Deformation Waves in Microstructured Materials: Theory and Numerics

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Abstract. A linear model of the microstructured continuum based on Mindlin theory is adopted which can be represented in the framework of the internal variable theory. Fully coupled systems of equations for macro-motion and microstructure evolution are represented in the form of conservation laws. A modification of wave propagation algorithm is used for numerical calculations. Results of direct numerical simulations of wave propagation in periodic medium are compared with similar results for the continuous media with the modelled microstructure. It is shown that the proper choice of material constants should be made to match the results obtained by both approaches.

1. Introduction

The classical theories of continua describe the behaviour of homogeneous materials. In reality, however, materials are always characterized by a certain microstructure at various scales. The character of a microstructure can be regular (like in laminated composites) or irregular (like in polycrystalline solids or alloys). Even more, regularity and irregularity may be combined like for some FGMs. The characteristic scale of a microstructure must always be compared with the spatial scale of excitation. The choice of proper mathematical models is extremely important in order to describe the wave fields with needed accuracy.

In general terms, the starting point for describing a microstructure could be either the discrete or the continuum approach. In the discrete approach the volume elements are treated as point masses with interaction [1]. Or, especially for laminated composites, the effective stiffness theory has been used [2]. The homogenization methods based on properties and geometry of constituents are widely used

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for static and quasi-static problems [3]. From the viewpoint of continua, the straight-forward modelling leads to assigning all the physical properties to every volume element dV in a solid which means introducing the dependence on space coordinates. Thus, the governing equations are so complicated that can be solved only by numerical methods.

Another way is to separate macro- and microstructure in continua. Then the conservation laws for both structures should be formulated separately [4, 5] or in a more sophisticated way the microstructural quantities could be introduced into one set of conservation laws for the macrostructure [6]. Quite recently it has been shown that the generalization of such theories can be obtained by using the concept of dual internal variables [7].

To check the capabilities of the theory, it is useful to compare the theoretical predictions with results of direct numerical simulation of wave propagation through a certain known microstructure. In what follows, the derivation of a microstructure model is presented in the one-dimensional setting. The concept of dual internal variables is applied for the physical description of continua with microstructure. The finite volume wave propagation algorithm is used for both direct numerical simulation and the microstructure modeling. Results of direct numerical simulations of wave propagation in a periodically layered medium are compared with similar results for the homogeneous medium with a modelled microstructure.

2. Governing Equations

The governing equations of thermoelasticity are local balance laws for linear momentum and energy [8]. In the one-dimensional case these governing equations are reduced to (no body forces)

$$\frac{\partial}{\partial t}\left(\rho_0 v\right) - \frac{\partial \sigma}{\partial x} = 0, \tag{2.1}$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_0 v^2 + E\right) - \frac{\partial}{\partial x}\left(\sigma v - Q\right) = 0, \tag{2.2}$$

complemented by the second law of thermodynamics

$$\frac{\partial S}{\partial t} - \frac{\partial}{\partial x}\left(Q/\theta + K\right) \geq 0. \tag{2.3}$$

Here t is time, ρ_0 is the matter density, v is the physical velocity, σ is the Cauchy stress, E is the internal energy per unit volume, S is the entropy per unit volume, θ is temperature, Q is the material heat flux, and the "extra entropy flux" K vanishes in most cases, but this is not a basic requirement.

3. Internal Variables

Up to now the microstructure was not specified. In the framework of the phenomenological continuum theory it is assumed that the influence of the microstructure on the overall macroscopic behaviour can be taken into account by the introduction of an internal variable φ, which we associate with the integral distributed effect of the microstructure, and a certain dual internal variable ψ. We suppose that the free energy depends on the internal variables φ, ψ and their space derivatives $W = W^*(u_x, \varphi, \varphi_x, \psi, \psi_x)$. Then the constitutive equations follow

$$\sigma := \frac{\partial W^*}{\partial u_x}, \quad \tau := -\frac{\partial W^*}{\partial \phi}, \quad \eta := -\frac{\partial W^*}{\partial \phi_x}, \quad \xi := -\frac{\partial W^*}{\partial \psi}, \quad \varsigma := -\frac{\partial W^*}{\partial \psi_x}. \tag{3.1}$$

We include into consideration the non-zero extra entropy flux [9]

$$K = -\theta^{-1}\eta\dot{\phi} - \theta^{-1}\varsigma\dot{\xi}. \tag{3.2}$$

It can be checked that the dissipation inequality in the isothermal case reduces to

$$(\tau - \eta_x)\,\dot{\phi} + (\xi - \varsigma_x)\,\dot{\psi} \geq 0. \tag{3.3}$$

In the non-dissipative case the dissipation inequality can be satisfied by the choice

$$\dot{\phi} = m(\xi - \varsigma_x), \quad \dot{\psi} = -m(\tau - \eta_x), \tag{3.4}$$

where m is a coefficient. The latter two evolution equations express the duality between internal variables: one internal variable is driven by another one and vice versa.

