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MECHANICS

Models for essentially nonlinear strain waves in materials with internal structure

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Abstract. Phenomenological models of essential nonlinear processes in solids with internal structure are developed so as to obtain nonlinear and dispersive features of the material similar to those described by the structural model. The exact solitary wave solutions of the governing equations are used as a tool for a comparison of two kinds of modelling. It is found that the model containing nonlinearity at the microlevel provides maximum similarity with the structural model.

Key words: mechanics of solids, nonlinear waves, microstructure, dispersion, exact solution.

1. INTRODUCTION

The development of models describing structural rearrangements and formation of defects in materials with an internal structure (e.g., microstructure) is an important practical problem. However, any structural deviations are usually described by means of *essentially nonlinear* models when nonlinearity is not approximated by a power series in strains like in the weakly nonlinear problems. There exist at least two approaches to describe such deviations. One of them may be called structural modelling as it takes into account a concrete internal structure [1–3]. The other approach may be called a phenomenological one because it formally employs the stress-strain power series relationships obtained in the weakly nonlinear case. In particular, the last approach was applied for seismic materials and paramagnetic materials, also it might be developed for the materials with micro- or even nanostructure [4–10].

Structural models are more precise; however, their parameters are unknown as a rule. Hence application of these models to the real materials is questionable. At the same time power series approximations gave rise to measure the parameters of the phenomenological models (see [4] and references therein). However, an application of the last models also depends on whether the features of their solutions are close to those of the structural ones. One of the possible ways to check similarity between the models is to study solitary wave solutions of their governing equations. It is known that solitary waves describe a balance between nonlinearity and dispersion. This balance may be studied analytically by an analysis of the relationships for the amplitude, velocity, and the wave width of the solution, which allows us to characterize nonlinear and dispersive features of the material with internal structure.

The main problem addressed in this paper is the possibility of developing an essentially nonlinear phenomenological model possessing nonlinear and dispersive features similar to those of the structural one. In Section 2 the main results obtained for the structural model solution in [4] are reminded and an extra solution in the form of the solitary wave on a pedestal is obtained. Sections 3 and 4 are devoted to phenomenological modelling. First, a simpler model is considered based on a single governing equation. Then more complicated models are studied that give rise to the coupled governing equations for macro- and microfields. Travelling wave solutions are examined in all cases and compared with those obtained for the structural model.

2. STRUCTURAL ESSENTIALLY NONLINEAR MODEL

A structural model has been developed for ferroelectrics based on the assumption of a deformed chain of atoms modified by a rotating microstructure [1]. Later an essentially nonlinear model was proposed by Aero and co-workers [2,3]. In this model, besides interatomic forces between atoms, the relative sub-lattices motion is taken into account to describe structural deviations in the bi-atomic lattice. The governing equations in the 1D case read [2,3]

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

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

where

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

a is a period of sub-lattice, U is a macrodisplacement, and u is a relative microdisplacement for the pair of atoms with masses m_1, m_2. The parameter p is introduced to account for large interatomic micro-displacements according to the known one-dimensional Frenkel–Kontorova model of a crystalline chain. Moreover, a striction S was added in [2,3] to describe nonlinear coupling between macro- and microfields taking into account a periodicity of the lattice. This model is called essentially nonlinear since no power series approximations for nonlinear terms are used; instead, translational symmetry of the lattice is modelled by trigonometric functions. The governing equations for ferroelectrics in [1] are structurally similar.

To obtain travelling strain wave solutions depending on the phase variable $\theta = x - V\, t$ one can first resolve u from Eq. (1),

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

where σ is a constant of integration, $v = U_\theta$. Substitution of Eq. (3) into Eq. (2) gives rise to the equation for the macrostrains, v,

$$v_\theta^2 = a_0 + a_1\, v + a_2\, v^2 + a_3\, v^3 + a_4\, v^4, \tag{4}$$

where $a_i = a_i(V)$, see their expressions in [4]. Only the cubic nonlinear term appears here in comparison with the governing equation for macrostrains in the weakly nonlinear case. One can note that Eq. (4) is similar to the ODE of the Gardner equation arising for the description of large amplitude internal waves in fluids.

