NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2011, 2 (3), P. 65–70

UDC 539.3

NONLINEAR DYNAMIC VARIATIONS IN INTERNAL STRUCTURE OF A COMPLEX LATTICE

A. V. Porubov[1], B. R. Andrievsky[1]

[1]Institute for Problems in Mechanical Engineering of RAS, Saint Petersburg, Russia
alexey.porubov@gmail.com

PACS 46.25.Cc, 68.35.Rh

Essentially nonlinear model of a crystalline bi-atomic lattice described by coupled nonlinear equations, is considered. Its nonlinear wave solutions account for dynamic variations in an internal structure of the lattice due to an influence of a dynamic loading. Numerical simulations are performed to study evolution of a kink-shaped dynamic variations in an internal structure of the lattice. Special attention is paid on the transition from kink-shaped to bell-shaped variations. It is shown how predictions of the known exact traveling wave solutions may help in understanding and explanation of evolution of localized waves of permanent shape and velocity in numerical solutions.

Keywords: bi-atomic lattice, numerical simulations.

Introduction

The cardinal, qualitative variations of the cell properties, lowering of potential barriers, switching of interatomic connections, arising of singular defects and other damages, phase transitions require development of essentially nonlinear models of a crystalline lattice taking into account deep variations in the structure. Recently such a nonlinear model of a crystalline bi-atomic lattice has been developed in Refs. [1,2]. The variations in the internal structure are described by coupled nonlinear equations which are derived for the vectors of macro-displacement U and relative micro-displacement u for the pair of atoms with masses m_1, m_2,

$$\mathbf{U} = \frac{m_1\mathbf{U_1} + m_2\mathbf{U_2}}{m_1 + m_2}, \ \mathbf{u} = \frac{\mathbf{U_1} - \mathbf{U_2}}{a}$$

where a is a period of sub-lattice. The first variable allows us to describe macro-dispalcements, while the second variable accounts for the reference displacement of the atoms in the lattice. In the one-dimensional (1D) case, the coupled governing equations read [1,2]

$$\rho U_{tt} - E\, U_{xx} = S(\cos(u) - 1)_x, \tag{1}$$

$$\mu u_{tt} - \kappa u_{xx} = (SU_x - p)\sin(u). \tag{2}$$

Nonlinearity is introduced via the trigonometric functions that ensures description of translational symmetry in the crystalline lattice. The 1D formulation allows some analytical solutions to account for dynamic variations in the internal structure governed by function u while the strain function $v = U_x$ accounts for an external loading of the lattice. Of special interest are bell-shaped and kink-shaped localized solutions [3–7]. However, they belong to the traveling wave solutions, hence they cannot account for arising of localized internal variations. In particular, existence of the bell-shaped or kink-shaped dynamic structure depends on the phase velocity as follows from exact solutions [3]. However, how one or another velocity may be achieved from rather arbitrary input for u and v? Only numerical simulations may answer this question. Previously the domain of the wave velocities has been studied where both macro- and micro-

Table 1. Wave shapes for $\sigma = 0$

V^2	$(0; c_L^2 - c_0^2)$	$(c_L^2 - c_0^2; c_L^2)$	$(c_L^2; c_L^2 + c_0^2)$	$> c_L^2 + c_0^2$
Shape of v	Tensile (4)	Tensile (4)	Compression (5)	Compression (4)
Shape of u	Kink	Bell-shaped	Kink	Kink
Choice of $Q_\pm$	Q_+	Q_-	Q_+	Q_+

bell-shaped strain waves co-exist [4–6]. Only some preliminary results obtained for the kinks in Ref. [7]. Now we consider the kink-shaped waves for u. Like in Refs. [4–6] the use of particular exact solution to design and describe numerical results is studied.

1. Exact kink-type solution

The function u may be found from Eq.(1) when all functions depend only on the phase variable $\theta = x - Vt - x_{11}$,

$$\cos(u) = 1 - \frac{(E - \rho V^2)U_\theta - \sigma}{S}, \tag{3}$$

where σ is a constant of integration. It is known that only bell-shaped exact localized traveling wave solutions exist for the macro-strain v [3]:

$$v_1 = \frac{A}{Q\cosh(k\,\theta) + 1}, \tag{4}$$

$$v_2 = -\frac{A}{Q\cosh(k\,\theta) - 1}. \tag{5}$$

whose parameters are defined for two values of σ, $\sigma = 0$ and $\sigma = -2S$ [3]. Thus, for $\sigma = 0$ we obtain

$$A = \frac{4\,S}{\rho(c_0^2 + c_L^2 - V^2)}, Q_\pm = \pm\frac{c_L^2 - V^2 - c_0^2}{c_L^2 - V^2 + c_0^2}, k = 2\sqrt{\frac{p}{\mu(c_l^2 - V^2)}} \tag{6}$$

where $c_L^2 = E/\rho$, $c_l^2 = \kappa/\mu$, $c_0^2 = S^2/(p\,\rho)$.

