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On modelling of wave propagation in microstructured solids

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Abstract. The basic concepts for modelling wave propagation in solids with microstructure are described. It is shown that the Green method, based on postulating the potential energy function, has certain advantages compared with the widely used Cauchy method, which postulates directly the stress-strain relations. Simple examples demonstrate how the Green method together with internal variables permits to determine the microstress and the interactive force between the constituents of solids. The structure of governing equations and possible physical effects captured by such modelling are described. The microstress and interactive force lead to the dispersion of waves at the macrolevel.

Key words: microstructured solids, internal variables, dispersion.

1. INTRODUCTION

In engineering, the strength of materials is the most important feature for design of reliable structures. That is why the governing stress–strain relation must be determined with sufficient accuracy. The classical theories are based on the assumption of homogeneity of materials and this assumption has been justified for many applications. The contemporary technology is, however, characterized by the wide usage of alloys, polycrystalline solids, composites, functionally graded materials, etc. All these materials have an inherent internal structure – microstructure – at smaller scales. The question is how to take such a microstructure into account and how it affects the behaviour at the macroscale. In statics, homogenization methods allow to establish the averaged material characteristics, needed for design following the classical theories. On the other hand, dynamical loading is often characterized by high-frequency excitations. In

this case, wavelengths of excitations may be comparable with characteristic scales of embedded microstructure(s). It is obvious that then the homogenization methods are not applicable because the fluctuations at microscale may affect the behaviour at the macroscale. This leads to the need to derive physically well-grounded methods for the description of material properties. For an engineer, the important question is: how does the stress-strain relation reflect the material properties and what are the consequences of this.

In this paper, the ideas of mathematical modelling of stress fields and deformation waves in microstructured solids are briefly described. First, it is argued that the Green approach, which starts from a function of potential energy, has some preferences compared with the Cauchy approach, based on proposing a suitable stress–strain relation. Mathematical models are then derived by using balance laws, introducing internal variables for capturing the effects of the internal structure of solids. For the sake of transparency, the modelling is described in the one-dimensional setting. The focal point of the paper is devoted to physical effects, which can be described by derived mathematical models. These effects (both qualitative and quantitative) can be used in nondestructive testing (NDT) of material characteristics.

2. GREEN OR CAUCHY?

Given the balance laws (of mass, momentum and energy) in continuum mechanics, the crucial problem for an engineer is: how to describe (or derive) the stress–strain relations. In other words, the question can be formulated as follows: how to determine the constitutive equations? For solving this problem, two methods are available [1]: the Green method and the Cauchy method. According to the Green method, the potential (free) energy is assumed to be a function of the strain and the stress–strain relation is followed from the potential energy. According to the Cauchy method, it is assumed that the stress is a function of the strain, determined experimentally. Both methods haven certain advantages and disadvantages when compared with each other.

Let us envisage briefly the essence of both methods. For the sake of simplicity, rectangular Lagrange coordinates are used within the framework of the theory of elasticity [2]. The potential energy W in the Green approach is assumed as a general sufficiently regular function of the strain ε_{ij}:

$$W = W(\varepsilon_{ij}), \tag{1}$$

where the strain tensor ε_{ij} can be written as

$$\varepsilon_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j} + u_{k,i}\ u_{k,j}). \tag{2}$$

Here u_i is the displacement, indices run over $1, 2, 3$ and the differentiation with respect to the space coordinate x_i is separated by comma. Then the stress tensor

σ_{ij} is calculated by

$$\sigma_{ij} = \frac{\partial W}{\partial \varepsilon_{ij}}. \tag{3}$$

According to the Cauchy method, one has to postulate directly

$$\sigma_{ij} = \sigma_{ij}(\varepsilon_{kl}). \tag{4}$$

In principle, there seems to be only a little difference between the two methods and, consequently, between relations (3) and (4). However, the potential energy W should be written in terms of invariants of e_{ij} in order to guarantee the material invariance under a coordinate system rotations [1]. It is not obvious following the Cauchy method. In addition, the potential energy W might involve also temperature and then the generalization to thermoelastic problems is obvious. As we see further, the potential energy W may be even a more complicated function with a clear physical background and then the stress–strain relationship will reflect more effects rather than strain only.

