Nonlinear Generalizations of the Born-Huang Model and Their Continuum Limits

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Abstract One previously developed essentially nonlinear continuum model for a bi-atomic lattice is examined by comparing with the continuum limit of generalized Born-Huang model. It is found that these models do not correspond to each other, while the coefficients of the last model may be evaluated for real bi-atomic crystals. Some new features of the strain waves in the lattice are revealed on the basis of exact traveling wave solutions of the generalized Born-Huang model.

1 Introduction

Deep variations in the structure of a crystalline lattice, allows description of the cardinal, qualitative variations of the cell properties, lowering of potential barriers, switching of interatomic connections, arising from singular defects and other damages, phase transitions. Recently an essentially proper structural nonlinear model has been developed in [1, 2] that treats a continuum approach and a crystal translational symmetry of the bi-atomic lattice without making a continuum limit of its discrete model. According to [1, 2], the following variables are introduced in the 1D case:

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

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where a is a period of the lattice, U is a macro-displacement and u is a relative micro-displacement for the pair of atoms with masses m_1, m_2. Then the density of kinetic energy is introduced,

$$K = \frac{\rho U_t^2}{2} + \frac{\mu u_t^2}{2} \tag{1}$$

where ρ and μ are an average density of the mass of the atoms and a so-called density of the reduced masses of the pair of the atoms respectively. The internal density energy Π is suggested in [1, 2] as

$$\Pi = \frac{E\, U_x^2 + \kappa\, u_x^2}{2} + (p - SU_x)(1 - \cos(u)) \tag{2}$$

where E and κ are the second order macro-and micro-elastic constants, p is an energy of activation of interatomic connections in the elementary cell, S is the coefficient of nonlinear striction (re-arrangement of the microstructure under the action of macroscopic strains). The term $(1-\cos(u))$ was chosen to take into account a translational symmetry of the crystalline lattice. It accounts for a strong or essential nonlinearity allowing transition of atoms in neighboring cells to realize the micro-mechanism of the cardinal re-arrangement of the structure. The weakly nonlinear models give rise to only the description of small variations in the position of the atoms around undisturbed state.

The governing equations are obtained using the variation Hamilton-Ostrogradsky principle, and the coupled equations for U and u are obtained in the form

$$\rho U_{tt} - E\, U_{xx} = S(\cos(u) - 1)_x, \tag{3}$$

$$\mu u_{tt} - \kappa u_{xx} = (SU_x - p)\sin(u) \tag{4}$$

The model eqs. (3), (4) possess interesting localized wave solutions describing variations in the amplitude of the localized defect u as well as simultaneous propagation of the bell-shaped and kink-shaped defects u due to an influence of an external loading U_x, see [3–5]. However, the model (3), (4) is based on some suggestions, mentioned above. These suggestions are given on the basis of physical reasons, but they are not justified enough. Also the constants E, S, μ, κ and p are not defined for real bi-atomic materials, and application of the solutions to Eqs. (3), (4) is questionable. To overcome this difficulty, a comparison may be done with a continuum limit of the discrete equations accounting for the bi-atomic lattice. A natural candidate is the familiar Born-Huang model for bi-atomic lattices [6, 7]. However, this model is linear, and its extension by the nonlinear case is needed. It will be done further in this paper. It seems that possible correspondence may help to check the suggestions about the expressions for the energies (1), (2) and to estimate the values of the constants of the model (3), (4).

2 Generalization of the Born-Huang Lattice Model

The Born-Huang model accounts for a lattice that is a chain of the atoms of two kinds interacting with each other. The interaction is modeled by elastic springs with equal stiffness, see Fig. 1. Consider an elementary cell (marked in Fig. 1) with displacement u_l for the mass m_1 and displacement v_l for the mass m_2. Two possible elementary cells are marked in Fig. 1, the choice depends on the mass that is placed ahead, heavier or lighter. First the Born-Huang model is generalized up to a weakly nonlinear level. The discrete equations of motion for the elementary cell are written as

$$m_1\, u_{l,tt} = C[(v_{l+1} - u_l) - (u_l - v_{l-1})] + P[(v_{l+1} - u_l)^2 - (u_l - v_{l-1})^2],$$
$$m_2\, v_{l,tt} = C[(u_{l+1} - v_l) - (v_l - u_{l-1})] + P[(u_{l+1} - v_l)^2 - (v_l - u_{l-1})^2],$$

where C and P are the coefficients of the linear and nonlinear stiffness respectively. The continuum long-wave limit of these equations up to the terms of order $O(a^3)$ is

$$m_1\, u_{tt} = 2C\,(v - u) + 4a\,P(v - u)v_x + C\,a^2 v_{xx}, \tag{5}$$
$$m_2\, v_{tt} = 2C\,(u - v) + 4a\,P(u - v)u_x + C\,a^2 u_{xx}. \tag{6}$$