2.1. Solitary waves

The known bell-shaped solutions of Eq. (4) have the form

$$v_1 = \frac{A}{Q\,\cosh(k\,\theta) + 1},\ v_2 = -\frac{A}{Q\,\cosh(k\,\theta) - 1}. \tag{5}$$

It was found in [4] that these solutions exist for two values of σ. Thus for $\sigma = 0$ the parameters read

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

while for $\sigma = -2S$ it was obtained that

$$A = \frac{4\,S}{\rho(c_0^2 + V^2 - c_L^2)}, Q_\pm = \pm\frac{V^2 - c_L^2 - c_0^2}{V^2 - c_L^2 + c_0^2}, k = 2\sqrt{\frac{p}{\mu\,(V^2 - c_l^2)}}, \tag{7}$$

where $c_L^2 = E/\rho$, $c_l^2 = \kappa/\mu$, $c_0^2 = S^2/(p\,\rho)$. An analysis performed in [4] revealed an absence of simultaneous existence of bounded solutions v_1 and v_2, hence the compression and tensile macrostrain waves cannot co-exist. The last expressions in (6) and (7) account for the dispersion properties giving the mode with cut-off or the optical mode, respectively, while no acoustical one exists.

The expression for u is obtained from Eq. (3) depending on whether the first derivative u_θ exists or not at $\theta = 0$. In the former case the bell-shaped wave,

$$u = \pm\arccos\left(\frac{(\rho V^2 - E)v}{S} + 1\right) \text{ for } -\infty < \theta < \infty,$$

accounts for deviations in the internal structure. In the latter case the kink-shaped wave arises of the form

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

$$u = \pm 2\pi \mp \arccos\left(\frac{(\rho V^2 - E)v}{S} + 1\right) \text{ for } \theta > 0.$$

The signs $\pm$ or $\mp$ mean that two mirror profiles of u appear for any macrostrain profile v, and the bell-shaped macrostrains give rise either to the bell-shaped or to the kink-shaped waves u of the internal structure. The choice of the profile is defined by the phase velocity V. The corresponding intervals for V for both values of σ may be found in [4].

2.2. Solitary waves on a pedestal

An obvious generalization of the solitary wave solution (5) may be suggested by adding a constant pedestal

$$v_3 = \frac{A}{Q\,\cosh(k\,\theta) + 1} + F,\; v_4 = -\frac{A}{Q\,\cosh(k\,\theta) - 1} + F. \tag{8}$$

Substitution of this ansatz to Eq. (4) gives rise to two sets of the parameters. The first one arises for

$$F = \frac{\sigma}{\rho(c_L^2 - V^2)} \tag{9}$$

and reads

$$A = \frac{4\,S(V^2 - c_L^2 + c_p^2)}{\rho(V^2 - c_L^2)(c_0^2 + c_L^2 - c_p^2 - V^2)},\; Q_\pm = \pm\frac{c_L^2 - V^2 - c_0^2 - c_p^2}{c_L^2 - V^2 + c_0^2 - c_p^2},$$
$$k = 2\sqrt{\frac{p(c_p^2 - c_L^2 + V^2)}{\mu(c_l^2 - V^2)(V^2 - c_L^2)}}, \tag{10}$$

where $c_p^2 = \sigma S/(p\rho)$.

Comparing it with the parameters (6) found for the solitary wave solutions (5), one can note a difference in the dispersive features. Indeed, the last expression in (10) gives rise to two solutions for V^2, one of them, V_1^2, belongs to the acoustical mode. It tends to

$$V_1^2 = c_L^2 - c_p^2$$

as $k \to 0$. The second solution, V_2^2, belongs to the mode with cut-off and it tends to

$$V_2^2 \;=\; c_l^2 + c_p^2 \;-\; \frac{4p}{\mu\, k^2}$$

as $k \to 0$. It coincides with the last relation (6) for the solitary wave solution when $\sigma \;=\; 0$ ($c_p \;=\; 0$).

The solution (8) also arises for

$$F \;=\; \frac{\sigma + 2S}{\rho(c_L^2 - V^2)}$$

and possesses similar dispersive features as for the F defined by Eq. (9) with the existence of an additional acoustical mode besides the optical one found for the solution (5) with parameters defined by (7).

