<sup>†</sup>

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Particular solutions of the Burgers equations (BE) with zero boundary conditions are investigated in an analytical form. For values of the shape parameter a greater than 1, but approximately equal to 1, the amplitude of the initial periodic perturbations depends nonmonotonically on the spatial coordinate, i.e. the initial perturbation can be considered as a shock wave. Particular BE solutions with zero boundary conditions describe a time decrease of the amplitude of initial nonmonotonic perturbations, which indicates the decay of the initial shock wave. At large values of the shape parameter  $a \gg 1$ , the amplitude of the initial periodic perturbations depends harmoniously on the spatial coordinate. It is shown that over time, the amplitude and the spatial derivative of the profile of such a perturbation decrease and tend to zero. Emphasis was put on the fact that particular BE solutions can be used to control numerical calculations related to the BE-based description of shock waves in the region of large spatial gradients, that is, under conditions of a manifold increase in spatial derivatives. These solutions are employed to describe the profile of a one-dimensional train of elementary steps with an orientation near <100>, formed during the growth of a NaCl single crystal from the vapor phase at the base of a macroscopic cleavage step. It is shown that the distribution of the step concentration with distance from the initial position of the macrostep adequately reflects the shock wave profile at the decay stage. The dimensionless parameters of the wave are determined, on the basis of which the estimates of the characteristic time of the shock wave decay are made.

**Keywords:** Burgers equation, analytical solutions, zero boundary conditions, shock wave, decay

PACS: PhySH: Surface & interfacial phenomena

It is known that vicinal surfaces during crystal growth from the vapor phase or solutions are subject to a certain type of morphological instability – bunching of steps [1-4]. The formation of step bunching is a very serious problem when growing perfect crystals and obtaining surfaces that are atomically smooth on a macroscale [5-7]. On the other hand, such instabilities lead to the formation of large-scale nanostructured surfaces, which can be used to obtain low-dimensional structures actual for various technological applications [8-13]. A theoretical description of the nonlinear processes that result in the development of such kind of instabilities is very complicated due to a variety of causes leading to the step bunching in real experimental conditions (stochasticity of growth processes in general, presence of impurities, surface electromigration effect, Ehrlich-Schwöbel effect, elastic stress fields, variable macroscopic fields, non-quasi-static effects, etc.) [14-20]. The current state of research of step bunching, in particular, induced by electric currents, is presented in the references given in [21], where it is shown how the general picture of the process of bunching depends on the short-range repulsive force between the steps. It is customary to distinguish between the steps bunching as a result of morphological instability and as a shock in a kinematic wave, when the flux of steps is determined only by their local density [3].

The study of kinematic ("shock") waves of steps on crystal surfaces was first carried out by Frank [22], and by Cabrera and Vermilyea [23], who used the results of the general analysis of kinematic waves done by Lighthill and Whitham [24]. Later, it was shown that the appearance of shock waves is accompanied by a characteristic curvature of the vicinal surface profile, reflecting the space-time distribution of the step density[25]. At the level of optical microscopy, kinematic waves are usually perceived as steps of macroscopic height. At that, they should be distinguished from another type of macro-steps associated with the anisotropy of the surface energy ("true" macro-steps) [25]. Subsequently, based on the experimental data, it was concluded that the characteristic macroscopic relief of shock waves can be formed under certain conditions of crystal growth (evaporation) on vicinal thermodynamically stable surfaces [26, 27]. As follows from [25], the appearance of shock waves with a curved profile of the vicinal surface under such conditions is the main result of the diffusion interaction of moving elementary steps.

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The dynamics of the macroscopic curved vicinal surface profile of a crystal growing from the vapor phase was studied in [28], in which the expressions for the average values of the ad atom concentration and the velocity of elementary steps were obtained by averaging over large spatial intervals. The nonlinear Korteweg-de Vries-Burgers (KVB) equation was obtained from the continuity equation for average values of the ad atom concentration and the velocity of elementary steps, taking phenomenological account of surface curvature [3, 29]. This equation describes the nonlinear dynamics of a train of parallel elementary steps on a macroscopically curved vicinal crystal surface. In a particular case, the KVB equation can transform into the Burgers equation (BE), which describes the formation and dynamics of shock waves.