A comparison with the model (3), (4) requires transition to the variables,

$$U = \frac{m_1 u + m_2 v}{m_1 + m_2},\; V = \frac{u - v}{a}.$$

that have the same meaning as for the model (3), (4). Then the continuum eqs. (5), (6) are transformed to the coupled equations for the new variables,

$$(m_1 + m_2)U_{tt} - 2a^2\, CU_{xx} - 4a^3\, PVV_x + \frac{a^3\, C(m_1 - m_2)}{m_1 + m_2}\, V_{xx} = 0, \tag{7}$$

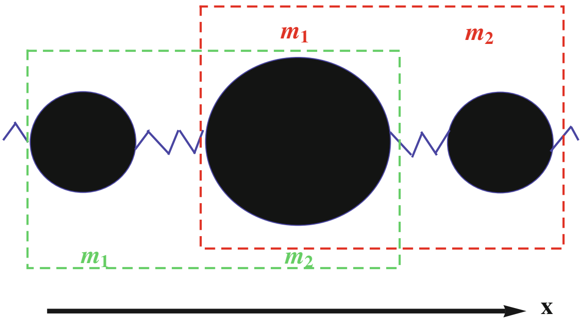

Fig. 1 Two kinds of establishing elementary cells in bi–atomic Born–Huang lattice. Two choices of an elementary cell are marked by dashed lines

$$\frac{m_1 m_2 a^2}{m_1+m_2} V_{tt} + \frac{a^4\, C m_1 m_2}{(m_1+m_2)^2}\, V_{xx} + 2a^2(C + 2a\, P U_x)V$$
$$+ \frac{a^3\, C(m_1-m_2)}{m_1+m_2}\, U_{xx} = 0. \tag{8}$$

A comparison will be done first between the linearized versions of Eqs. (3), (4) and (7), (8). Then Eqs. (7), (8) will be compared with the weakly nonlinear limit of Eqs. (3), (4) resulting from application of the power series expansions of the trigonometric functions. Finally, an essentially nonlinear extension of Eqs. (7), (8) will be suggested to compare with Eqs. (3), (4).

3 Comparison of the Models

The linearized equations (3), (4),

$$\rho U_{tt} - E\, U_{xx} = 0, \tag{9}$$
$$\mu u_{tt} - \kappa u_{xx} = 0. \tag{10}$$

demonstrate no coupling and no acoustical and optical branches in the dispersion relation. On the contrary, the Born-Huang model (linearized Eqs. (7), (8)),

$$(m_1+m_2)U_{tt} - 2a^2\, C U_{xx} + \frac{a^3\, C(m_1-m_2)}{m_1+m_2}\, V_{xx} = 0, \tag{11}$$
$$\frac{m_1 m_2 a^2}{m_1+m_2} V_{tt} + \frac{a^4\, C m_1 m_2}{(m_1+m_2)^2}\, V_{xx} + \frac{a^3\, C(m_1-m_2)}{m_1+m_2}\, U_{xx} = 0, \tag{12}$$

possesses both branches [6]. Also, one can note that the coefficients in Eqs. (9), (10) are independent, while they depend on each other in Eqs. (11), (12).

The weakly nonlinear limit of Eqs. (3), (4) is obtained by expanding the trigonometric functions and retaining only the first terms in the expansions,

$$\rho U_{tt} - E\, U_{xx} = -S\, u u_x, \tag{13}$$
$$\mu u_{tt} - \kappa u_{xx} = (S U_x - p)\, u. \tag{14}$$

A comparison with Eqs. (7), (8) may be done using exact traveling wave solutions depending only on the phase variable $\theta = x - c\, t$. Two kinds of decoupling are possible for Eqs. (13), (14). The Eq. (13) may be resolved for U_θ,

$$U_\theta = \frac{S\, u^2 - 2\sigma}{2(E - \rho\, c^2)}, \tag{15}$$

and Eq. (14) becomes an equation for finding the function u after substitution of Eq. (15). Alternatively, Eq. (13) gives rise to the relationship for u,

$$u = \frac{\sqrt{2((E-\rho\, c^2)U_\theta - \sigma)}}{S}, \tag{16}$$

while the function U is defined from Eq. (14) after substitution of Eq. (18). In both cases σ is a constant of integration.

