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Waves in microstructured solids with nonlinearities in microscale

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Abstract. Consistent modelling of wave motion in microstructured solids is discussed. Based on the Mindlin model, the simplest model equation of motion is derived. The fundamental properties of such a model are (i) hierarchical structure distinguishing the macro- and microbalance, (ii) changes in the wave speed, and (iii) definite influence of dispersion. The nonlinearity in the microlevel, although presented by a simple energy density function, leads to a complicated nonlinear term in the equation of motion as well as in the corresponding evolution equation. Such consistent modelling opens up direct ways for determining material constants characterizing the microstructure.

Key words: microstructured solids, wave hierarchy, nonlinearity, evolution equation.

1. INTRODUCTION

Attention to microstructured materials has increased enormously over the last decade. One reason is that materials like alloys, crystallites, ceramics, composites, functionally graded materials, etc. have gained wide application. On the other hand, the dynamical excitations have the same wavelengths as the spatial scale of inhomogeneities, and even intuitively one could understand that the internal structure of the material should influence the wave field. In order to model possible physical phenomena related to various scales, both macro- and microscales should be distinguished. Actually, the theory of continua foresaw such problems long ago [1–3]. Contemporary understanding of basic mechanics of such materials is presented in Maugin [4]. The microstructure involves additional degrees of

freedom to the motion of the macrostructure. There are several possibilities of describing the influence of such a phenomenon depending upon the assumptions: Cosserat continuum, continua with planar and ordinary spins, continua with vector microstructure, micromorphic continua, etc. [5,6].

Here attention is focused on the modelling of wave motion in microstructured solids following the idea of the hierarchy of waves in the sense of Whitham [7]. The idea is to construct a governing equation, say for a longitudinal wave which should be able to distinguish between the scales, i.e. between long- and short-wave excitations. Considering recent findings on nonlinear behaviour of the microstructure [8], the model should be able to catch that effect.

An overview of several models can be found in [9]. More recently, the ideas of Mindlin [3] have been used in several studies [10−12] for analysing the one-dimensional (1D) wave motion. It has been shown that the concept of internal variables [13] can be extremely useful in deriving the evolution equations [11]; this approach corresponds to the case where microbalance is assumed not to be inertial. Several models for granular media have been derived accounting either for the rotation of particles [14] or full deformation of grains [15].

Despite the existence of several models, we would like here to clarify the essence of the approach based on splitting the macro- and microforce balances. In other words, this is a search for a "skeleton" to which "flesh" could be added depending on various physical constitutive assumptions. Section 2 gives the basic statements and a short description of the Mindlin theory. In Section 3 the basic model is derived and analysed. Section 4 describes nonlinearity in microscale. Finally, in Section 5 the discussion on modelling and the corresponding evolution equations is presented.

2. BASIC STATEMENTS

The starting assumption is to distinguish between the macro- and microscales (i.e. gross and fine structure, respectively [10,16]). Actually, the terminology is not yet fixed and here we stress that the microscale corresponds to a scale of about 1 μm. This scale excludes nanoeffects and is sometimes called a mesoscale (the notion of mesoscopic materials is used [8]). According to [2,16], the fundamental balance laws accounting for two scales can be formulated as follows: macroscopic momentum balance:

$$\int_{\partial P} \mathbf{S}\,\mathbf{n} da + \int_P \mathbf{b}_{\rm mac} dV = \frac{d}{dt} \int_P \mathbf{v} dV, \tag{2.1}$$

and microscopic momentum balance:

$$\int_{\partial P} \mathbf{N}\,\mathbf{n} da + \int_P (\mathbf{b}_{\rm mic} + \mathbf{T}) dV = \frac{d}{dt} \int_P \mathbf{w} dV. \tag{2.2}$$

Here P is a control volume, $\mathbf{n}$ is the outward unit normal to ∂P, $\mathbf{S}$ is the macrostress tensor (Piola stress), $\mathbf{N}$ is the microstress tensor, $\mathbf{b}_{\mathrm{mac}}$ and $\mathbf{b}_{\mathrm{mic}}$ are the body macro- and microforces, respectively, $\mathbf{T}$ is the interactive microforce. The kinematics include the following notations: $\mathbf{v} = \rho\dot{\mathbf{y}}$ is the linear momentum, ρ is the mass density, and $\dot{\mathbf{y}}$ is the macroscopic velocity; $\mathbf{w} = I_{\mathrm{in}}\dot{\boldsymbol{\delta}}$, where I_{in} is the inertia tensor and $\dot{\boldsymbol{\delta}}$ is the microscopic velocity.