Depending on the value of the phase velocity, see Table 1, Eq.(3) gives rise to the solution for u in the kink-shaped or in the bell-shaped form [3–6]. In this paper we consider only the former solution which reads

$$u = \pm\arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right) \text{ for } \theta > 0, \tag{7}$$

$$u = \pm 2\pi \mp \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right) \text{ for } \theta \le 0, \tag{8}$$

In particular, the kink-shaped solution exists in the interval $(0; c_L^2 - c_0^2)$ as follows from Table 1. while the bell-shaped solution for u [3]

$$u = \pm\arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right), \tag{9}$$

exists in the neighboring interval of velocities $(c_L^2 - c_0^2; c_L^2)$. Previously we have obtained in [7] that moving kink-shaped wave of internal variations u may arise in a lattice even if its initial velocity lies within the neighboring interval $(c_L^2 - c_0^2; c_L^2)$. The kink velocity is changed due to

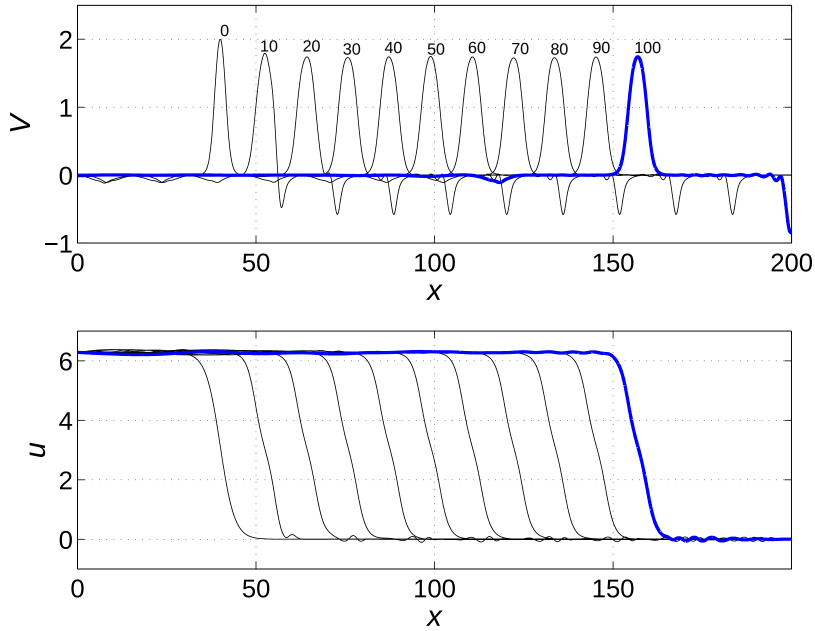

Fig. 1. Simultaneous propagation of localized bell-shaped macro-strain wave v and the kink-shaped wave u in the interval of velocities prescribed by the exact solution. Points of time correspond to the neighboring peaks. Final wave profiles are allocated in bold.

variations in the amplitude of the input of external loading v. Now we call attention to the waves evolution caused by variation in the relative position of the inputs for u and v.

2. Transition from kink to bell-shaped moving variations in the structure

To solve Eqs. (1), (2) numerically the standard MATLAB routine *ode45* is used [8]. The parameters chosen are $S = 1$, $p = 1$, $\rho = 1$, $c_0 = 1$, $c_L = 1.6$, $c_l = 2$, then the suitable for kinks values of V lie in the interval $(0, 1.25)$. The initial condition for v is chosen in the form (4) with $Q = Q_+$ and with initial velocity V. The condition for u is used in the form slightly differing form that of described by Eqs.(7), (8), namely, $u = \pi(1 - \tanh(k(x - x_{12})))$ where $k = 0.25$ is chosen to be as close as possible to the shape of the solution (7), (8).

First the case is considered when initial positions x_{11} of the input for v and x_{12} of that of u coincide and equal to 40 units. Shown in Fig. 1 is rather fast transition of the input u to that of the exact solution (7), (8) and further simultaneous stable propagation of this kink with the bell-shaped wave of v or an external loading. The velocity of the waves propagation lies in the interval $(c_L^2 - c_0^2; c_L^2)$ prescribed by the exact solution.

