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MICROSTRUCTURED SOLIDS AND INVERSE PROBLEMS

Abstract. Microstructured solids are characterized by their dispersive properties and dispersive effects can be used for solving the inverse problems, i.e. for Nondestructive Testing. In this paper the Mindlin-type one-dimensional model is derived for longitudinal wave motion in such solids. In case of linear approximation, the inverse problems based on harmonic waves and localized boundary conditions are posed and solved, using the measurements of phase and group velocities and phase shifts. The full nonlinear model leads to solitary waves due to the balance of dispersive and nonlinear effects resulting in an asymmetric solitary wave. In this case the characteristics of wave profiles are used for solving an inverse problem.

1. Introduction

Contemporary materials are often characterized by their complex structure at various scales. For short, such materials are refered to as "microstructured materials". The microstructural properties influence strongly the macro-behaviour of compound materials and/or structures, that is why stress analysis should be based on proper modelling of possible physical effects caused by the microstructure. Two possible classes of problems must be distinguished: (i) given the properties of the material and its constituencies, and external disturbance, determine the global behaviour; (ii) given the external disturbance and the global behaviour, determine the properties of the material. The first class is identified as direct problems, the second – as inverse problems. In technical terms, the second class (inverse problems) is the Nondestructive Testing (NDT) with the aim to determine the physical and/or geometrical properties of materials (specimens) by measuring the wave fields at given excitations. By using ultrasound, NDT has found wide range of applications not only in engineering but also in medicine.

The ideas of using ultrasound in NDT have been developed since the discovery of the piezoelectric effect in quartz in 1880 (see [1]). The ideas were developed further for detecting objects in water (or air) and for detecting flaws in solids. Overviews on later applications are given in [2] - [5], for example.

Quite often in engineering applications of NDT, simplified mathematical models are used and the origin of these models, based on continuum mechanics, is forgotten. In [6], a simple straight-forward idea is advocated: for theoretical background of NDT, the conservation and constitutive laws should be stated first in the full correspondence to the axioms of continuum mechanics. The outcome could be rather complicated but all the possible simplifications (approximations) of the basic model should be based on clear procedures retaining the effects of the same order of accuracy. Only then the solutions of the inverse problems reflect reality.

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In most general terms, microstructured materials mean polycrystalline solids, ceramic composites, functionally graded materials, granular materials, etc. The existence of grains, inclusions, layers, block walls, etc. – all that refers to microstructure. There are powerful methods in continuum mechanics in order to describe such materials or the existence of irregularities in materials starting from early studies of Cosserats and Voigt up to contemporary formulations [7]. The straight-forward modelling of microstructured solids leads to assigning concrete physical properties to every irregularity or to every volume element in a solid. This means introducing direct dependencies of all the physical properties on material coordinates and consequently leads to an extremely complex system. Another approach is to separate macro- and microstructure in continua. Then the conservation laws for both structures should be separately formulated [7, 11] or the microstructural quantities are separately taken into account in one set of conservation laws [8].

In this paper, we present a mathematical model for microstructured solids following the ideas of separating macro- and microstructure [11]. The details of modelling are described in [12, 13]. Based on that model, inverse problems in one-dimensional (1D) setting are posed and solved by making use of wave field characteristics. Presented are the main ideas whereas the uniqueness and stability theorems are published elsewhere [14, 15].

In Section 2 the basic assumptions are presented and the mathematical model is derived. The physical effects described by such a model are listed in Section 3. The focal point of this paper is Section 4 where three inverse problems are posed and their solutions briefly envisaged. In Section 5, results are summed up.

2. Mathematical model

We start from the Mindlin model [11] for microstructured solids. This model has a clear physical background interpreting the microstructure as deformable cells which can be "a molecule of a polymer, a crystallite of a polycrystal or a grain of a granular material". The displacement $\mathbf{u}$ of a material particle in terms of macrostructure is defined as usual by its components $u_i \equiv x_i - X_i$, where $x_i, X_i (i = 1, 2, 3)$ are the components of the spatial and material position vectors, respectively. Within each material volume there is a microvolume (microstructure) and the microdisplacement $\mathbf{u}'$ is defined by $u'_i \equiv x'_i - X'_i$, where the origin of the coordinates x'_i moves with the displacement $\mathbf{u}$. The displacement gradient is assumed to be small and that permits to use the basic assumption of the Mindlin model

$$u'_j = x'_k \varphi_{kj}(x_i, t) \tag{1}$$

and consequently

$$\frac{\partial u'_j}{\partial x'_i} = \partial'_i u'_j = \varphi_{ij}. \tag{2}$$

Further we limit ourselves to the 1D case (see discussion in Section 5) and denote $u_1 = u$, $\varphi_{11} = \varphi$. The fundamental balance laws are formulated separately for macroscopic and microscopic scales.