In the 1D case, Eqs. (2.1), (2.2) yield

$$\rho u_{tt} = \sigma_x + b_{\mathrm{mac}}, \tag{2.3a}$$

$$I\delta_{tt} = \eta_x + \tau + b_{\mathrm{mic}}, \tag{2.3b}$$

where $\sigma,\ \eta$, and τ denote the single components of $\mathbf{S}, \mathbf{N}$, and $\mathbf{T}$, respectively, and the indices x, t denote differentiation. Further on the influence of $b_{\mathrm{mac}}, b_{\mathrm{mic}}$ is neglected.

Several studies are based on simplifications of (2.3). In [11] the inertia of the microstructure was neglected, and the microstructure was treated as an internal variable taking the dissipative effects into account. In [12] the influence of inertia was analysed together with several assumptions concerning the nonequilibrium parts of macro- and microstresses. Here we revisit [3] in order to build up a clear basis for further generalizations.

Mindlin [3, p. 51] has interpreted the microstructure "as a molecule of a polymer, a crystallite of a polycrystal or a grain of a granular material". Such an inclusion is a unit cell, and if this cell is rigid, the Cosserat model is obtained. The displacement $\mathbf{u}$ of a material volume P is defined 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 (particle) there is a microvolume P' and the microdisplacement $\mathbf{u}'$ is defined by $x_i',\ u_i' \equiv x_i' - X_i'$, where the origin of x_i' moves with the displacement $\mathbf{u}$. The displacement gradients are assumed to be small. This leads to the *basic assumption* that "the microdisplacement can be expressed as a sum of products of specified functions of x_i' and arbitrary functions of x_i and t" [3, p. 52]. The first approximation is then

$$u_j^{'} \ = \ x_k^{'}\psi_{kj}(x_i, t). \tag{2.4}$$

The *microdeformation* is

$$\frac{\partial u_j^{'}}{\partial x_i^{'}} \equiv \partial_i^{'} u_j^{'} = \psi_{ij}. \tag{2.5}$$

Clearly, beside macrostrain ϵ_{ij} one should account for a *relative deformation*

$$\gamma_{ij} = \partial_i u_j - \psi_{ij}, \tag{2.6}$$

which is actually the difference between the macrodisplacement gradient and the microdeformation, and also for a *microdeformation gradient*

$$\chi_{ijk} = \partial_i \psi_{jk}, \tag{2.7}$$

i.e. for the macrogradient of the microdeformation. Note that $\epsilon_{ij},\ \gamma_{ij},\ \chi_{ijk}$ are independent of $x_i^{'}$. Mindlin [3] has treated the full set of equations based on a homogeneous quadratic function of the potential energy density. The maximum number of independent coefficients is then 1764, but it can be reduced considerably by using additional assumptions. Here we use the basic kinematics of Mindlin and derive the governing equations for the 1D case: $\epsilon_{11} = u_x$, $\gamma_{11} = u_x - \psi,\ \ \chi_{111} = \psi_x$.

3. GOVERNING EQUATIONS

On the basis of the discussion in Sec. 2, we proceed with the simplest 1D model

$$\rho u_{tt} = \sigma_x, \quad I\psi_{tt} = \eta_x + \tau, \tag{3.1}$$

where there is no need to distinguish between material and space coordinates. Further we need the free energy function $W = W(u_x,\ \psi,\ \psi_x, ...)$ and the constitutive equations. These equations are split up into equilibrium and non-equilibrium (dissipative) components:

$$\sigma = \sigma_{\rm eq} + \sigma_{\rm neq}, \quad \eta = \eta_{\rm eq} + \eta_{\rm neq}, \quad \tau = \tau_{\rm eq} + \tau_{\rm neq}. \tag{3.2}$$