The simplest free energy dependence is a quadratic function [10]

$$W^* = \frac{\rho_0 c^2}{2} u_x^2 + A\phi u_x + \frac{1}{2}B\phi^2 + \frac{1}{2}C\phi_x^2 + \frac{1}{2}D\psi^2, \tag{3.5}$$

where A, B C, D, and c are material constants.

Here we include only the contribution of the second internal variable itself. In this case, the evolution equation for the internal variable φ is a hyperbolic equation [7]

$$\ddot{\phi} = m^2 D(\tau - \eta_x) . \tag{3.6}$$

As a result, we can represent the equations of motion in the form

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + A\phi_x, \tag{3.7}$$
$$I\phi_{tt} = C\phi_{xx} - Au_x - B\phi, \tag{3.8}$$

where $I = 1/(m^2 D)$ is an internal inertia measure. In terms of stresses introduced by Eq. (3.1), the same system of equations is represented as

$$\rho_0 \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x}, \qquad I\frac{\partial^2 \phi}{\partial t^2} = -\frac{\partial \eta}{\partial x} + \tau. \tag{3.9}$$

It is worth to note that same equations are derived in [11] but based on different considerations.

3.1 Single Wave Equation

The governing equations (3.7) and (3.8) can be reduced to one equation. We can determine the first space derivative of the internal variable from Eq. (3.8) and its third derivatives from Eq. (3.7). Inserting the results into the balance of linear momentum (3.7), we obtain a higher order equation [9] with clearly separated wave operators which describe the influence of the microstructure

$$u_{tt} = \left(c^2 - \frac{A}{\rho_0 B}\right) u_{xx} + \frac{C}{B}(u_{tt} - c^2 u_{xx})_{xx} - \frac{I}{B}(u_{tt} - c^2 u_{xx})_{tt}. \tag{3.10}$$

3.2 System of Equations

At the same time, in terms of strain and velocity, Eq. (3.7) is rewritten as

$$\rho_0 v_t = \rho_0 c^2 \varepsilon_x + A\phi_x. \tag{3.11}$$

The particle velocity and the strain are related by the compatibility condition

$$\varepsilon_t = v_x, \tag{3.12}$$

which form the system of equations for these two variables.

Similarly, introducing a microvelocity w as follows:

$$w_x := -D\psi, \tag{3.13}$$

and using Eq. (3.6) with $m = 1$, we have

$$\phi_t = w_x, \tag{3.14}$$

that is nothing else but the compatibility condition at micro-level. It follows from Eqs. (3.14) and (3.8) that

$$I\dot{w}_x = C\phi_{xx} - A\varepsilon - B\phi. \tag{3.15}$$

Integrating the latter equation over x, we arrive at

$$Iw_t = C\phi_x - \int \left(A\varepsilon + B\phi\right) dx \tag{3.16}$$

Thus, we have two coupled systems of equations (3.11), (3.12) and (3.14), (3.16) for the determination of four unknowns: ε, v, φ, and w. These two systems of equations are solved numerically to describe the microstructure dynamics.

4. Numerical Simulations

4.1 Algorithm Description

There are many computational methods used to describe wave propagation phenomena (see, e.g. [12]). In our computations we apply a modification of the wave propagation algorithm [13] that was successfully applied to the simulation of wave propagation in inhomogeneous media with rapidly-varying properties [14]. In simulations of wave propagation in a layered medium with known location of inhomogeneities, the numerical scheme is the same as described in [14]. However, the wave propagation algorithm is modified in order to solve the coupled systems of equations in the modelling of the microstructure. This modification is needed to treat the source terms which appeared in equations due to their coupling.

4.2 Linear Waves

As an example, the propagation of a pulse in an one-dimensional medium which can be represented as an elastic bar is analysed. This bar is assumed homogeneous except of a region of length d, where periodically alternating layers of size l are inserted. The density and longitudinal velocity in the bar are chosen as $\rho_0 = 4510$ kg/m^3 and $c = 5240$ m/s, respectively. The corresponding parameters for the material of the inhomogeneity layers are $\rho_1 = 2703$ kg/m^3 and $c_1 = 5020$ m/s, respectively. The shape of the pulse before the crossing of the inhomogeneity region is formed by an excitation of the strain at the boundary for an limited dimensionless time period ($0 < t < 100$)

$$\varepsilon(0,t) = (1 + \cos(\pi(t-50)/50)) . \tag{4.1}$$

The time step used in calculations is by definition a unit. The length of the pulse $L = 100\,\Delta x$ is comparable with the size of inhomogeneity ($l = 128\,\Delta x$). Using the notion of the bar, it must be stressed that l and L are much smaller than the diameter of the bar [15].