For the simplest one-dimensional elastic case, the potential energy is a quadratic function of e_{11}:

$$W = \frac{1}{2}(\lambda + 2\mu)\varepsilon_{11}^2, \tag{5}$$

where λ and μ are Lamé parameters. Then for the linear case

$$\sigma_{11} = (\lambda + 2\mu)\varepsilon_{11} = (\lambda + 2\mu)u_{1,1}, \tag{6}$$

where we recognize the widely used case in engineering.

It has been stressed [1] that the elastic constants in Eq. (2) are directly related to the energy function whereas the relation of elastic constants of Eq. (4) to the energy W is unclear. It is also shown [1] that it is easier to satisfy the conditions of objectivity and material invariance for the Green method while the Cauchy method has found more usage for dissipative systems [3].

In order to derive constitutive equations for microstructured solids, one should have a clear understanding about the internal structure of such solids and forces between the constituents. In this case, the Green method could have a clear advantage before the Cauchy method, because at the energy level it is easier to guarantee stability of the energy function and thermodynamic consistency, if needed. Proposing a stress–strain function directly like it is done by the Cauchy method, it will be more like a guessing exercise. Most of the studies, related to microstructured solids, follow the Green method for deriving the governing equations [4–6].

3. MICROSTRUCTURE MODELLING

Our attention is focused to microstructured solids. One can certainly imagine that at the molecular level a solid might be composed by different particles and one should know the forces between the particles in order to derive governing equations. Such a discrete approach will involve a large system of equations and usually this system is brought to a continuum limit [7]. However, the question how the forces at the molecular level can be treated at the continuum limit, is difficult to answer. That is why the modelling usually starts from the viewpoint of continua. As far as conventional continuum mechanics is based on the assumption of homogeneity, the generalized continuum theories are proposed which incorporate the properties of the microstructure into the governing equations [4–6,8]. The balance laws for macro- and microstructures can be formulated separately [4,5] or all macro- and microstructural effects can be introduced in one set of balance laws. The last approach reflects very clearly the structure of the solid with corresponding forces, caused by the internal structure. Moreover, it is easy to generalize this idea introducing the internal variables into modelling. The concise overview on generalized continuum mechanics is given in [9].

We shall demonstrate now the main stages of the modelling of wave propagation in microstructure solids. For the sake of simplicity, we focus on one-dimensional problems only. The full three-dimensional theory is presented in [10,11].

3.1. Mindlin's microelasticity

To describe the influence of a microstucture on the macromotion, we need to take into consideration a new variable: microdeformation. The microdeformation is treated as an internal degree of freedom. According to Mindlin [5], macrodisplacement is denoted by $u = u_1$ and microdeformation – by φ. Then the kinetic and potential energies are governed by following expressions,

$$K = \frac{1}{2}\rho u_t^2 + \frac{1}{2} I \varphi_t^2, \tag{7}$$

$$W = \frac{1}{2}(\lambda + 2\mu) u_x^2 + A u_x \varphi + \frac{1}{2} B \varphi^2 + \frac{1}{2} C \varphi_x^2, \tag{8}$$

respectively. Here ρ is the macrodensity, I is the microinertia, and the indices x and t denote differentiation. The material parameters A, B, and C characterize the given microstructured solid. The corresponding Euler–Lagrange equations in terms of the Lagrangian $\mathcal{L} = K - W$ are

$$\left(\frac{\partial \mathcal{L}}{\partial u_t}\right)_t + \left(\frac{\partial \mathcal{L}}{\partial u_x}\right)_x - \frac{\partial \mathcal{L}}{\partial u} = 0, \tag{9}$$

$$\left(\frac{\partial \mathcal{L}}{\partial \varphi_t}\right)_t + \left(\frac{\partial \mathcal{L}}{\partial \varphi_x}\right)_x - \frac{\partial \mathcal{L}}{\partial \varphi} = 0. \tag{10}$$