The BE is a partial differential equation and it can be derived from the Navier-Stokes equations in the special case when the system under consideration has one spatial dimension [30]. Following [30], the BE for the fluid flow velocity u(x,t) is written in the next form:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \mu \frac{\partial^2 u}{\partial x^2},\tag{1}$$

where t and x are the time and coordinate along the flow, respectively,  $\mu > 0$  is the kinematic viscosity of the fluid. We consider the quantities t, x, and  $\mu$  to be dimensionless.

Equation (1) is used in various fields of applied physics: to study the appearance of shock waves in hydrodynamic mediums[31], to describe the steepening and overturning of waves on the water surface [32]. The BE is also used in nonlinear acoustics to study cylindrical and spherical shock waves, as well as waves in relaxing mediums[33,34].

It is known that the BE can be reduced to the heat conduction equation using the Hopf-Cole transformation [35, 36]. The analytical solution obtained in this case describes the velocity of the medium for an arbitrary initial spatial distribution [37]. However, the integrals included in the solution cannot be always represented in an analytical form. Therefore, preference is given to such analytical solutions that are expressed in terms of elementary functions and can be easily applied to the problem being solved.

The scientific literature provides analytical and numerical methods for solving the BE [31, 35-37]. The asymptotic of solutions of the BE with initial or boundary conditions on a finite interval with periodic boundary conditions is analyzed in [38]. It is shown that in a viscous medium, the profile initially at rest transforms into a traveling wave with decreasing amplitude. At viscosity values approaching zero, the asymptotic profile takes on a saw tooth shape with periodic derivative discontinuities, similar to Fay's solution on the half-line.

Numerical calculations of the BE on a finite interval allow us not only to find new solutions, but also to verify experimentally their asymptotic using analytical estimates. It is noted that the numerical simulation of functions with a discontinuous derivative complicates the calculations, because in the vicinity of the discontinuities, the standard methods become unstable. The latter fact causes multiple oscillations, leading to a loss of accuracy and incorrect results. The only way to avoid that is to use an adaptive step length on the spatial coordinate, which corresponds to a step reduction of 10-20 times compared to the original step length. But the marked possibility is limited. Therefore, all calculations must be checked using model analytical solutions.

Analytical solutions of the BE with periodic boundary conditions were obtained in [39]. These solutions are proposed to be considered as a model for the development of stable and convergent grid methods for the numerical analysis of viscous media motion. However, the analytical solutions obtained in this work, as reference ones, do not describe the formation of a shock wave, but its decay.

The purpose of this work is to obtain analytical solutions of the BE that describe both the formation of a shock wave, which is expressed in an increase in the steepness of the wave profile, and its decay, accompanied by a decrease in the steepness of its profile in a sufficiently wide time interval. The obtained solutions are used to describe some experimental results related to growth from the vapor phase (or evaporation) of alkali-haloid crystals.

### ANALYTICAL SOLUTIONS OF THE BE FOR SPATIALLY PERIODIC PERTURBATIONS WITH ZERO BOUNDARY CONDITIONS

Let us find the bounded solutions  $|u(x,t)| < \infty$  of the BE (1) on the interval  $x \in [0,L]$ , for times  $t \in [0,\infty]$  with the boundary conditions:

$$u(0,t) = u(L,t) = 0.$$
 (2)

The Hopf-Cole transformation (HC)  $u(x,t) = -2\mu \frac{1}{v(x,t)} \frac{\partial v(x,t)}{\partial x}$  [37] reduces the nonlinear equation (1) to the

linear heat equation for the function v(x,t):

$$\frac{\partial \mathbf{v}(\mathbf{x},t)}{\partial t} = \mu \frac{\partial^2 \mathbf{v}(\mathbf{x},t)}{\partial \mathbf{x}^2}.$$
 (3)

The boundary condition (2) implies the property of the function v(x,t) in the range of its variation and its boundary conditions are the following:

$$\mathbf{v}(x,t) \neq 0,\tag{4}$$

$$\frac{\partial \mathbf{v}(0,t)}{\partial x} = \frac{\partial \mathbf{v}(L,t)}{\partial x} = 0,$$
(5)

where  $0 \le x < L$ ,  $0 \le t < \infty$ .

Equation (3) has an infinite set of functions and conditions (4), (5) [39]:

$$\mathbf{v}_{n}(x,t) = \cos(\lambda_{n}x)\exp(-\mu\lambda_{n}^{2}t),\tag{6}$$

where  $\lambda_n = n\pi/L$ , n = 1, 2, 3, ...