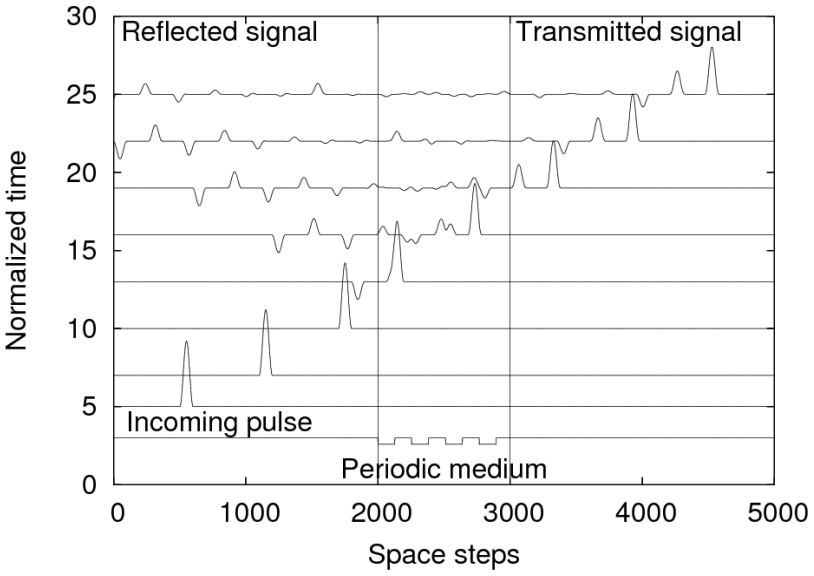

Fig. 4.1 Scattering of a pulse by a periodic multilayer.

Direct numerical simulation of linear elastic wave propagation in the medium with variable properties shows that the pulse holds its shape up to the entering into the inhomogeneity region. After the interaction with the periodic multilayer, the single pulse is separated into many reflected and transmitted parts as it can be seen in Fig. 4.1. Normalized time shown in Fig. 4.1 is measured in hundreds of time steps. During the propagation in the periodic medium, the amplitude of the pulse is diminished due to multiple reflections.

The same pulse propagation was simulated by the microstructured model described above with the following choice of material parameters: $A = 49\ \rho_0 c^2$, $I = \rho_1$, $C = Ic_1^2$, $B = 24.6\ A^2\rho_0 c^2$. In this case, there is no assumption of periodicity of microstructure, however, in calculations of the pulse propagation, the internal length l for the microstructure is kept the same as in the case of periodic multilayer. The ratio of scales l and L together with the value of the parameter A determines the contribution of the microstructure to the macromotion.

Here the coupled systems of equations (3.11), (3.12) and (3.14), (3.16) are solved simultaneously. It should be noted that no boundary conditions for the internal variable are prescribed. A non-zero solution for the microstructure is induced due to the coupling.

Results of numerical simulation are presented in Fig.4.2, where the corresponding transmitted pulses from the solution of the problem with periodic multilayer are also shown.

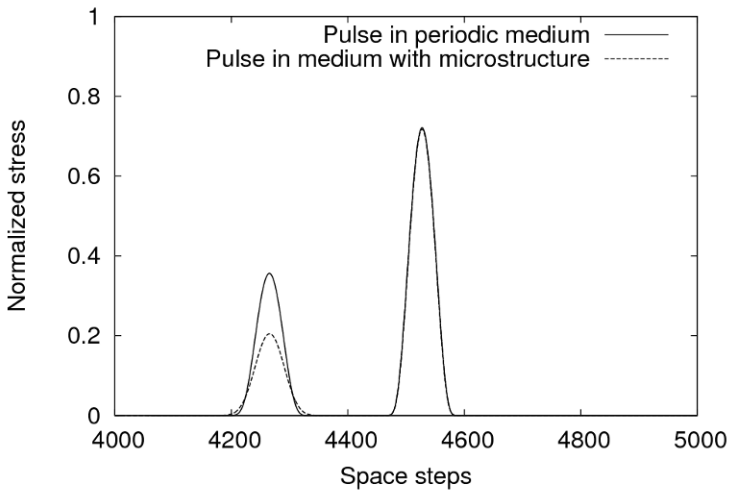

Fig. 4.2 Transmitted pulses.