The equilibrium components are deduced from the free energy

$$\sigma = \frac{\partial W}{\partial u_x}, \quad \eta = \frac{\partial W}{\partial \psi_x}, \quad \tau\ =\ \frac{\partial W}{\partial \psi}, \tag{3.3}$$

while for nonequilibrium components the assumptions are needed, based on the principle of equipresence:

$$\sigma_{\rm neq} = D_{11}u_{xt} + D_{12}\varphi_t + D_{13}\psi_{xt}, \tag{3.4a}$$

$$\eta_{\rm neq} = D_{21}u_{xt} + D_{22}\psi_t + D_{23}\psi_{xt}, \tag{3.4b}$$

$$\tau_{\rm neq} = D_{31}u_{xt} + D_{32}\psi_t + D_{33}\psi_{xt}. \tag{3.4c}$$

Clearly, these equations are phenomenological and the dissipation inequality imposes restrictions on parameters D_{kl}. These assumptions need detailed analysis; here we leave them out from the further discussion and analyse only the dissipationless case.

The simplest free energy function describing the influence of a microstructure is a quadratic function

$$W = \frac{1}{2}\,\alpha u_x^2 - A\psi u_x + \frac{1}{2}\,B\psi^2 + \frac{1}{2}\,C\psi_x^2, \tag{3.5}$$

with α, A, B, C constants.

The balance equations are now specified as follows:

$$\rho u_{tt} = \alpha u_{xx} - A\psi_x, \tag{3.6a}$$

$$I\psi_{tt} = C\psi_{xx} - Au_x + B\psi. \tag{3.6b}$$

For further analysis we introduce dimensionless variables (note that ψ is already dimensionless)

$$U \;=\; uU_0^{-1}, \quad X \;=\; xL^{-1}, \quad T \;=\; tc_0L^{-1}, \tag{3.7}$$

where $c_0^2 \;=\; \alpha\rho^{-1}$; U_0 and L are certain constants (intensity and wavelength of the initial excitation). We also need a scale of the microstructure l. Then two dimensionless parameters can be introduced: $\delta \sim l^2L^{-2}$, $\epsilon \sim U_0L^{-1}$. Following [12], we suppose $I = \rho l^2 I^*,\; C = l^2 C^*$, where I^* is dimensionless and C^* has the dimension of the stress. Then (3.6) yields

$$U_{TT} \;=\; U_{XX} \;-\; \frac{A}{\epsilon\rho_0 c_0^2}\,\psi_X, \tag{3.8a}$$

$$\delta\alpha I^*\psi_{TT} \;=\; \delta C^*\psi_{XX} \;-\; A\epsilon U_X \;+\; B\psi. \tag{3.8b}$$

In order to reduce system (3.8) into one governing equation, the slaving principle could be used [12,17]. Indeed, (3.8b) yields

$$\psi \;=\; \frac{\epsilon A}{B}\,U_X \;+\; \frac{\delta}{B}\left(\alpha I^*\psi_{TT} - C^*\psi_{XX}\right). \tag{3.9}$$

If we consider $\psi = \psi_0 + \delta\psi_1 + ...$, we get

$$\psi_0 \;=\; \epsilon AB^{-1}U_X, \tag{3.10}$$

$$\psi_1 \;=\; \epsilon\alpha AI^*B^{-2}U_{XTT} \;-\; \epsilon AC^*B^{-2}U_{XXX}. \tag{3.11}$$

Inserting (3.10), (3.11) into (3.8), we get the final equation in terms of U as follows:

$$U_{TT} \;=\; \left(1 \;-\; \frac{A^2}{\alpha B}\right)U_{XX} \;+\; \delta\frac{A^2I^*}{B^2}\left(U_{TT} \;-\; \frac{C^*}{\alpha I^*}\,U_{XX}\right)_{XX}. \tag{3.12}$$

This is the sought "skeleton" of the wave equation for microstructured solids, much in the sense of the Lorenz system for the Navier–Stokes equations. Equation (3.12) has several remarkable properties:

(i) it reflects the *wave hierarchy* in Whitham's sence [7]; if δ is small, then the last two terms are negligible; if δ is large, then the first two terms are negligible and the process is governed by properties of the microstructure;

(ii) the *wave speed* in the compound material is affected by the microstructure (1 vs. $A^2\alpha^{-1}B^{-1}$) and clearly only $A = 0$ excludes this dependence. This is directly observed in numerical calculations of the wavefield in materials with randomly distributed inclusions [18];

(iii) the influence of the microstructure is, as expected, characterized by *dispersive terms*; however, contrary to the idealized models (see [19]), the double dispersion (different terms U_{TTXX} and U_{XXXX}) is of importance (see [20] where a similar effect is described in detail for waves in rods).