We assume that free energy function W has the form $W = W_2 + W_3$, where W_2 is the simplest quadratic function

$$W_2 = \frac{1}{2}\left(\alpha u_x^2 + B\varphi^2 + C\varphi_x^2 + 2A\varphi u_x\right) \tag{3}$$

and W_3 includes nonlinearities on both the macro- and microlevel

$$W_3 = \frac{1}{6}\left(Nu_x^3 + M\varphi_x^3\right). \tag{4}$$

Here α, A, B, C, N and M are constants and indices here and below denote differentiation. The non-quadratic potential W_3 is the first approximation towards nonlinear theory. Then the governing equations (for details, see [12, 13] are the following:

$$\rho u_{tt} = \alpha u_{xx} + N u_x u_{xx} + A\varphi_x, \tag{5}$$

$$I\varphi_{tt} = C\varphi_{xx} + M\varphi_x\varphi_{xx} - Au_x - B\varphi, \tag{6}$$

where ρ is the macrodensity, and I is the microinertia. It can be shown that this system can also be interpreted as a balance of pseudomomentum [14] - for that see [16].

Let us rewrite this system (5), (6) in dimensionless variables $X = x/L$, $T = tc_0/L$, $U = u/U_0$, where U_0 is the amplitude of an excitation, and L - the wavelength of an excitation, and $c_0^2 = \alpha/\rho$. Note that φ is already dimensionless. We introduce also the geometric parameters $\delta = l^2/L^2$, $\epsilon = U_o/L$, where l is the scale of the microstructure. System (5), (6) yields then

$$U_{TT} = U_{XX} + \frac{N\epsilon}{\rho c_0^2} U_X U_{XX} + \frac{A}{\rho c_0^2 \epsilon}\varphi_X, \tag{7}$$

$$\delta\alpha I^*\varphi_{TT} = \delta C^*\varphi_{XX} + \delta^{3/2}M^*\varphi_X\varphi_{XX} - A\epsilon U_X - B\varphi, \tag{8}$$

where $I = I^*\rho l^2$, $C = C^* l^2$ and $M = M^* l^3$.

For further analysis we eliminate microdeformation φ from (7), (8) by making use of the slaving principle [16, 17]. This results in the following hierarchical governing equation for U

$$\begin{aligned} U_{TT} &= (1-b)\, U_{XX} + \frac{\mu}{2}(U_X^2)_X + \delta(\beta U_{TT} - \gamma\, U_{XX})_{XX} - \\ &- \delta^{3/2}\frac{\lambda}{2}(U_{XX}^2)_{XX}, \end{aligned} \tag{9}$$

where

$$b = \frac{A^2}{\alpha\ B}, \quad \mu = \frac{N\varepsilon}{\alpha}, \quad \beta = \frac{A^2 I^*}{B^2}, \quad \gamma = \frac{A^2\ C^*}{\alpha\ B^2}, \quad \lambda = \frac{A^3\ M^*\ \varepsilon}{\alpha\ B^3}.$$

This is the sought model equation for longitudinal waves in 1D setting.