The initial position of the inputs should coincide according to the exact solution. Small difference in the relative position, $x_{11} = 40$, $x_{12} = 37.5$, yields perturbations on the profiles of the waves propagating with the velocity from the interval $(0; c_L^2 - c_0^2)$, see Fig. 2. Further increase in the relative initial positions, $x_{11} = 40$, $x_{12} = 36$, gives rise to a splitting of the wave v into two localized bell-shaped parts what is clearly seen at the final bold curve in Fig. 3. One can see that one part continues to move together with the kink-shaped wave u while the second one propagates faster. The last wave gives rise to an appearance of perturbations in the shape of u trapped by this part of v. Finally, at larger relative initial distance, $x_{11} = 40$, $x_{12} = 35$, the initial condition for u also splits into two parts as shown in Fig. 4. The kink-shaped part propagates with corresponding part of v like in Fig. 3 while the new bell-shaped part moves faster together

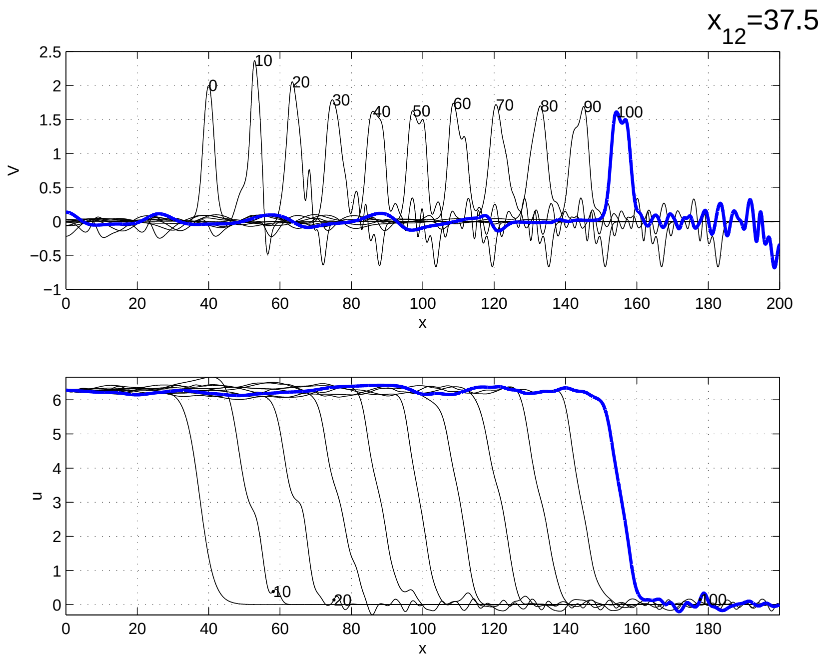

Fig. 2. Perturbations on the profiles of moving localized bell-shaped macro-strain wave and kink-shaped wave u when its initial position is slightly shifted behind that of v. Points of time correspond to the neighboring peaks. Final wave profiles are allocated in bold.

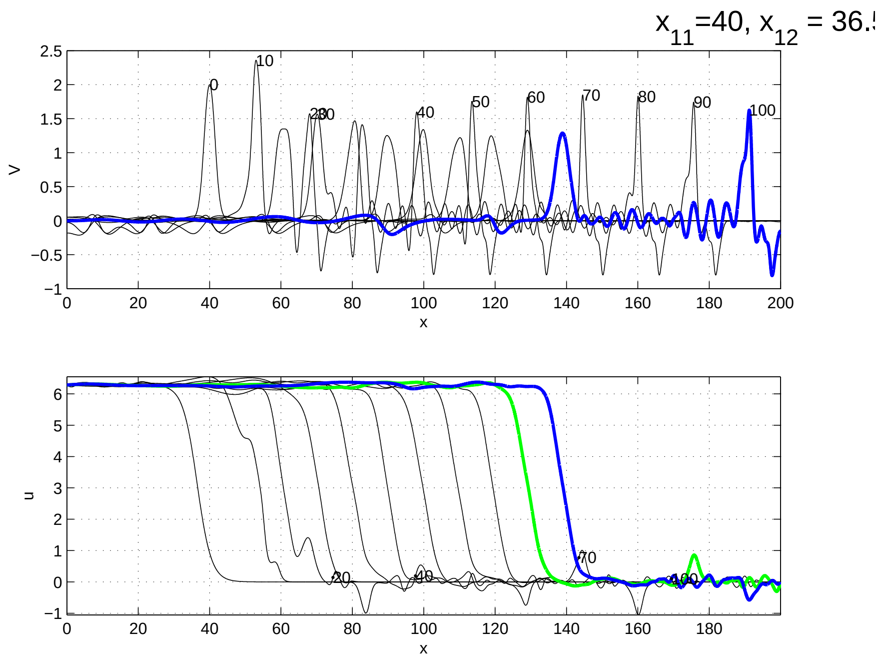

Fig. 3. Splitting of moving localized bell-shaped macro-strain wave v when the kink-shaped input for u is shifted more behind that of v. Points of time correspond to the neighboring peaks. Final wave profiles are allocated in bold.