The model of the one-dimensional chain of dumbbell-like particles, exhibiting transverse displacements V_n and rotations ψ_n, yields a similar result [6]. Indeed, after passing to the continuum limit, the final system of equations of that model, describing micropolar Cosserat-type elasticity, coincides in principle with (3.6). Notice that the Maxwell–Rayleigh model [21] leads also to the double dispersion. However, the dispersive terms (U_{TTTT} and U_{XXTT}) are different from those in (3.12), which means a differerent operator for the wave hierarchy. While (3.12) includes the space derivatives of the wave operator in brackets, this model [21] indicates the role of time derivatives of the wave operator.

4. NONLINEARITY OF THE MICROSTRUCTURE

We focus now on possible nonlinear effects on the microstructural level motivated by experiments [8]. In order to understand again the basic effects, the description of the macrolevel is kept linear, and only one term in the free energy function is added compared to (3.5). Suppose

$$W = \frac{1}{2}\,\alpha u_x^2 - A\psi u_x + \frac{1}{2}\,B\psi^2 + \frac{1}{2}\,C\psi^2 + \frac{1}{6}\,M\psi^3. \tag{4.1}$$

Then instead of (3.6) we have

$$\rho u_{tt} = \alpha u_{xx} - A\psi_x, \tag{4.2a}$$

$$I\psi_{tt} = C\psi_{xx} + M\psi_x\psi_{xx} - Au_x + B\psi. \tag{4.2b}$$

Note that if $A = 0$, then Eq. (4.2b) is the familiar nonlinear equation of motion (term $\psi_x\psi_{xx}$). Following the slaving procedure (see Sec. 3), we obtain

$$\begin{aligned}\psi_1 = \epsilon\alpha A I^* B^{-2} U_{XTT} - \epsilon A C^* B^{-2} U_{XXX} \\ - \epsilon\delta^{1/2} A^2 M^* B^{-3} U_{XX} U_{XXX},\end{aligned} \tag{4.3}$$

where $M = l^2 M^*$. Due to basic assumptions about the microstructure, the nonlinearity is now described by higher-order derivatives. The final governing equation is then

$$U_{TT} = \left(1 - \frac{A^2}{\alpha B}\right) U_{XX} + \delta \frac{A^2 I^*}{B^2} \left(U_{TT} - \frac{C^*}{\alpha I^*} U_{XX}\right)_{XX}$$

$$- \ \delta^{3/2} \, \epsilon \frac{A^3 M^*}{\alpha B^3} \left[\frac{1}{2} \left(U_{XX}\right)^2\right]_{XX}. \qquad (4.4)$$

The effect of the nonlinearity is emphasized by the last term of Eq. (4.4). Its effect on wave profile distortion should be examined in detail. Obviously, the evolution equation could be derived on the basis of Eq. (4.4). For that we introduce the moving frame $a^2 = 1 - A^2 \alpha^{-1} B^{-1}$. The evolution equation governing the wave propagating to the right is then derived in terms of $v \sim U_x$:

$$\frac{\partial v}{\partial \tau} + \frac{\delta}{\epsilon} m \frac{\partial^3 v}{\partial \xi^3} + \delta^{3/2} n \left[\left(\frac{\partial^2 v}{\partial \xi^2}\right)^2 + \frac{\partial v}{\partial \xi} \left(\frac{\partial^3 v}{\partial \xi^3}\right)\right] = 0, \qquad (4.5)$$

where

$$m \sim \frac{A^2 C^*}{2\alpha a^2 B} - \frac{A^2 I^*}{2B^2}, \quad n = \frac{A^3 M^*}{2\alpha a^2 B^3}. \qquad (4.6)$$

