

WAVES IN MICROSTRUCTURED MATERIALS: COMPARATIVE ANALYSIS OF MODELS

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Abstract

Several mathematical models describing wave propagation in microstructured materials are comparatively analysed. The basic model is taken along Mindlin (1964) and its asymptotic simplification (Engelbrecht and Pastrone, 2003). This asymptotic model describes (i) hierarchical character of wave motion; (ii) changes in wave speed; (iii) influence of dispersion. The comparative analysis of lattice models (Maugin, 1999) and models for periodic structures (Santosa and Symes, 1991) permits to clarify the nature of dispersive effects including the role of inertia of the microstructure. In addition, the straightforward modelling can be used assigning all the physical parameters to every volume element in a material. In this case, the numerical simulation (Berezovski et al., 2001; 2003) by finite volume method supports the theoretical considerations. Having the clear understanding about the physical effects and the accuracy of models, the experiments can be outlined in order to verify the theories and to determine the physical parameters.

Keywords: deformation waves, microstructure, dispersion

1 Introduction

The complex dynamic behaviour of microstructured materials at high speeds of deformation cannot be explained by the classical theory of continuous media. This concerns granular materials, polycrystalline solids, ceramic composites, functionally graded materials, alloys, damaged materials, etc. Such materials are characterized by the existence of intrinsic space-scales in matter, like the lattice period, the size of a crystallite or a grain, the distance between the microcracks, etc. that introduce the scale-dependence into the governing equations. The theories of continua have actually foreseen the problems of irregularities of media long time ago (Cosserats, Voigt, Eringen [1], Mindlin [2], et al). The elegant mathematical theories of continua with voids, planar or ordinary spin, vector microstructure, Cosserat continuum, micromorphic continuum, etc. have been elaborated (see overviews in Eringen [3], Capriz [4]). Clearly every irregularity (or inclusion) creates an additional stress field around itself, consequently the most general approach in modelling should be the presentation of all the conservation laws and constitutive equations taking such a stress field into account. This approach is in detail described by Maugin [5] using the concept of pseudo-momentum and material inhomogeneity force.

Beside the theory, experiments provide often only indirect data on physical effects related to the behaviour of materials with microstructure. We have to confess that there is a gap between the theoretical models and experimental studies in this field. The obvious reason for such a mismatch is that the macroscopic theories involve physical parameters (or even functions) that cannot be determined directly from the experiments. In addition, the influence of nonlinearities causes nonadditivity of physical effects. That is why all the physical effects must be carefully studied. The list of structurally sensitive effects is long including complicated dispersion, emergence of solitary waves, stress-induced phase-transition, kinetic localisation of damage, attenuation characterized by asymmetric resonance curves, etc. The situation becomes even more complicated when dealing with ferromagnetic effects, physical-chemical reactions, molecular crystals and nanomaterials.

This way or another, the starting point in describing a certain microstructure is to determine the scales. However, the scales are not uniquely determined although many studies are going on. Generally speaking, a characteristic internal length of microstructured materials is up to $1 \mu m$ (Sih [6]; Suresh and Mortensen [7]; Suquet [8]; Engelbrecht and Braun [9]; Phillips [10]; etc. and references therein). Below that limit come nanostructured materials with a characteristic length on the order of few (typically 1-10) nm (Gleiter [11]). In this limit, the full attention should be paid to

lattice models (Maugin [12]). If the attention is focused primarily to the formation of physical substructures in materials under loading, then also the concept of mesomechanics is used (Sih, [6]), especially reflecting the features of plasticity and dislocation theory. Another approach in mesoscopic modelling is the dynamics of microcracks (Van et al. [13]) where the macroscopic-phenomenological and microscopic-statistical descriptions are used. Notice also Guyer and Johnson [14] on mesoscopic elasticity. In what follows below, we keep the notion of microstructure in the scale up to $1\mu m$ that could be related to the size of a grain of a granular material, a crystallite of a polycrystal or a molecule of a polymer (Mindlin [2]). One should also notice that in terms of field theories, microstructure induces nonlocality (Eringen [3]; Engelbrecht and Braun [9]).