Only the first kind of decoupling is realized for solving Eqs. (7), (8). Thus, Eqs. (7) yields

$$U_\theta = \frac{2a^3PV^2 + \sigma}{c^2(m_1+m_2) - 2Ca^2} + \frac{(m_2-m_1)C\, a^3 V_\theta}{(m_1+m_2)(c^2(m_1+m_2) - 2Ca^2)} \tag{17}$$

that is used for derivation of the governing equation for V from Eq. (8). One can note that the second term in Eq. (17) depends on the difference of the masses m_i.

Despite the relationships for U_θ for both models are different due to the last term in Eq. (17), the resulting ordinary differential equations (ODE) for the functions u and V are similar. Thus, Eq. (14) transforms to the ODE reduction of the modified Korteweg - de Vries (mKdV) equation,

$$(u_\theta)^2 = b_1u^4 + b_2u^2 + b_3,$$

$$b_1 = \frac{S^2}{4\left(\kappa - c^2\mu\right)\left(E - c^2\rho\right)},\ b_2 = -\frac{\left(p(E-c^2\rho) + S\sigma\right)}{\left(\kappa - c^2\mu\right)\left(E - c^2\rho\right)},\ b_3 - \text{const.}$$

while for the generalized Born- Huang model substitution of Eq. (17) into Eq. (8) results in the same ODE for the function V,

$$(V_\theta)^2 = q_1V^4 + q_2V^2 + q_3,$$

but with different coefficients,

$$q_1 = \frac{2a^4P^2}{C^2a^4 - m_1m_2c^4},\ q_2 = \frac{2(2aP\sigma C(m_1+m_2)c^2 - 2C^2a^2)}{C^2a^4 - m_1m_2c^4},\ q_3 - \text{const.}$$

The known solitary wave solution of the mKdV equation is be written for u,

$$u = \frac{2\sqrt{p\left(c^2\rho - E\right) - S\sigma}}{S}\text{sech}\left(\frac{\sqrt{p\left(E - c^2\rho\right) + S\sigma}}{\sqrt{\left(\kappa - c^2\mu\right)\left(E - c^2\rho\right)}}(\theta - \theta_0)\right) \tag{18}$$

while the same solution for V is

$$V = \frac{\sqrt{2C^2a^2 - c^2C(m_1 + m_2) - 2aP\sigma}}{\sqrt{2}a^2P}$$

$$\text{sech}\left(\frac{\sqrt{2}\sqrt{2C^2a^2 - c^2C(m_1 + m_2) - 2aP\sigma}}{\sqrt{-C^2a^4 + c^4m_1m_2}}(\theta - \theta_0)\right). \quad (19)$$

However, the reality of the parameters of the solutions depend on the coefficients of the equation. The coefficients are independent for the model (13), (14), then the solution (18) exists, in particular, for $\sigma = 0$. It follows from Eq. (15) that U_θ vanishes at $\theta \to \pm\infty$, and the solitary wave of the moving defect u is accompanied by the solitary wave of an external loading, or a macro-strain, U_θ. However, the coefficients of Eqs. (7), (8) do not allow the value of the velocity c at $\sigma = 0$ for the solution (19). It means that the macro-strain wave U_θ (17) cannot vanish at infinities, and a constant external loading is needed to support the localized wave of defects V in this case. Typical shapes of the wave (17) are shown in Fig. 2 in the form of a localized wave but with constant negative shift that has a meaning of an external longitudinal compression. The shape of the wave is not symmetric with respect to its peak contrary to the symmetric shape of the solution (15). Also a trough appears ahead or behind the wave depending on the ratio of the masses, m_i.