Introducing Eqs (7), (8) into system of equations (9), (10), we obtain

$$\rho u_{tt} - \left(\frac{\partial W}{\partial u_x}\right)_x = 0, \tag{11}$$

$$I\varphi_{tt} - \left(\frac{\partial W}{\partial \varphi_x}\right)_x + \frac{\partial W}{\partial \varphi} = 0. \tag{12}$$

Here we recognize

$$\sigma = \frac{\partial W}{\partial u_x} = (\lambda + 2\mu)u_x + A\varphi, \tag{13}$$

$$\eta = \frac{\partial W}{\partial \varphi_x} = C\varphi_x, \tag{14}$$

$$\tau = \frac{\partial W}{\partial \varphi} = Au_x + B\varphi, \tag{15}$$

where σ is the macrostress (Piola–Kirchhoff stress), η is the microstress and τ is the interactive force. Clearly $(\lambda+2\mu)$ is the longitudinal modulus, C is the microstress modulus, A describes coupling effects and B – the strength of the interactive force. Compared with the simplest case of a homogeneous solid (see Eq. (6)) the situation is much more complicated but physically clear.

The governing system of equations derived from Eqs (11), (12), is the following:

$$\rho\, u_{tt} = (\lambda + 2\mu)u_{xx} + A\varphi_x, \tag{16}$$

$$I\, \varphi_{tt} = C\varphi_{xx} - Au_x - B\varphi. \tag{17}$$

If there is no coupling between macro- and microstructure then $A = 0$ and

$$\rho\, u_{tt} = (\lambda + 2\mu)u_{xx}, \tag{18}$$

$$I\, \varphi_{tt} = C\varphi_{xx} - B\varphi, \tag{19}$$

i.e. two uncoupled equations of motion yield.

The coupling in system of equations (16), (17) means that the micro- and macromotion interact with each other. This model of microstructure is called *micromorphic*. It suggests the knowledge of the values of materials parameters A, B, C, and I, as well as boundary conditions both for the macrodisplacement and for the microdeformation. The latter is the most disputed problem, which is still under question.

3.2. Dual internal variables

A more general description of the internal structure of a continuum can be achieved by introducing dual internal variables. Contrary to observable variables (like measurable strain, for example), the internal variables are "measurable but not controllable" [12] and give insight about the integrally distributed effect of a microstructure within a solid [13]. In the dual internal variables approach, one internal variable permits to model the rate of changing of another internal variable [14].

We start with the balance of pseudomomentum [15] within the material formulation. Multiplying Eq. (18) by u_x we then check that Eq. (18) yields the following material balance of momentum

$$\frac{d\mathcal{P}}{dt} - \frac{\partial b}{\partial x} = f^{int} + f^{inh}, \tag{20}$$

where the *material momentum* $\mathcal{P}$, the material *Eshelby stress* b, the material *inhomogeneity force* f^{inh}, and the material *internal force* f^{int} are defined by [15]

$$\mathcal{P} := -\rho_0 u_t u_x, \tag{21}$$

$$b := -\left(\rho_0 u_t^2/2 - W + \sigma\varepsilon\right), \tag{22}$$

$$f^{inh} := \left(\frac{1}{2}{u_t}^2\right)\frac{\partial \rho_0}{\partial x} - \left.\frac{\partial W}{\partial x}\right|_{expl}, \tag{23}$$

$$f^{int} := \sigma u_{xx} - \left.\frac{\partial W}{\partial x}\right|_{impl}. \tag{24}$$

Here the subscript notations $expl$ and $impl$ mean, respectively, the derivative keeping the fields fixed (and thus extracting the explicit dependence on x), and taking the derivative only through the fields present in the function.