3. PHENOMENOLOGICAL MODEL BASED ON A SINGLE GOVERNING EQUATION

The stress–strain relationship in the 1D weakly nonlinear case is often modelled by a truncated expansion

$$P \;=\; E^* U_x + C_1 U_x^2 + C_2 U_x^3. \tag{11}$$

Indeed, the typical elastic strain in classic elastic materials is $U_x \;\sim\; 10^{-3} - 10^{-5}$, while $E^*/C_1 \sim 0.1$, $C_1/C-2 \sim 0.1$, then $C_2 U_x^3 \;<<\; C_1 U_x^2 \;<<\; E^* U_x$ that justifies the use of truncated expansions. However, non-classic materials (rocks, soils, some crystals) possess an internal structure that gives rise to an equal contribution $C_2 U_x^3 \;\sim\; C_1 U_x^2 \;\sim\; E^* U_x$ even for the typical elastic strain $U_x \;\sim\; 10^{-4} - 10^{-5}$ (see [4] and references therein). Abnormally large values of higher-order nonlinear elastic moduli C_1, C_2 relative to the linear modulus E^* make strain processes in these materials essentially nonlinear. There is lack in the values of higher-order nonlinear moduli of the conventional microstructured materials; however, a similarity in the formalism with that of the rocks allows us to suggest Eq. (11) also for their modelling.

Then Eq. (11) cannot be used as a truncated expansion, and the idea of phenomenological modelling is to use it as an exact expression. It allows us to derive the governing equation like in the weakly nonlinear theory. Then the equation for longitudinal strains reads [4]

$$v_{tt} - a\, v_{xx} - c_1\,(v^2)_{xx} - c_2\,(v^3)_{xx} + \alpha_3\, v_{xxtt} - \alpha_4\, v_{xxxx} = 0, \tag{12}$$

where $v \;=\; U_x$, $a \;=\; E^*/\rho$, $c_1 \;=\; 2C_1/\rho$, $c_2 \;=\; 3C_2/\rho$. There is no equation for a microfield, but internal structure is introduced first via dispersion and secondly because the abnormally large coefficients in Eq. (11) arise due to the influence of internal structure.

The equation for travelling wave solutions obeys the ODE similar to Eq. (4) [4]. However, due to the difference in the coefficients of the equation and the absence of coupling with an equation for the internal field, nonlinear and dispersive features of the solution differ from those of the structural model. Namely, now there is a possibility for simultaneous existence of the compression and tensile macrostrain solitary waves, and the waves always belong to the acoustical mode. Certainly, the microfield deviations noted at the end of Section 2.2 are not described within this model. Therefore, a more general phenomenological model is required.

4. PHENOMENOLOGICAL MODEL BASED ON COUPLED GOVERNING EQUATIONS

An internal field or a microfield may be introduced within phenomenological modelling. Thus, linearized coupled governing equations for the macrodisplacement $U(x,t)$ and microstrain $\psi(x,t)$,

$$\rho\; U_{tt} - a\; U_{xx} \;=\; D\; \psi_x, \tag{13}$$

$$I\; \psi_{tt} - C\; \psi_{xx} \;=\; -D\, U_x - B\; \psi, \tag{14}$$

where I is the microinertia, may be suggested (see [5] and references therein). The dispersion relation analysis performed in [5] revealed the existence of both acoustical and optical modes, which make dispersive features closer to those of the structural model.

4.1. Nonlinearity at the macrolevel

The nonlinear generalization of (13), (14) may be made at the macrolevel similarly to [7,10]. Now a cubic nonlinear term is added following the arguments for essentially nonlinear model in Section 3,

$$\rho\, U_{tt} - a\, U_{xx} \;=\; N\, U_x U_{xx} + M\, U_x^2 U_{xx} + D\, \psi_x, \tag{15}$$

$$I\, \psi_{tt} - C\, \psi_{xx} \;=\; -D\, U_x - B\, \psi. \tag{16}$$

The equations may be decoupled in a different manner. First, the slaving principle [10] may be used when ψ is expressed via U_x from Eq. (16) asymptotically,

$$\psi \;=\; -\frac{D}{B}\, U_x + \frac{D}{B^2}(I\, U_{ttx} - C\, U_{xxx}).$$

Substitution of this expression into Eq. (15) yields the governing equation for v similar to Eq. (12), whose solution possesses the same features as that of the model based on a single equation; in particular, no optical mode exists. Alternatively, the microfield may be expressed using Eq. (15) via the macrofield [4],

$$\psi_x \;=\; \frac{1}{D}\left(\rho\, U_{tt} - AU_{xx} - N\, U_x U_{xx} - M\, U_x^2 U_{xx}\right). \tag{17}$$