Similarly the essentially nonlinear case may be considered. However, the weakly nonlinear Eqs. (7), (8) should be extended up to the essential level in the same manner as Eqs. (3), (4) are reduced up to the weakly nonlinear level, (13), (14). Now we assume that the nonlinear terms in Eqs. (7), (8) are the "traces" of the expansions of the trigonometric functions. Then the essentially nonlinear generalization of the continuum limit of the Born-Huang model is suggested in the form

$$(m_1 + m_2)U_{tt} - 2a^2CU_{xx} - 4a^3P(1 - \cos V)_x + \frac{a^3C(m_1 - m_2)}{m_1 + m_2}V_{xx} = 0 \quad (20)$$

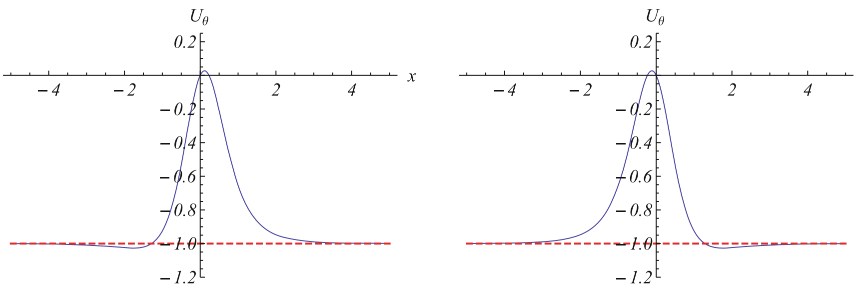

Fig. 2 Solitary wave with a constant shift (shown by dashed line), $m_1 < m_2$ (left), $m_1 > m_2$ (right)

$$\frac{m_1 m_2 a^2}{m_1+m_2} V_{tt} + \frac{a^4\, C m_1 m_2}{(m_1+m_2)^2}\, V_{xx} \\ +2a^2(C+2a\, PU_x)\sin V + \frac{a^3\, C(m_1-m_2)}{m_1+m_2}\, U_{xx} = 0. \tag{21}$$

Again a comparison is done using exact traveling wave solutions to Eqs. (3), (4) and Eqs. (20), (21). Two kinds of decoupling are possible for Eqs. (3), (4):

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

or

$$u = \arccos\left(\frac{(\rho\, c^2 - E)U_\theta - \sigma}{S} + 1\right).$$

Only the first kind is realized for the generalized essentially nonlinear Born-Huang model, (20), (21),

$$U_\theta = \frac{a^3 P(1-\cos V) + \sigma}{c^2(m_1+m_2) - 2Ca^2} + \\ \frac{(m_2-m_1)C\, a^3 V_\theta}{(m_1+m_2)(c^2(m_1+m_2)-2Ca^2)} \tag{22}$$

The equations both for the functions u and V have the form of the ODE reduction of the Double Sine-Gordon equation. In particular, substitution of Eq. (22) into Eq. (21) of the generalized essentially nonlinear Born-Huang model results in

$$\left(\frac{m_1 m_2 a^2(c^2 + C\, a^2)}{m_1+m_2} - \frac{(m_1-m_2)^2 C^2\, a^6}{(m_1+m_2)^2((m_1+m_2)c^2 - 2C\, a^2)}\right) V_{\theta\theta} \\ + 2a^2\left(C + \frac{2AP(4a^3 P + \sigma)}{(m_1+m_2)c^2 - 2C\, a^2}\right)\sin V - \frac{4a^4 P}{(m_1+m_2)c^2 - 2C\, a^2}\sin(2V) = 0. \tag{23}$$

The substitution of variable $V = 2\arctan W(\theta)$ allows us to convert Eq. (23) to the form of the mKdV equation for the function W. Then a comparison is done using already noted solitary wave solution. It turns out that the main deviations in the solutions are the same as in the weakly nonlinear case. Again the generalized essentially nonlinear Born-Huang model does not possess the bell-shaped solution for U_θ without constant shift, σ, while the shape of the wave U_θ is similar to that shown in Fig. 2.

4 Conclusions

The essentially nonlinear continuum model (3), (4) and the continuum limit of the discrete Born-Huang model do not correspond to each other at the linearized, weakly nonlinear and essentially nonlinear levels. The distinct features of the last model are the dependence of the profile of the solution on the ratio between the masses m_i of the atoms of the lattice and the need in a shift σ for the existence of the solution for the macro-strain U_θ needed for propagation of localized defects V. Therefore, both models similarly describe propagation of localized defects but under different loading, U_θ (with or without constant part or a pedestal). The coefficients in the continuum equations of the generalized Born- Huang model depends on the interaction forces of the lattice that makes possible their evaluation for real bi-atomic materials.

However, the essentially nonlinear continuum model (3), (4) corresponds well to the structural essentially nonlinear model after G. Pouget, G.A. Maugin and M.K. Sayadi [8, 9] for a one-dimensional atomic chain equipped with rotatory molecular groups. Therefore, all the solutions obtained in Refs. [3–5] may be successfully applied in this problem.

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