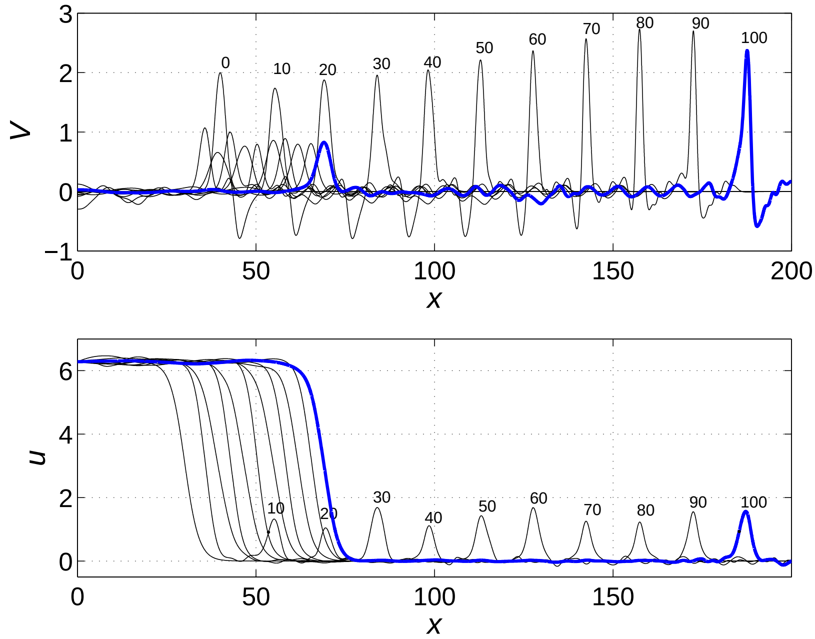

Fig. 4. Generation of moving localized bell-shaped micro-strain wave in a lattice from the kink-shaped input for u whose initial position is shifted behind that of v. Points of time correspond to the neighboring peaks. Final wave profiles are allocated in bold.

with corresponding bell-shaped wave v with the velocity from the interval $(c_L^2 - c_0^2; c_L^2)$ prescribed by the bell-shaped exact solutions.

3. Conclusions

It is shown that exact kink-shaped solution prescribes well the velocity interval required for propagation of the kink-shaped wave accounting for variations in the internal structure of the lattice. However, variation in the initial positions of the inputs for u and v gives rise to their splitting into two parts. These parts yield two pairs of the waves u and v propagating with different shapes and velocities. However, correspondence between the wave shape and its velocity is in an agreement with the analysis following from the traveling wave exact solution.

Acknowledgements

The work has been supported by the Russian Foundation for Basic Researches, projects No. 09-01-00469a and 10-01-00243-a.

References

[1] Aero E. L. Micromechanics of a double continuum in a model of a medium with variable periodic structure // J. Eng. Math. — 2002. — V. 55. — P. 81–95.

[2] Aero E. L., Bulygin A. N. Strongly nonlinear theory of nanostructure formation owing to elastic and nonelastic strains in crystalline solids // Mechanics of Solids. — 2007. — V. 42. — P. 807–822.

[3] Porubov A. V., Aero E. L., Maugin G. A. Two approaches to study essentially nonlinear and dispersive properties of the internal structure of materials // Phys. Rev. E. — 2009. — V. 79, 046608.

[4] Porubov A. V., Aero E. L., Andrievsky B. R. Dynamical properties of essentially nonlinear generalized continua // In: Maugin G. A., Metrikin A. V. (eds.), Mechanics of Generalized Continua. — Berlin: Springer, 2009. — P. 161–168.

[5] Porubov A. V., Andrievsky B. R., Aero E. L. Nonlinear dynamic processes in media with internal structure // In: Altenbach H., Maugin G. A., Erofeyev V. I. (eds.), Mechanics of Generalized Continua. — New York: Springer, 2011. — P. 245–254.

[6] Porubov A. V., Andrievsky B. R. Influence of coupling on nonlinear waves localization // CNSNS. — 2011. — V. 16. — P. 3964–3970.

[7] Porubov A. V., Andrievsky B. R. Localized nonlinear strain waves in media with internal structure // In: Vibration Problems, ICOVP2011. — Berlin: Springer, 2011. — P. 687–692.

[8] Shampine L. F., Reichelt M. W. // SIAM J. Scientific Computing. — 1997. — V. 18. — P. 1–22.