Substitution of Eq. (17) into Eq. (16) gives rise to the governing for macrostrain waves v, which is not similar to Eq. (12) since the higher-order nonlinear terms appear (see Eq. (23) in [4]). It provides different nonlinear features in the solution: as follows from [7], the solution does not describe symmetric profiles for v. At the same time, dispersive features allow existence of both acoustical and optical modes but independent of whether a solitary wave or a wave on a pedestal is considered.

4.2. Nonlinearity at the microlevel

Nonlinear generalizations of the phenomenological models (13), (14) may be made at the microlevel. Let us introduce them as follows

$$\rho\, U_{tt} - a\, U_{xx} \;=\; D\, \psi\psi_x, \tag{18}$$

$$I\, \psi_{tt} - C\, \psi_{xx} \;=\; -(D\, U_x + B)\, (\psi - \psi^3/6). \tag{19}$$

Then, for travelling wave solutions ψ is expressed from Eq. (18) as

$$\psi^2 \;=\; (2\rho/D)((V^2 - s_L^2)v + \sigma_1/\rho), \tag{20}$$

where $s_L^2 \;=\; a/\rho$, σ_1 is a constant of integration. Substitution of this expression into Eq. (19) yields the ODE for v in the form similar to Eq. (4). Analysis of this equation allows us to conclude that the solitary wave solutions (5) exist only for some values of σ_1. Thus, for $\sigma_1 \;=\; 0$ we have for the parameters of the wave

$$A \;=\; \frac{6D}{\rho(V^2 - s_L^2 - 3s_0^2)},\; k^2 \;=\; \frac{2B}{I(s_l^2 - V^2)},\; Q_\pm \;=\; \pm\frac{\sqrt{(s_L^2 - V^2 - s_0^2)^2 + 8s_0^4}}{3s_0^2 + s_L^2 - V^2},$$

where $s_l^2 \;=\; C/I$, $s_0^2 \;=\; D^2/(\rho B)$.

Both dispersive and nonlinear features of this solution are closer to those of the structural model, i.e., the mode with cut-off for the solitary wave solution and absence of simultaneous existence of compression and tensile waves. It is possible to obtain also two symmetric profiles of microstrain waves from Eq. (20) corresponding to the same macrostrain wave. However, the last equation still describes only bell-shaped microstrains, not kinks.

5. CONCLUSIONS

An attempt was made to develop an essentially nonlinear model based on the formal use of power series approximations for the strains used in the weakly nonlinear theory. The solitary wave solutions of the governing equation were efficiently employed for comparison of nonlinear and dispersive features of the developed models and those of the structural model. The closest similarity was achieved for the phenomenological model based on coupled equations with nonlinearity at the microlevel. However, the description of the kink-shaped microstrain wave corresponding to the bell-shaped macrostrain one remains an open problem. Its solution may allow us to answer the still open question: What kind of modelling, structural or phenomenological, is more suitable for a description of internal structural deviations in complex materials?

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Tugevalt mittelineaarsete deformatsioonilainete mudelid kompleksmaterjalides

Alexey V. Porubov

Struktuurselt põhjendatud liikumisvõrrandid sisestruktuuriga materjalide käitumise kirjeldamiseks saab tuletada atomaarsest mudelist [2,3]. Samas on võimalik liikumisvõrrandid tuletada pideva keskkonna teooria baasil, võttes näiteks aluseks Mindlini teooria [5]. Mõlemad mudelid lubavad solitoni-tüüpi lahendeid. Artiklis on näidatud, et nende solitoni-tüüpi lahendite võrdlemine lubab ühildada kaht nimetatud lähendust eelkõige lahendite tasandil ja siis juba liikumisvõrrandite tasandil. Sellest võib tuletada ka seosed mudelite parameetrite vahel, mis on olulised materjali iseloomustamiseks.