Particular solutions (3) is determined up to a constant. Therefore, they can be represented as:

$$\mathbf{w}_{n}(x,t) = \mathbf{v}_{n}(x,t) + a,\tag{7}$$

where a is a constant. It follows from (4) that a > 1.

As a result of the HC transformation, we obtain particular BE solutions:

$$u_n(x,t) = 2\mu\lambda_n \frac{\sin(\lambda_n x)}{\cos(\lambda_n x) + a\exp(\mu\lambda_n^2 t)}.$$
 (8)

Solution (8) describes an infinite number of BE particular solutions for different values of constants  $a, \mu, n$ . Further, we call a the shape parameter of BE particular solutions, since its value determines the shape of the initial perturbation. Let us consider the dependence of solutions (8) on the value of the parameter a.

## DEPENDENCE OF THE BE SOLUTIONS ON TIME FOR DIFFERENT VALUES OF THE SHAPE PARAMETER $\,a$

At the initial moment of time (t = 0), ordinary BE particular solutions are described by a periodic function in the following form:

$$u_n(x,0) = 2\mu \frac{n\pi}{L} \frac{\sin(n\pi x/L)}{\cos(n\pi x/L) + a}.$$
(9)

For large positive values of the shape parameter  $a \gg 1$ , the initial perturbation is close to a harmonic signal:

$$u_n(x,0) \approx 2\mu \frac{n\pi}{aL} \sin\left(n\pi x/L\right) \left(1 - a^{-1} \cos\left(n\pi x/L\right)\right). \tag{10}$$

For finite values of the shape parameter  $a = 1 + \zeta$ , where  $0 \le \zeta << 1$ , a particular solution of the BE at the initial moment of time (9) is a periodic function which, at points x = (2k+1)L/n when  $\zeta \to 0$  ( $a \to 1$ ), has a singularity of the form:

$$u_n(x,0) = 2\mu \frac{n\pi}{L} \operatorname{tg}\left(\frac{n\pi x}{2L}\right),\tag{11}$$

where  $k = 0; \pm 1; \pm 2..., (2k+1) \le n$ .

It follows from (11) that solutions (8) are inapplicable for the shape parameter a = 1, since the boundedness condition of solutions is violated already for the initial perturbations (t = 0). Therefore, the range of variation of the shape parameter a, as noted above, is determined by the condition a > 1.

Let us determine the extreme values of the initial perturbation in the specified intervals of change in the shape

parameter. For  $0 < \zeta < 1$  at the initial moment of time (9) at points  $x_{\rm ext}^{\pm} = \frac{2L}{n\pi} \arccos\left(\frac{\Delta_{\pm}}{\sqrt{1+2\Delta_{\pm}^2}}\right)$ , the BE positive

particular solutions are bounded and have extreme values:

$$u_n\left(x_{\text{ext}}^{\pm},0\right) = \pm 2\frac{\mu\lambda_n}{\sqrt{\zeta}\sqrt{2+\zeta}},\tag{12}$$

where 
$$\Delta_{\pm} = \pm \sqrt{\frac{\zeta}{2}}$$
.

It follows from (12) that, for example, for n=2, when  $\zeta$  increases from zero to infinity, the parameter  $\Delta_-$  changes from zero to minus infinity, and the coordinate of the maximum shifts from L/2 to L/4. When  $\zeta$  increases from zero to infinity, the parameter  $\Delta_+$ , on the contrary, changes from zero to plus infinity, and the coordinate of the minimum shifts from L/2 to 3L/4. In all these cases, as  $\zeta$  increases, the initial wave profile spreads and its amplitude decreases.