3. Direct problem: physical effects

Equation (9) is a comparatively simple model but surprisingly rich. For the sake of further analysis we separate linear ($N = M = 0$) and nonlinear ($N \neq 0, \quad M \neq 0$) cases. In the linear case

$$U_{TT} = (1-b)\, U_{XX} + \delta(\beta U_{TT} - \gamma\, U_{XX})_{XX} \tag{10}$$

the hierarchical structure is explicitly seen. Indeed, Eq. (10) includes two wave operators - one for macrostructure ($\mathcal{L}_{macro} = U_{TT} - (1-b)\, U_{XX}$), another for microstructure ($\mathcal{L}_{micro} = \beta U_{TT} - \gamma\, U_{XX}$). If the scale parameter δ is small then $\mathcal{L}_{micro}$ can be neglected; if δ is large then on contrary the influence of macrostructure is weaker and $\mathcal{L}_{macro}$ can be neglected; clearly the intermediate case includes both effects. The wave speed in the compound material is affected by the microstructure (1 *versus* b) and clearly only $A = 0$ excludes this dependence. The influence of the microstructure on wave motion is, as expected, characterized by dispersive terms. However, the double dispersion occurs due to the different higher order terms (U_{TTXX} and U_{XXXX}) – cf. [16, 18].

The dispersion analysis [12, 13] shows that the phase velocity depends strongly on the wave number, i.e. on frequency of the excitation. Consequently, this effect could be used for solving the inverse problem in the linear setting.

In nonlinear case of Eq. (9) with ($N \neq 0, M \neq 0$), dispersive and nonlinear terms act together. From the theory of nonlinear waves it is known that if dispersive and nonlinear effects are balanced, then solitary waves may emerge. It would be of interest to analyse this case separately from the viewpoint of an inverse problem – can the form of a solitary wave (if it exists) give information about the properties of microstructure?

In what follows, we present the main ideas of solving the inverse problems in linear (Eq. (10)) and nonlinear (Eq. (9)) cases. In other words, we are going to determine the coefficients of these equations related to physical parameters in (3), (4), (5), (6).

4. Inverse problems

4.1. Linear case, harmonic waves

For sake of simplicity, we rewrite Eq. (10) with lower case letters

$$u_{tt} = (1-b)\, u_{xx} + \delta(\beta\, u_{ttxx} - \gamma\, u_{xxxx}). \tag{11}$$

Obviously (see Eq. (3)) b, δ, β, γ are positive and $b < 1$. If we consider the scale parameter δ to be known, then the number of parameters to be determined for the inverse problem is three.

Assume that Eq. (11) has a solution in the form of harmonic waves

$$u(x,t) = exp[i(kx - \omega t)], \tag{12}$$

where k and ω are the wave number and frequency, respectively. Then the phase velocity c_{ph} is determined by

(13) $$c_{ph}(k) = \left(\frac{\delta\gamma k^2 + 1 - b}{\delta\beta k^2 + 1}\right)^{1/2}.$$

The inverse problem is the following: given three phase velocities $c_{ph}(k_1)$, $c_{ph}(k_2)$, and $c_{ph}(k_3)$ which correspond to wave numbers k_1, k_2, k_3 such that $k_1^2 \neq k_2^2$, $k_1^2 \neq k_3^2$, $k_2^2 \neq k_3^2$, determine the parameters b, β, and γ. The qualitative behaviour of phase velocities is shown in Fig. 1. This means solving the system of nonlinear equations with three unknowns

(14) $$c_{ph}(k_j) = \left(\frac{\delta\gamma k_j^2 + 1 - b}{\delta\beta k_j^2 + 1}\right)^{1/2}, \qquad j = 1, 2, 3,$$

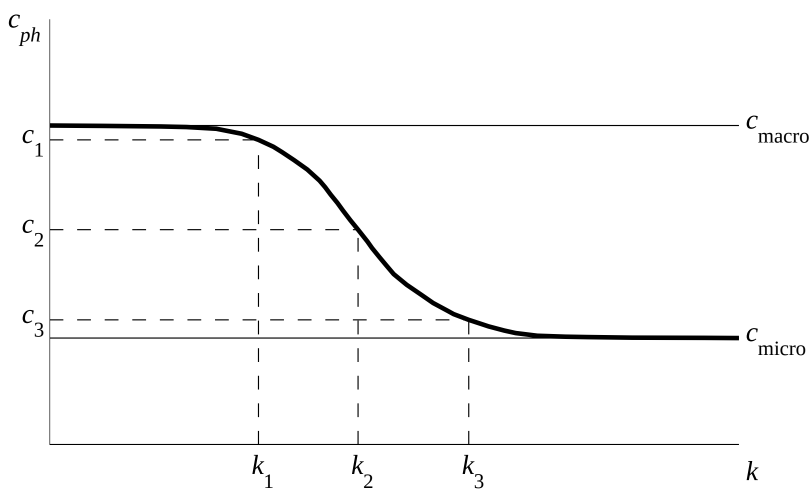

Figure 1: Qualitative behaviour of phase velocities. Here c_{macro} and c_{micro} denote the velocities in pure macro- and microstructure, respectively; c_j, $j = 1, 2, 3$ are phase velocities $c_{ph}(k_j)$.