A crucial point in modelling is to choose the theory. The first decision should be made to choose between discrete and continuum models. In discrete approach the volume elements of the matter are treated as pointmasses with a proposed topological structure and the interaction between the discrete masses. This gives a good chance to model crystal lattices with certain symmetries, vacancies, impurities, defects, walls, etc. (Maugin [12]). The governing equations are then deduced following the Newton's law and the key problem is the modelling of forces between the pointmasses. Starting from the Born-von Karman model for an one-dimensional atomic chain such models have gained much attention (Maugin [12] and references therein).

From the viewpoint of continua, the straight-forward modelling of microstructured solids leads to assigning all the physical parameters to every volume element dV in a solid introducing so the dependence on coordinates X^k . Then the governing equations include space-dependent parameters and the most effective way to solve the governing equations is the numerical integration. Another probably much more effective way is to separate macro- and microstructure in continua. Then the conservation laws for both structures should be separately formulated (Eringen [1, 3]; Mindlin [2]) or the microstructural quantities are separately taken into account in one set of conservation laws (Maugin [5]). Separating the macro- and microstructure gives two possibilities: either to consider both structures inertial or to suppose the microstructural quantities to behave noninertially. The first case is exactly following Eringen [1, 3] and Mindlin [2], the second case leads to the formalism of internal variables (Maugin [15], Maugin and Muschik [16]).

Both approaches - discrete and continuous - are closely related. One could, for example, to replace the set of n differential equations with its continuum analogy using the Taylor-series expansions. The most celebrated case is that of the Zabusky-Kruskal approximation of the Fermi-Pasta-Ulam problem, producing the Korteweg-de

Vries equation for the description of waves influenced by the quadratic nonlinearity and the cubic dispersion.

One should also stress the importance of a special case of microstructure - periodic (or laminated) structures (mostly composites). In this case, contrary to functionally graded materials, the periodic layering is important. One of the possibilities to account for such layers is to analyse the frequency spectrum of time-harmonic Bloch expansion (Ziegler [17]). An important presentation in the form of a dispersive effective medium is given by Santosa and Symes [18]). This approach is recently generalized for linear (Fogarty [19]; Fogarty and LeVeque [20]) and nonlinear (LeVeque and Yong [21]) cases. The dispersion relation is derived from Bloch expansion and then the equation of motion is restored accounting for dispersive effects caused by periodicity. The clear correspondence of this model to the Mindlin-type model (Engelbrecht and Pastrone [22]) is obvious and explains the role of the scale parameter related to periodicity. In addition, the comparison of two models (see Fogarty and LeVeque [20]; Engelbrecht and Pastrone [22]) permits to analyse the effects of inertia prescribed to microstructure.

Here we concentrate our attention to modeling dispersive effects due to the presence of microstructure in solids. Our further aim is to understand the possible balance of nonlinear and dispersive effects in wave motion, however the dispersion analysis is within the linear framework, that is why this part needs a special attention. Section 2 describes our basic model where for the sake of clarity one-dimensional (1D) approach is used. In Section 3 other possible models are briefly presented. Section 4 includes the comparative analysis and conclusions.

2 The basic model

Here we follow Mindlin [2] who has interpreted the microstructure "as a molecule of a polymer, a crystallite of a polycrystal or a grain of a granular material". This microelement is taken as a deformable cell. Note that if this cell is rigid, then the Cosserat model follows. The displacement \mathbf{u} of a material particle in terms of macrostructure 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 and the microdisplacement \mathbf{u}' is defined by its components $u'_i \equiv x'_i - X'_i$, where the origin of the coordinates x'_i moves with the displacement \mathbf{u} . The displacement gradient assumed to be small. This leads to the *basic assumption* of Mindlin [2] - "the microdisplacement can be

expressed as a sum of products of specified functions of x'_i and arbitrary functions of x_i and t ". The first approximation is then

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

The *micro deformation* is

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

Clearly, beside macrostrain $\epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$ in linear approximation, we need also a relative deformation

$$\gamma_{ij} = \partial_i u_j - \varphi_{ij}, \quad (3)$$

which is actually the difference between the macrodisplacement gradient and the microdeformation. Mindlin [2] has also used a microdeformation gradient $\partial_i \varphi_{jk}$, but here we do not go so far.