### NUMERICAL ANALYSIS OF THE TEMPORAL DYNAMICS OF THE BE PARTICULAR SOLUTIONS

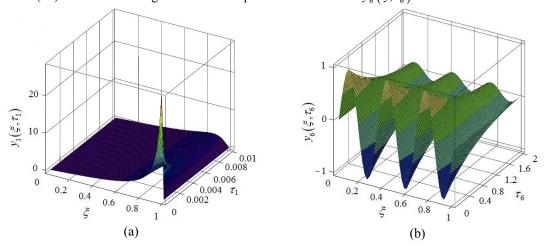
As an example of how the profile of (8) changes over time, let us plot the dependence of the dimensionless velocity  $y_n(x,\tau_n) = u_n(x,t)/(2n\pi\mu/L)$  on the dimensionless time  $\tau_n = \mu(n\pi/L)^2 t$  and the dimensionless coordinate  $\xi = x/L$  for a given mode n. At that, the areas of time and coordinate changes remain the same:  $0 \le \tau_n < \infty$ ,  $0 \le \xi \le 1$ .

The BE particular solution in new variables takes the form:

$$y_n(\xi, \tau_n) = \frac{\sin(n\pi\xi)}{\cos(n\pi\xi) + a\exp(\tau_n)}.$$
 (13)

Figure 1(a) shows the time dynamics of the BE particular solution (13) for the mode n=1 and for the shape parameter value a=1.001. Such particular solution describes the decrease in the nonmonotonical initial perturbation amplitude (11) with time, which corresponds to shock waves. The figure shows an exponential decrease in  $y_1(\xi, \tau_1)$  over time.

Figure 1(b) shows the time dynamics of the BE particular solution (13) for the mode n=6 and for a large value of the shape parameter a=15. The ordinary BE particular solution describes the decrease in the initial perturbation amplitude (10) with time. The figure shows an exponential decrease in  $y_6(\xi, \tau_6)$  over time.



**Figure. 1.** Time dynamics of the BE particular solution (13): (a) - for n = 1 and the shape parameter a = 1.001; (b) - for n = 6 and the shape parameter a = 15.

Thus, the study of periodic particular BE solutions shows that the amplitude of the perturbation, as well as its spatial derivative, decreases with time to zero. This behavior of the perturbation indicates its decay and does not describe the formation of shock waves.

### RESULTS AND DISCUSSION

### Experimental results on the study of the growth of alkali halide crystals from the vapor phase

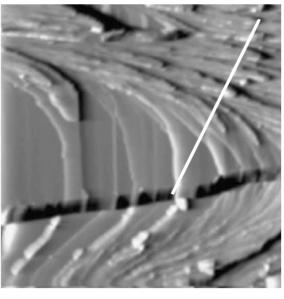
In [28], the density waves of monatomic steps with <10> orientation on thermodynamically stable vicinal surfaces of NaCl(100) were investigated under conditions of very low super saturation ( $10^{-5}$ - $10^{-4}$ ) and high temperatures ( $\sim 10^{3}$  K). The wave structure is adequately described on the basis of the analytical solution of the KVB equation obtained by the

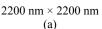
averaging method for the one-dimensional (1D) model of the train of steps. This allows, on the one hand, to confirm the conclusion that the observed step bunches have a kinematic origin, on the other hand, to show that they are monotonic shock waves without oscillations. Dimensionless characteristics of shock waves, such as the average step density  $\rho_0 \lambda_s$ , amplitude  $A_0$ , wave number  $q_0$  and velocity  $u_0$  were determined. Here  $\lambda_s$  is the ad molecule mean free path,  $\rho_0 = 1/l_0$ ,  $l_0$  is the average width of the vicinal surface terrace. Since the dimensionless coefficients of the obtained KVB equation are determined by the crystal parameters at the growth (evaporation) stage, this allowed us to take a fresh look at the physics of the process and take into account the effects of dispersion and dissipation in the experimental studies. The value of the parameter  $v^{-1} = \rho_0 \lambda_s / q_0 \ge 1$  obtained in [28] indicated that, during the formation of the investigated kinematic waves, the contribution of the dispersion effect to the competition with nonlinear effects is quite significant. This value agrees with the ratio of the coefficients at spatial derivatives of higher order in the KVB equation obtained using the method of many scales [29], and allows us to conclude that shock waves described by the BE should be expected on vicinal NaCl (100) surfaces in the temperature range under study at higher values of super saturation, when  $v \ll 1$ . Such shock waves, characterized by the presence of a saw tooth profile and discontinuities in the density of elementary steps, were found on the pore growth surfaces formed during the thermally induced motion of pores in NaCl single crystals [40].