Actually it is possible to transform Eq. (14) to a more suitable form for practical solution

(15) $$b + \delta k_j^2 c_{ph}^2(k_j)\beta - \delta k_j^2\gamma = 1 - c_{ph}^2(k_j), \qquad j = 1, 2, 3.$$

The detailed analysis of uniqueness of solution to Eq. (15) is given in [14].

4.2. Linear case, localized boundary condition

In practice of NDT, the excitations (boundary conditions) are usually localized. The general solution to Eq. (11) satisfying the boundary condition $u(0,t) = g(t)$ is the following:

$$u(x,t) = \frac{1}{2\,\pi}\int_{-\infty}^{\infty} G(\omega)\exp\left[i\,(k(\omega)x - \omega t)\right]d\omega, \tag{16}$$

$$G(\omega) = \int_{-\infty}^{\infty} g(t)\exp(i\omega t)dt. \tag{17}$$

We assume now

$$g(t) = A\exp\left(-\frac{t^2}{4\nu^2}\right)\exp(-i\eta t), \tag{18}$$

where A, ν are given and η is the fixed frequency.

Then expression (16) yields (for details see [17])

$$u(x,t) = \frac{A\nu}{\sqrt{\pi}}\int_{-\infty}^{\infty}\exp\left[-\nu^2(\omega-\eta)^2\right]\exp\left[i\,(k(\omega)x - \omega t)\right]\,d\omega. \tag{19}$$

Further on, we use an approximation and derive $k(\omega)$ into the Taylor series around $\omega = \eta$. Keeping three first terms, we have

$$k(\omega) \approx k(\eta) + k'(\eta)(\omega-\eta) + \frac{1}{2}k''(\eta)(\omega-\eta)^2, \tag{20}$$

where prime denotes differentiation. From the definition of phase and group velocities we determine

$$k\,(\eta) = \frac{\eta}{c_{ph}}, \quad k'(\eta) = \frac{1}{c_g} \tag{21}$$

and denote $d = \frac{1}{2}k''(\eta)$.

The real part of the integral (19) can now be evaluated [14] ($\tilde{u}$ denotes the approximation):

$$Re\tilde{u}(x,t) = A_1(x)\exp\left[-\nu^2 f_1(x,t)\right]\cos\left[\eta\left(\frac{x}{c_{ph}} - t\right) + \Phi(x) - \right. \\ \left. - \, xdf_1(x,t)\right], \tag{22}$$

$$A_1 = A\nu(\nu^4 + x^2d^2)^{-\frac{1}{4}}, \tag{23}$$

$$f_1(x,t) = \frac{1}{4}\left(\frac{x}{c_g} - t\right)^2(\nu^4 + x^2d^2)^{-1}, \tag{24}$$

$$\Phi(x) = \frac{\arctan \frac{1}{2} x d}{\nu^2}. \tag{25}$$

From (22) - (25) it follows that the amplitude of the wave is decreasing with increasing x and the dispersion of the normal distribution in $g(t)$ is increasing. So it is possible to determine the number d from the measurement.

The inverse problem stated now is the following: given the phase and group velocities c_{ph}, c_g and the number d, determine the parameters b, β, γ. This problem has the unique solution provided $c_{ph} \neq c_g$:

$$\beta = \frac{1}{\delta m^2}(4F(m) - 1), \tag{26}$$

$$\gamma = \frac{c_{ph}}{\delta m^2}(4c_g F(m) - c_{ph}), \tag{27}$$

$$b = 1 + c_{ph}\left[4(c_g - c_{ph})F(m) - c_{ph}\right] \tag{28}$$

with

$$F(m) = \left[\frac{c_g}{c_{ph}} - \frac{2dmc_g^3}{c_g - c_{ph}}\right]^{-1}, \tag{29}$$

where m is the wave number corresponding to the frequency η and the condition $0 < F^{-1}(m) < 4$ must be satisfied in order to get positive β.