In addition, the dissipation inequality reads in the isothermal case

$$-W_t + \sigma\varepsilon_t \geq 0, \tag{25}$$

where σ is the Piola–Kirchhoff stress tensor. The advantage of Eq. (20) compared with the conventional balance laws is that the r.h.s. is clearly formulated in terms of forces within the solid and allows to describe better the effects of microstructure.

If we use the concept of dual internal variables, then there is an important difference compared with theories derived by Mindlin [5] or Eringen [8]. Instead of two separate balance laws for the macro- and microstructure, only one balance law (20) is at our disposal. The governing equation for the internal variable(s) is derived from dissipation inequality (25). In this way, the advantages of using potential energy and the dissipation inequality as an energy constraint, are clearly taken into account.

As an example, let the potential energy $W = W(u_x, \varphi, \psi)$ be represented by

$$W = \frac{1}{2}\,(\lambda + 2\mu)\,u_x^2 + Au_x\varphi + \frac{1}{2}B\,\varphi^2 + \frac{1}{2}\,C\,\varphi_x^2 + \frac{1}{2}\,D\,\psi^2, \qquad (26)$$

where φ and ψ are internal variables and A, B, C, D are constants. Then the balance law for linear momentum yields

$$\rho u_{tt} = (\lambda + 2\mu)\,u_{xx}^2 + A\varphi_x. \qquad (27)$$

As before, we have

$$\sigma = (\lambda + 2\mu)\,u_x + A\varphi, \qquad (28)$$

$$\eta = C\varphi_x, \qquad (29)$$

$$\tau = Au_x + B\varphi, \qquad (30)$$

$$\xi = \frac{\partial W}{\partial \psi} = D\psi. \qquad (31)$$

Dissipation inequality (25) yields

$$(\tau - \eta_x)\varphi_t + (\xi - \zeta_x)\psi_t \geq 0, \qquad (32)$$

where $\zeta = \partial W/\partial \varphi_x$. It is clear that in the non-dissipative case dissipation inequality (32) can by satisfied by the choice

$$\varphi_t = R(\xi - \zeta_x), \quad \psi_t = -R(\tau - \eta_x), \qquad (33)$$

where R is a constant. Finally, from Eqs (33) we obtain

$$I\varphi_{tt} = C\varphi_{xx} - Au_x - B\varphi, \qquad (34)$$

where $I = 1/(R^2 D)$. Note that here $\zeta = 0$. Evidently, systems of equations (16), (17), and (27), (34) look like equivalent. However, in the case of dual internal variables there exist natural boundary conditions following from the condition of zero extra entropy flux at boundaries.

There are several theories proposed for enlarging the concepts of micro-structured continua [16,17]. It is shown that many so-called gradient theories can be derived by using the concept of dual internal variables [18].

3.3. Further generalizations

Certain materials (e.g., biomaterials) are essentially nonlinear. It is straightforward to introduce also physical nonlinearities at macro- and microscale in the

framework of dual internal variables. For this the potential energy W should also include the following terms:

$$\frac{1}{6}Nu_x^3 + \frac{1}{6}M\varphi_x^3, \tag{35}$$

where coefficients N and M are responsible for the nonlinearity in macro- and microscale, respectively. In this case, the final governing equations (cf. Eqs (16), (17)) are the following [19]:

$$\rho u_{tt} = (\lambda + 2\mu)u_{xx} + A\varphi_x + Nu_x u_{xx}, \tag{36}$$

$$I\varphi_{tt} = C\varphi_{xx} - Au_x - B\varphi + M\varphi_x\varphi_{xx}. \tag{37}$$

This system of equations describes wave propagation in nonlinear microstructured solids.