As one can see, the adjustment of material parameters in the microstructure model allows us to reproduce the first pulse with perfect accuracy while the second one is essentially smaller in amplitude, because of the absence of a reflected trail in the case of the microstructure model.

4.3 Weakly Nonlinear Waves

We consider again the propagation of a pulse in a layered 1D medium (elastic bar) where the length of inhomogeneity $l = 4\,\Delta x$ is much smaller than the length of the pulse $L = 100\,\Delta x$. The properties of materials are the same as previously with a weak nonlinearity for the less stiff material (cf. [16])

$$\sigma = \rho_0 c^2 u_x \left(1 + N u_x\right) , \tag{4.2}$$

where N is a parameter of nonlinearity.

Direct computations in this weakly nonlinear case ($N = 0.04$) show that the initial bell-shaped pulse is transformed in a train of soliton-like pulses propagating with amplitude-dependent speeds (Fig. 4.3) like for the celebrated KdV case.

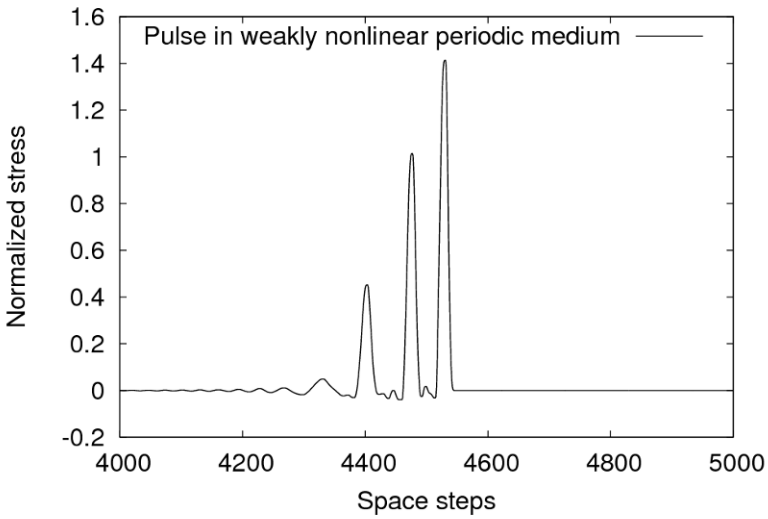

Fig. 4.3 Transformation of a bell-shaped pulse in a weakly nonlinear periodic medium (after 4600 time steps).

If we return to the microstructure model then the linear governing equations (3.7), (3.8) must be modified. Instead of the free energy function (3.5), a cubic function is used:

$$W^* = \frac{\rho_0 c^2}{2} u_x^2 + A\phi u_x + \frac{1}{2} B\phi^2 + \frac{1}{2} C\phi_x^2 + \frac{1}{2} D\psi^2 + \frac{\rho_0 c^2}{6} M\phi^3 + \frac{\rho_0 c^2}{6} N u_x^3, \tag{4.3}$$

where M and N are new material constants (see [17]).

Now the governing equations yield (cf. (3.7), (3.8))

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + \rho_0 c^2 N u_x u_{xx} + A\phi_x, \tag{4.4}$$

$$I\phi_{tt} = C\phi_{xx} + M\phi_x\phi_{xx} - Au_x - B\phi. \tag{4.5}$$

Besides dispersive effects (see [10]), the governing equations (4.4) and (4.5) include also nonlinear effects in macro- and microscale. The dispersive effects are analysed in [10] while the influence of nonlinearities is described in [18]. It is not surprising that the balance between the dispersive and nonlinear effects can occur resulting in emergence of solitons.

For numerical simulation, the system of equations (4.4), (4.5) can be represented in the form of a single (4^{th} order) equation (like Eq. (3.10)). The initial value problem for such a model nonlinear equation is solved by the pseudospectral method [18]. The initial pulse-type excitation leads to the train of solitons similar to that shown in Fig. 4.3.

5. Conclusions

If we know all the details of a given microstructure, namely, size, shape, composition, location, and properties of inclusions as well as properties of a carrier medium, the classical wave theory is sufficient for the description of wave propagation. Usually our knowledge about the microstructure is limited – we know only the characteristic scale of microstructure and its physical properties. Then the accuracy of classical theories is not sufficient and the more advanced theories of continua should be used.