The microcrystallization conditions that can be created in pores (high temperatures and low super saturations [28]) are difficult to implement in conventional growth experiments. This is mainly due to the technical difficulties in maintaining and controlling both the required super saturation values and the temperatures themselves. The value of (super-) under saturation on the (growing) evaporating surfaces of pores inside a crystal can be controlled either by the value of the temperature gradient during their thermally induced motion, or by the difference in local surface curvatures during relaxation of their shape under isothermal conditions (see, references in [28]).

A similar technique for studying the processes of dissolution and growth of crystals from solutions has been developed for liquid inclusions (see references in [41, 42]). In the case of saturated solution inclusions in alkali-halide crystals, the activation energies of dissolution (growth) processes are quite small. This makes it possible to study the spontaneous displacement of inclusions as a whole by creating inhomogeneous distributions of structural defects in the crystal (point defects of radiation origin, dislocations, etc.) [41], as well as the transition from the kinetic regime of motion of inclusions, when the processes at the inclusion-matrix interface are determining, to the diffusion regime, when the processes of substance transfer through the inclusion volume are decisive [42].

Meanwhile, the use of the moving pore (liquid inclusion) technique excludes the possibility of studying the dynamics of elementary steps in-situ and allows one to study only stationary stages of the growth processes of alkali halide crystals. And in order to obtain data on the characteristic times of formation (decay) of shock waves of the elementary steps density, necessary for the interpretation of theoretical results, it is important to study exactly the non-stationary stages of the growth (evaporation) on the vicinal surfaces of crystals.





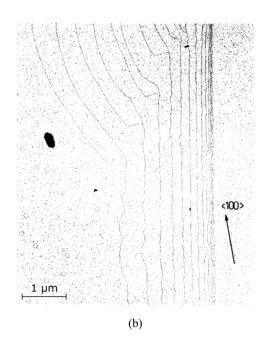


Figure 2.(a) - AFM micrograph showing the macrostep formed on the KCl(100) surface during crystal cleavage in vacuum [44] and (b) – the electron microscope image of the surface decorated with gold particles showing the "decay" of a similar macrostep into elementary steps during growth of NaCl(100) from the vapor phase (T = 620 K,  $R/R_0 = 5$ ,  $\Delta\mu = 0.09 \text{ eV}$ , A = 10 nm) [43].

Figure 2 shows the atomic force microscopy (AFM) image of the KCl(100) surface (a) and the electron microscope image of the NaCl(100) surface decorated with gold particles (b). The image (b) of the "decay" process during the growth

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from the vapor phase of a macroscopic step formed on NaCl(100) upon cleavage of the crystal in vacuum is taken from [43]. The presence of such steps and their height can be reliably monitored by AFM, as it seen from Figure 2(a) taken from [44]. By decay we mean the process of forming a train of elementary steps of variable density at macrostep's base. At a distant stage of this process, one should expect a complete "splitting" of the macrostep into elementary steps. The reason is that vicinal NaCl surfaces near (100) are thermodynamically stable and the existence of such macrosteps is thermodynamically disadvantageous [28]. In this case, the elementary steps have a height of 2a, which is obviously due to a relatively high value of super saturation in the vapor phase at a given temperature (T = 620 K) [43]. However, Figure 2(b) clearly shows the process of simultaneous decay of double-height steps into monoatomic ones. This process is assisted by the deviation of the orientation of both the macrostep itself and the double steps attached to it from the dense packing direction. The observed faceting of the double steps indicates that their disintegration into monoatomic steps begins from the <10> directions, for which the speeds of the steps are greater than that in the <10> direction.

The area of the NaCl(100) growth surface decorated with gold particles, shown in Figure 2(b), allows us to reconstruct its topography quite accurately and estimate the formation time of the studied train of elementary (2a) steps of variable density. Therefore, the experimental data presented in Figure 2(b) were used to interpret the obtained theoretical results describing the decay of shock waves, i.e. the space-time evolution of perturbations with the amplitudes  $a \ge 1$  at the initial moment of time. Here A is the thickness of the evaporated layer, R is the evaporation rate,  $R/R_0$  is the super saturation coefficient calculated from T and R on the basis of the temperature dependence of the saturated vapor pressure  $P_0$  [45],  $\Delta \mu = kT \ln (R/R_0)$ . The train of elementary (2a) steps in Figure 2(b) was digitized and the obtained values of the concentration ( $\rho \lambda_s$ ) of steps, taking into account the width ( $l = 1/\rho$ ) of the terraces adjacent to them, are presented as a function of the longitudinal coordinate x (in units  $\lambda_s$ ) in Figure 3.