5. DISCUSSION

First we give some ideas about the assumptions of the Mindlin theory. One might think about a more sophisticated description of the microstructure. For example, suppose $u_j^{'} = u_j^{'}(x_i^{'}, X^h, t)$. Then

$$\partial_i^{'} u_j^{'} = \frac{\partial}{\partial x_i^{'}} u_j^{'} \left(x_h^{'}, X^h, t\right) = \psi_{ij}^{'} \left(x_h^{'}, X^h, t\right). \qquad (5.1)$$

If we now magnify this to the level of the macrostructure, we get

$$\bar{\psi}_{ij} = \lim_{\Omega \to \mathbf{X}} \frac{1}{\Omega} \int_{\Omega} \psi_{ij}^{'} dx_1^{'} dx_2^{'} dx_3^{'}, \qquad (5.2)$$

where Ω is any portion of the body. Clearly, $\bar{\psi}_{ij}$ depends only on X^h. Hence, the microdeformation is expressed as a function of the macrocoordinates only in an "exact way" and not as a first approximation in (2.5). Obviously (2.5) can also be written in terms of Lagrangian coordinates. Moreover, the mathematical restrictions on the field function $\psi_{ij}^{'}$, such that the limit (5.2) exists, are weaker than the linearity assumed by Mindlin. Finally, the linear approximation is surely included in (5.2): if (5.1) holds and if we assume (2.4), then ψ_{ij} coincides with $\bar{\psi}_{ij}$, i.e. we recover the Mindlin model, only one assumption is included. Generally, the description (5.2) might be useful when we study the acceleration waves where jumps of the second derivatives for the macrofield and of the first derivative for the microfield occur (see [10]).

Within the framework of the Mindlin theory the simplest nonlinear evolution equation is Eq. (4.5). Although the dispersion is of the third order like in the KdV equation, the nonlinearity involved is much more complicated. The constraints due to the double-dispersion character of Eqs. (3.12) and (4.4) need to be analysed in detail (cf. [20]), but the influence of two terms is directly seen for the expression of the parameter m. Evidently the dispersion could be either normal or anomalous, depending on the material parameters. The nonlinear effects are crucial and the main question is whether the dispersive and nonlinear effects could be balanced. One should note here that we have kept kinematics linear and introduced only physical nonlinearity. This can be justified by the usual balance of geometrical and physical nonlinearities (see, for example, [22]) because the physical nonlinearity has leading qualitative and quantitative effects.

The model equations demonstrate clearly the fundamental influence of a microstructure on the wave motion – changes in the wave speed, dispersive character of motion, and the influence of a scale parameter. This permits us also to relate the experimental measurements directly to theoretically introduced parameters (cf. for example, the changes in wave speeds calculated by Berezovski et al. [18]).

In this paper nonlinearity in the microscale was introduced by smooth terms in the energy function (Section 4). There is experimental evidence that for some materials the microstructural nonlinearity has hysteretic character [8], modelled by phenomenological expressions. Further interest is to combine both descriptions: theory of continua and phenomenological approaches.

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Lainelevi mikrostruktuuriga materjalides ja mikrostruktuuri mittelineaarsus

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Lähtudes Mindlini teooriast on mikrostruktuur modelleeritav iseseisva kinemaatikaga osakestena, mille kohta kehtivad sarnaselt makroelemendi liikumisega jäävusseadused. On tuletatud lihtsaim ühemõõtmeline liikumisvõrrand, mille analüüs lubab tuvastada järgmised füüsikalised efektid. Esiteks on mudelil hierarhiline struktuur, mis eristab makro- ja mikroefektid sõltuvalt dünaamilise mõjutuse lainepikkusest. Teiseks ilmneb mudelist lainelevi kiiruse otsene sõltuvus mikrostruktuuri parameetritest. Kolmandaks on mudelist tuvastatav nn topeltdispersioon, kus lisaks tavapärasele sõltuvusele mikrostruktuuri ruumilisest jaotusest lisandub sõltuvus mikroelemendi inertsiaalsusest. Mikrostruktuuri mittelineaarsus (vastavalt kõige lihtsamale siseenergiafunktsioonile) põhjustab tavapärasest keerukamad mittelineaarsed efektid. Esitatud matemaatiline mudel lubab leida otseseid meetodeid mikrostruktuuri parameetrite määramiseks.