In the paper, we have compared results of direct numerical simulations of wave propagation in given layered media with the corresponding results obtained by a continuous model of the microstructure. The presented model looks like a promising variant of the theory, complicated enough to describe various effects of the

microstructure. This model can be naturally extended to include non-linear effects and dissipation [19]. However, numerical simulations demonstrate that the straight-forward numerics and the modelling on the basis of continuum theories need a careful matching of material coefficients.

Some general remarks should be made in addition. The concept of dual internal variables introduced in [7] permits to model consistently microstructure(s) for both dissipative (not analysed here) and non-dissipative processes (see above). Such an approach gives an excellent basis to clarify the structure of generalised continuum theories such like linear Cosserat, micromorphic, and second gradient elasticity theories. This will be a subject of our forthcoming publications.

Once the wavefields in microstructured materials are described with needed accuracy, the respective mathematical models can also be used for solving the inverse problems. In linear cases, the dependence of phase velocities on the microstructure can be used for determining the material properties. In nonlinear cases, when the balance between dispersive and nonlinear effects supports the propagation of solitary waves, the algorithms for solving the inverse problems can be based on the analysis of shapes of solitary waves. It has been shown namely [17] that the nonlinearity of the microstructure leads to asymmetric solitary waves. This property can be used for constructing an algorithm which determines the parameters of the microstructure from measured asymmetry (see [17]).

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References

[1] Maugin, G.A.: *Nonlinear Waves in Elastic Crystals*, Oxford University Press (1999).
[2] Sun, C.T., Achenbach, J.D., Herrmann, G.: Continuum theory for a laminated medium. *J. Appl. Mech*. **35** 467–475 (1968).
[3] Nemat-Nasser, S., Hori, M.: *Micromechanics: Overall Properties of Heterogeneous Materials*, Elsevier, Amsterdam (1993).
[4] Mindlin, R.D.: Microstructure in linear elasticity. *Arch. Rat. Mech. Anal* **16** 51-78 (1964).
[5] Eringen, A.C., Suhubi, E.S.: Nonlinear theory of micro-elastic solids II. *Int. J. Eng. Sci.* **2** 189-203 (1964).
[6] Maugin, G.A.: On the thermomechanics of continuous media with diffusion and/or weak nonlocality. *Arch. Appl. Mech.* **75** 723-738 (2006).
[7] Ván, P., Berezovski, A., Engelbrecht, J.: Internal variables and dynamic degrees of freedom. *J. Non-Equilib. Thermodyn.* **33** 235-254 (2008).
[8] Nowacki, W.: *Thermoelasticity*. Pergamon/PWN, Oxford/Warszawa (1962).
[9] Maugin, G.A.: Internal variables and dissipative structures. *J. Non-Equilib. Thermodyn*. **15** 173-192 (1990).
[10] Engelbrecht, J., Berezovski, A., Pastrone, F., Braun, M.: Waves in microstructured materials and dispersion. *Phil. Mag*. **85** 4127-4141 (2005).

[11] Engelbrecht, J., Cermelli, P., Pastrone, F.: Wave hierarchy in microstructured solids. In: Maugin, G.A. (ed.) Geometry, *Continua and Microstructure*, pp. 99-111. Hermann Publ., Paris (1999).
[12] *Effective Computational Methods for Wave Propagation*. Kampanis, N. A., Dougalis, V.A., Ekaterinaris, J.A. (eds.) , Chapman & Hall/CRC, Boca Raton (2008).
[13] LeVeque, R.J.: *Finite Volume Methods for Hyperbolic Problems*. Cambridge University Press (2002).
[14] Berezovski, A., Engelbrecht, J., Maugin, G.A.: *Numerical Simulation of Waves and Fronts in Inhomogeneous Solids*. World Scientific, Singapore (2008).
[15] Lakes, R.S.: Experimental method for study of Cosserat elastic solids and other generalized continua. In: Mühlhaus, H.-B. (ed.) *Continuum Models for Materials with Microstructure,* pp.1-22. Wiley, New York (1995).
[16] Berezovski, A., Berezovski, M. and Engelbrecht, J.: Numerical simulation of nonlinear elastic wave propagation in piecewise homogeneous media. *Mater. Sci. Engng. A* **418** 364-369 (2006).
[17] Janno, J., Engelbrecht J.: An inverse solitary wave problem related to microstructural materials. *Inverse Problems.* **21** 2019-2034 (2005).
[18] Engelbrecht, J. Berezovski, A., Salupere, A.: Nonlinear deformation waves in solids and dispersion. *Wave Motion*. **44** 493-500 (2007).
[19] Pastrone, F., Cermelli, P. and Porubov, A.: Nonlinear waves in 1-D solids with microstructure. *Mater. Phys. Mech.* **7** 9-16 (2004).