To make the values of the step density ( $\rho$ ) and longitudinal coordinate dimensionless, we used the value  $\lambda_s$ , obtained at T=620 K on the basis of the empirical temperature dependence presented in [29]. This value agrees to within tenths with the data presented in [43] for the conditions of the considered growth experiment.

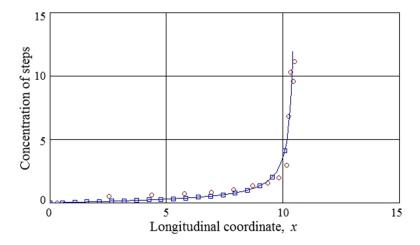


Figure 3. The structure of the shock wave of the elementary step density, shown in Figure 2(b), at the decay stage: symbols "o" are the experimental values of the step concentration in the wave; the solid line and symbols "o" are the result of calculations using formula (8).

### Description of the experimental results of the NaCl crystal growth from the vapor phase by the BE particular solutions

The structure of the kinematic wave, represented by the grouping of elementary (2a) steps shown in Figure (b), is distinguished by the following characteristic features: the presence of a segment of the sharp change in the profile of the initial perturbation and its subsequent smooth decrease to the minimum value. Such the change in the step concentration with the distance from the macrostep initial position is in qualitative agreement with the profile of the shock wave described by the BE particular solution at the stage of its decay at a given mode n = 1 (Figure 1(a)).

Before moving on to the interpretation of the experimental data based on the analytical solutions (8) and (13), we made the estimates of the coefficient  $\mu$  [28] taking into account the equilibrium concentration of ad molecules on an atomically smooth surface  $\xi_{a0}$ . Estimating  $\xi_{a0} \sim 10^{-9}$  by the saturated vapor pressure of NaCl [45] and assuming  $q \sim 0.01(\rho_0 \lambda_s)$ , with the known  $\sigma$  and  $\lambda_s$  [28], we found that the coefficient at the dissipative term in the BE is  $\mu \sim 1$ .

Using the Wolfram Mathematica package, the obtained experimental dependence of the step concentration on the longitudinal coordinate was approximated by the theoretical dependence based on equation (8) at n = 1 (solid line and symbols" or in Figure 3). This made it possible to obtain the values of the dimensionless parameters of the shock wave at

the decay stage (Table 1). Here  $f_A$  is the amplitude of the wave,  $f_0$  is its pedestal, a is the shape parameter of the initial perturbation, L is the half-width of the wave front, t is the dimensionless time.

Table 1. Parameters of the shock wave (Figure 3) at the decay stage.

μ	L	а	t	$f_0$	$f_{\scriptscriptstyle A}$
0.55	10.35	1.0001	0.005	1.37	11.50

To interpret the obtained values of the dimensionless parameters under the conditions of the considered experiment, the data on the real time of formation of the train of double-height steps in Figure 2(b) are needed. Unfortunately, these data are not given in [43]; however, the image of a spiral consisting of monoatomic height steps under the same experimental conditions at the nonstationary growth stage is presented. Earlier, when studying the morphology of evaporation (growth) spirals and the dynamics of motion of monatomic and double-height steps in a wide range of temperatures and under saturations, the normalized velocities of isolated steps were measured [46]. On their basis, the velocities of steps in the spiral and in the train (Figure 2(b)) were calculated, which, when reduced to the same effective super saturation under the experimental conditions [43], were  $3.3 \cdot 10^{-10}$  m/s and  $1.3 \cdot 10^{-10}$  m/s, respectively. This allowed us to estimate the time of the nonstationary growth stage in Figure 2(b) as  $t_{\rm exp} \sim 1$  hour, taking into account the value  $R/R_0 = 5$ .