4.3. Nonlinear case, solitary wave

As in Section 4.1, we rewrite the basic equation – Eq. (9) with lower case letters. As far as here is no need to distinguish the wave speed components for microstructure, we denote by $b_1 = 1 - b$. Equation (9) reads then in terms of $v = u_x$

$$v_{tt} = b_1\, v_{xx} + \frac{\mu}{2}(v^2)_{xx} + \delta(\beta v_{tt} - \gamma v_{xx})_{xx} - \delta^{3/2}\frac{\lambda}{2}(v_x^2)_{xxx}. \tag{30}$$

First we establish a solution to the direct problem and then analyse the possibilities to solve the inverse problem. We seek the travelling waves

$$v(xt) = w(x - ct) = w(\xi) \tag{31}$$

where c is a free parameter (velocity of the wave) and $w(\xi)$ satisfies the equation

$$(c^2 - b_1)w'' - \frac{\mu}{2}(w^2)'' - \delta(\beta c^2 - \gamma)w^{IV} + \delta^{3/2}\frac{\lambda}{2}\left[(w')^2\right]''' = 0. \tag{32}$$

When looking for solitary waves, the conditions $\omega(\xi), \omega'(\xi), \omega''(\xi) \to 0$ as $|\xi| \to \infty$ should be satisfied. After integrating Eq. (32) three times (before the last integration multiplying by ω'), we obtain

$$\frac{1}{2}\delta\left(\beta c^2 - \gamma\right)\left(w'\right)^2 - \frac{1}{3}\delta^{3/2}\lambda\left(w'\right)^3 = \frac{1}{2}\left(c^2 - b_1\right)w^2 - \frac{1}{6}\mu w^3. \tag{33}$$

It can be proved [18] that for the existence of the solitary wave solution the following in equalities should be satisfied

$$\beta c^2 - \gamma \neq 0, \quad c^2 - b_1 \neq 0, \quad \mu \neq 0. \tag{34}$$

In addition, the necessary solvability condition is

$$\left(c^2 - b_1\right) / \left(\beta c^2 - \gamma\right) > 0. \tag{35}$$

Now we introduce the following three parameters which have certain physical or geometrical meaning:

$$\kappa = \sqrt{\frac{c^2 - b_1}{\delta(\beta c^2 - \gamma)}}, \quad A = \frac{3(c^2 - b_1)}{\mu}, \quad \theta = 2\left[\frac{c^2 - b_1}{\beta c^2 - \gamma}\right]^{3/2} \frac{\lambda}{\mu}. \tag{36}$$

In terms of these parameters, Eq. (33) has the form

$$(w')^2 - \frac{\theta}{\kappa A}(w')^3 = \kappa^2 w^2 \left(1 - \frac{w}{A}\right). \tag{37}$$

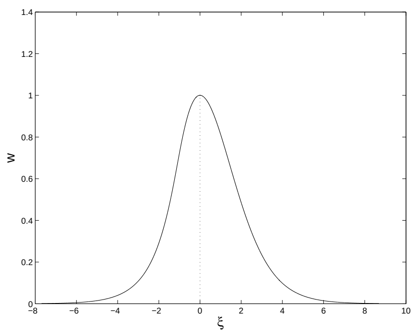

Figure 2: Solitary wave in case $\theta = 0.9$

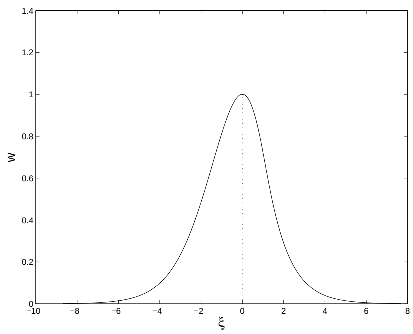

Figure 3: Solitary wave in case $\theta = -0.9$

The parameter κ is the exponential decay rate of the solution as $|\xi| \to \infty$. The inverse of decay rate $1/\kappa$ is usually referred to as the width of the wave. Parameter A is actually the amplitude of the wave and parameter θ is related to the asymmetry of the wave. We remind now that in our model two nonlinearities are taken into account: on the macrolevel ($\mu \neq 0$) and on the microlevel ($\lambda \neq 0$) – cf. Eq. (9). If $\lambda = 0$, i.e. nonlinearity on the microlevel is neglected then a symmetric bell-shaped solitary wave can be found [16, 18]