In many practical applications the microstructure has also multiple scales – they could be hierarchically ordered (a scale within a scale) or concurrent (same scale but different properties). It is possible to use the same procedure [20] for deriving the governing equations. For example, in the hierarchical case, the potential energy is written as

$$W = \frac{1}{2}\,(\lambda\ + 2\mu)\,u_x^2 + A_1\varphi_1 u_x + \frac{1}{2}B_1\varphi_1^2 + \frac{1}{2}\,C_1(\varphi_1)_x^2 + A_{12}(\varphi_1)_x\varphi_2 + \frac{1}{2}\,B_2\varphi_2^2 + \frac{1}{2}\,C_2(\varphi_2)_x^2, \tag{38}$$

where φ_1 and φ_2 are internal variables (microdeformations), and $A_1, B_1, C_1, A_{12}, B_2, C_2$ are material parameters. Then we obtain the following governing equations:

$$\rho u_{tt} = (\lambda\ + 2\mu)u_{xx} + A_1(\varphi_1)_x, \tag{39}$$

$$I_1\,(\varphi_1)_{tt} = C_1(\varphi_1)_{xx} - A_1u_x - B\varphi_1, \tag{40}$$

$$I_2\,(\varphi_2)_{tt} = C_2(\varphi_2)_{xx} - A_{12}(\varphi_1)_x - B_2\varphi_2. \tag{41}$$

The detailed analysis of this model is given in [21].

Finally, it is also possible to use the same approach for deriving the governing equations for the thermoelasticity where the microtemperature (temperature fluctuation due to microstructure) is taken into account [22,23].

3.4. Main features of the models

System of Eqs (16), (17) or other models derived above involve coupling between macro- and microstructure. In order to understand the effects of coupling, one should introduce a scale parameter δ, which is the ratio of the characteristic scale of a microstructure and the wavelength of the excitation.

First, let us note that system of Eqs (16), (17) can be represented in the form of a single equation by replacing the system of two second-order equations by one fourth-order equation in terms of macrodisplacement u [24]:

$$u_{tt} = \left(c_0^2 - c_A^2\right)\, u_{xx} - p^2 \left(u_{tt} - c_0^2\, u_{xx}\right)_{tt} + p^2 c_1^2 \left(u_{tt} - c_0^2\, u_{xx}\right)_{xx}, \qquad (42)$$

where $c_0^2 = (\lambda + 2\mu)/\rho$, $c_1^2 = C/I$, $c_A^2 = A^2/\rho B$ and $p^2 = I/B$. The velocities c_0, c_1 and c_A characterize the macromotion, the microstructure, and the slowing down effect due to the microstructure, respectively.

Further on, let us introduce dimensionless variables

$$U = u/U_o, \;\; X = x/L, \;\; T = c_0 t/L, \;\; \delta = l^2/L^2, \;\; \epsilon = U_0/L, \qquad (43)$$

where U_0 and L are the amplitude and the wavelength of an excitation and l is a characteristic scale of the microstructure. We also suppose that $I = \rho l^2 I^*$, $C = l^2 C^*$, where I^* is dimensionless and C^* has the dimension of stress. By an asymptotic analysis [19] we get in the first approximation

$$U_{TT} = \left(1 - \frac{c_A^2}{c_0^2}\right)\, U_{XX} + \frac{c_A^2}{c_B^2}\left(U_{TT} - \frac{c_1^2}{c_0^2}\, U_{XX}\right)_{XX}, \qquad (44)$$

where $c_B^2 = BL^2/I$. The scale parameter δ is involved in the ratio of velocities

$$\frac{c_A^2}{c_B^2} = \delta I^* \frac{A^2}{B^2}. \qquad (45)$$

Equation (44) exhibits directly the hierarchical nature of wave propagation in microstructured solids in the spirit of Whitham [25]:

– if c_A^2/c_B^2 is small then waves are governed by the properties of the macrostructure;
– if c_A^2/c_B^2 is large then waves "feel" more the properties of the microstructure.

Note that in absence of the interaction between macro- and microstructure ($A = 0$, which means also $c_A = 0$) the governing wave operator is simply the classical $U_{TT} - U_{XX}$. Another important feature is that even for small values of A, the velocity of waves at macroscale is influenced by the coupling (see Eq. (44)). This effect is also demonstrated by direct numerical analysis [26].