In the kinematic wave theory, the characteristic time of a shock wave decay is considered to be the time during which the wave amplitude decreases by a factor of e. For the shock wave parameters presented in Table 1, the characteristic decay time was  $t_{\rm d}=0.057$ . During this time, under the conditions of the considered experiment, a train of elementary steps could propagate over a distance  $L_{\rm 2} \approx 109.4$  in  $\lambda_{\rm s}$  units with the speed of double steps, or over a distance  $L_{\rm 1} \approx 277.9$  with the speed of monoatomic steps. Assuming  $q \sim 1/2L$ , we obtain for the parameter  $v \sim q/(\rho_0\lambda_s)=0.019$ , which is close to the value used to estimate the value of  $\mu$ . However, at that, the corresponding values of the average width of the terraces are several times greater than the value of  $2\lambda_{\rm s}$ . This indicates that the diffusion interaction of elementary steps, which is responsible for the formation of shock waves, is very weak under these experimental conditions. Since, theoretically, the processes of formation and decay of shock waves are mutually reversible, their detection under the considered experimental conditions is practically unlikely. Anyway, despite the numerous published results of studies of the morphology of the growth (evaporation) surfaces of alkaline-halide crystals in the considered temperature range, we do not know such data. It should be noted that the considered experiment is a model one in the sense that it is not the decay of the "true" shock wave that is investigated, but its model in the form of a macrostep on the singular crystal surface, the vicinals to which are thermodynamically stable.

#### **CONCLUSIONS**

In this paper, particular solutions of the BE with zero boundary conditions are investigated in an analytical form to describe the decay of shock waves. It is shown that the amplitude of the initial periodic perturbation for values of the shape parameter a greater than 1, but about 1, nonmonotonically depends on the spatial coordinate. The particular solution of the BE describes a time decrease of the amplitude of the initial nonmonotonic perturbation, which can be considered as a shock wave. Such behavior of the perturbation indicates the decay of the initial shock wave. For large values of the shape parameter a >> 1, the amplitude of the initial periodic perturbation depends harmonically on the spatial coordinate. It is shown that over time the amplitude and the spatial derivative of such perturbation decrease and tend to zero. Particular solutions of the BE with zero boundary conditions may be used to control numerical calculations related to the BE-based description of shock waves in the region of large spatial gradients, that is, under conditions of a manifold increase in spatial derivatives. Such solutions were employed to describe the profile of a one-dimensional train of elementary steps with an orientation near <100>, formed during the growth of a NaCl single crystal from the vapor phase at the base of a macroscopic cleavage step. It is shown that the distribution of the step concentration with a distance from the initial position of the macrostep adequately reflected the shock wave profile at the decay stage. The dimensionless wave parameters were determined, on the basis of which the estimates of the characteristic decay time of the shock wave were performed.

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### ЗАСТОСУВАННЯ ЧАСТИННИХ РОЗВ'ЯЗКІВ РІВНЯННЯ БЮРГЕРСА ДЛЯ ОПИСУ ЕВОЛЮЦІЇ УДАРНИХ ХВИЛЬ ГУСТИНИ ЕЛЕМЕНТАРНИХ СХОДИН

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Частинні розв'язки РБ з нульовими граничними умовами досліджені в аналітичній формі. Для значень параметра форми *а* більше, але приблизно рівному 1, амплітуда початкових періодичних збурень немонотонно залежить від просторової координати, тобто початкове збурення можна розглядати як ударну хвилю. Частинні розв'язки РБ з нульовими граничними умовами описують зменшення з часом початкової амплітуди немонотонних збурень, що свідчить про затухання початкової ударної хвилі. При великих значеннях параметра форми *а* >> 1 амплітуда початкових періодичних збурень гармонійно залежить від просторової координати. Показано, що з часом амплітуда та просторова похідна профілю такого збурення зменшуються і прагнуть до нуля. Наголошено, що періодичні аналітичні розв'язки РБ з нульовими граничними умовами можуть бути використані для контролю числових розрахунків, пов'язаних з описом ударних хвиль на основі РБ в області великих просторових градієнтів, тобто в умовах багаторазового збільшення просторових похідних. Ці розв'язки використані для опису профілю одновимірного ешелону елементарних сходинок з орієнтацією поблизу <100>, що сформувався при рості монокристала NaCl з парової фази біля основи макроскопічної сходини відколу. Показано, що розподіл концентрації сходинок з відстанню від початкового положення макросходини адекватно відображає профіль ударної хвилі на стадії розпаду. Визначено безрозмірні параметри хвилі, на підставі яких зроблено оцінки характерного часу її розпаду.

Ключові слова: рівняння Бюргерса, нульові граничні умови, аналітичні розв'язки, ударна хвиля, розпад