$$w(\xi) = A \cosh^2\left(\frac{\kappa\xi}{2}\right). \tag{38}$$

In case $\mu \neq 0$, $\lambda \neq 0$, the situation is more complicated and we have used numerical integration for finding the solitary wave. Two examples of solitary waves, computed by means of the second-order Adams-Bashforth method, are depicted in Figs 2, 3, where $\zeta = \kappa\xi$, $y = \omega/A$. The results are clearly asymmetric. Let us fix same relative level $y \in (0, 1)$ and consider the front and rear half-lengths of the wave at this level – namely the quantities $|\xi^-(yA)|$ and $|\xi^+(yA)|$. The asymmetry at this level is the ratio of those quantities which depends on [18]:

(39) $$\frac{|\xi^+(yA)|}{|\xi^-(yA)|} = F_y(\theta),$$

where $F_y(\theta)$ is an increasing function of θ in the interval (-1,1) and $F_y(0) = 1$. The details on complicated function F_y are presented in [15].

In the model equation (30) there are 5 material parameters: $b_1, \mu, \beta, \gamma, \lambda$ which need to be determined in the NDT. Measuring just a single solitary wave, one could recover maximally κ, A, and θ, i.e. only 3 parameters. That is why for solving the full problem, one should use the measurements of two independent solitary waves [19]. The full procedure is formed by two stages. As before, we assume δ to be known.

The first stage is to determine the parameters of macrostructure, b_1 and μ. Let be given two solitary waves ω_1 and ω_2 with the velocities c_1 and c_2, and amplitudes A_1 and A_2.

We expect that the conditions $c_1^2 \neq c_2^2$ and hence $A_1 \neq A_2$ are satisfied. Then from expressions (36) we have the system

(40) $$3b_1 + A_j\mu = 3c_j^2, \quad j = 1, 2,$$

which determine uniquely b_1 and μ.

The second stage is to find other unknowns β, γ, λ. For that not only the amplitudes A_j and c_j should be known but also some additional information. We fix two numbers w_{11}, w_{12} which lie between 0 and A_1 for the first solitary wave at both sides of the maximum amplitude A_1, respectively and a number w_{21} which lies between 0 and A_2 for the second solitary wave. We need also to registrer time when the first wave reaches w_{11}, $w = A_1$, and w_{12} and the second – w_{21} and $w = A_2$. Then knowing c_1 and c_2, the corresponding coordinates ξ_{11}, ξ_{12} and ξ_{21} can be calculated. Note that $\xi = 0$ for both A_1 and A_2. Now the inverse problem posed is the following: given b_1, μ, the points (ξ_{11}, w_{11}), (ξ_{12}, w_{12}) with $\xi_{11} > 0$, $\xi_{12} < 0$ on the graph of the first wave and the point (ξ_{21}, w_{21}) with $\xi_{21} \neq 0$ on the graph of the second wave, determine β, γ, λ. The details of solving this inverse problem with the proof of the uniqueness and a stability estimate are given in [19].

5. Summary

It has been demonstrated how to solve the inverse problem of determining the material parameters from wave characteristics in microstructured materials. The following physical effects have been used: (i) the dependencies of phase and group velocities on wave numbers and (ii) the asymmetric structure of solitary waves. The measurements of velocities are easily carried on, the measurements of wave profiles need higher accuracy. However, the experimental studies of strain waves in microstructured materials [20] have demonstrated the asymmetry of solitary waves. In this case tungsten-epoxy composites were used with reference samples made of aluminium.

In practical realizations the ultrasonic transducers are used for generating waves in samples. In principle, the generated wave beams are not one-dimensional but the diffractional expansion in the transverse direction is rather weak. On the axis of the wave beam, the 1D approximation is possible [21].

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