The presence of the microstructure leads to the dispersion of waves. This is explicitly seen from Eq. (44) where the influence of the microstructure is described by the second derivative of the wave operator

$$U_{TT} - c_1^2/c_0^2\, U_{XX}, \qquad (46)$$

i.e. the fourth-order derivatives U_{TTXX} and U_{XXXX} govern the dispersion effects.

The dispersion analysis for the derived model is represented in several studies [18,19,24,27]. From the results of the dispersion analysis it is worth to mention the following:

– the character of dispersion (normal or anomal) is studied [27];
– both boundary and initial value problems are analysed [27];
– the dispersion properties for different models are compared [28];
– the role of parameters, which govern the waves in microstructured solids, is demonstrated [29].

Another important feature to be understood is the possible balance of dispersion and nonlinear effects in microstructured solids. It is well known that this balance can lead to the emergence of solitary waves. In contrast with the celebrated evolution equations like the Korteweg–de Vries (KdV) equation, the leading terms are here (cf. Eq. (44)) of the second order. This means that the governing equations are of the Boussinesq type [30,31]. The analysis of waves, based on derived mathematical models, demonstrates clearly the existence of solitary waves and the emergence of strains of solitary pulses [32,33].

If the KdV equation models the emergence of soliton trains in one direction only then the Boussinesq-type equation models the emergence of trains of solitary pulses in two directions [33]. Moreover, the influence of nonlinearities at the microlevel leads to the asymmetry of a solitary wave. It is certainly possible to derive an evolution equation from the second-order system. In this case the results is a modified KdV-type equation, which in the standardized form reads [34]

$$q_t + 6qq_x + q_{xxx} + 3k(q_x^2)_{xx} = 0, \tag{47}$$

where q is related to deformation at the macroscale. Equation (47) exhibits the trend to asymmetry due to the last term in it but the inertial and elastic properties of the microstructure are described by one term (q_{xxx}) only.

4. FINAL REMARKS

This brief review summarizes recent results in studies on modelling of wave propagation in microstructured solids. It is clear that the proper modelling is a basis for engineering calculations. However, the description of coupling between macro- and microstructure together with inertial and elastic properties of the microstructure needs more physical parameters than in case of traditional homogeneous solids. Fortunately, the existence of microstructure means also additional measurable effects on the macroscale. This leads to the possibility to elaborate algorithms for nondestructive testing (NDT) of material properties. Mathematically it means solving the inverse problems – once we know the system with the accuracy of parameters then given the initial (boundary) values and the measured effects one can determine the parameters of the system. For one-dimensional problems several NDT algorithms are presented in the monograph [35].

These algorithms are based on the dispersion analysis and elaborated for harmonic waves and wave packets. In addition, a novel method is proposed to use solitary waves in the NDT. In this case, nonlinear effects are taken into account like asymmetry of a wave which increases during the propagation.

Further studies on modelling of waves in microstructured solids are in progress, involving thermoelastic waves, two-dimensional problems, etc.

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Lainelevi modelleerimisest mikrostruktuuriga tahkistes

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Materjalide mikrostruktuurist põhjustatud efektid peavad olema piisava täpsusega kirjeldatud ka lainelevi matemaatilistes mudelites. Inseneri seisukohalt on oluline täpsustada pinge ja deformatsiooni vahelist seost (nn olekuvõrrandit). Artiklis on analüüsitud Greeni ja Cauchy meetodeid olekuvõrrandite tuletamiseks ning kirjeldatud energeetilistel tingimustel põhineva Greeni meetodi eeliseid. On näidatud, kuidas sisemuutujate abil on võimalik makropingete kõrval määrata ka mikropingeid ja interaktiivseid jõude mikrostruktuuriga tahkiste dünaamilisel koormamisel. Selliselt konstrueeritud liikumisvõrrandites ilmneb dispersiooni oluline roll lainelevi protsessides taolistes materjalides.