According to [2, 4, 23], the fundamental balance laws for microstructured materials can be formulated separately for macroscopic and microscopic scales. Here we use the simplest 1D model and get (cf. [22, 24])

$$\rho u_{tt} = \sigma_x, \quad (4)$$

$$I \varphi_{tt} = \eta_x + \tau, \quad (5)$$

where τ is the macrostress (Piola stress), η is the microstress and τ is the interactive microforce; ρ is the macrodensity, I is the microinertia and indices x and t denote the differentiation. As usual, we have (cf [22])

$$\sigma = \frac{\partial W}{\partial U_x}, \quad \eta = \frac{\partial W}{\partial \varphi_x}, \quad \tau = \frac{\partial W}{\partial \varphi}, \quad (6)$$

where W is the free energy. At this moment, we neglect the dissipation which was discussed earlier in [24].

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

$$W = \frac{1}{2} \alpha u_x^2 - A \varphi u_x + \frac{1}{2} B \varphi^2 + \frac{1}{2} C \varphi_x^2, \quad (7)$$

with α, A, B, C - constants. The balance equations (15) are now specified as follows:

$$\rho u_{tt} = \alpha u_{xx} - A \varphi_x, \quad (8)$$

$$I \varphi_{tt} = C \varphi_{xx} - A u_x + B \varphi. \quad (9)$$

For further analysis we introduce dimensionless variables and use the slaving principle [25, 26] for eliminating φ . Omitting the details (for those see [22]), the final governing equation in terms of nondimensional displacement U reads:

$$U_{TT} = \left(1 - \frac{A^2}{\alpha B}\right) U_{XX} + \delta \frac{A^2}{B^2} \left(I^* U_{TT} - \frac{C^*}{\alpha} U_{XX}\right)_{XX}. \quad (10)$$

Here $\delta = l^2 L^{-2}$, l is the scale of the microstructure and L , for example, is the wavelength of the excitation. The quantities I^* and C^* are determined by $I = \rho l^2 I^*$ and $C = l^2 C^*$.

Equation (10) is the sought "skeleton" of the wave equation for microstructured solids.

3 Specific models

3.1 Lattice theory

There has been a wide interest to lattice theory and corresponding models (see [12] and the references therein). The simplest 1D model is that of Born-von Karman which describes the longitudinal wave in an infinite elastic chain of particles, placed at the equal distance a at equilibrium and linked by identical springs of stiffness k . The longitudinal motion in such a chain is described by the equations of motion

$$m \frac{d^2 U_n}{dt^2} = k(\xi_{n+1} - \xi_n), \quad (11)$$

$$\xi_n = U_n - U_{n-1}, \quad (12)$$

where m is the mass and U_n - the displacement. In continuum limit, U_n is derived into the Taylor-series and then the standard wave equation

$$U_{tt} - c_0^2 U_{xx} = 0, \quad c_0^2 = \frac{ka^2}{m} \quad (13)$$

follows. If, however, to replace eqs. (11) by equations of more general type

$$m \frac{d^2 U_n}{dt^2} = - \frac{\partial \phi}{\partial U_n}, \quad (14)$$

where ϕ is the potential then the situation may be more complicated. Considering more terms in Taylor expansion (for details see [12]), the continuum limit gives

$$U_{tt} - c_0^2 U_{xx} - \frac{1}{12} c_0^2 a^2 U_{xxxx} = 0 \quad (15)$$

in the linear version. It has been shown [12] that even higher-order terms (U_{xxxxxx}) can be taken into account.

3.2 Periodic structures

Periodic microstructure is quite a typical case of composite and functionally graded materials. A suitable model may be constructed by homogenization of periodic media that approximates well the dispersive nature of waves [18]. Homogenization is possible when the shortest wavelength of the initial excitation is several times larger than the of the microstructure and the time scale is large. Santosa and Symes [18] have used the Bloch wave expansion for that, i.e. the solution of an eigenvalue problem is used. The medium with cell size $2\pi p$ is considered and $\epsilon = p/\lambda \ll 1$, where λ is the lower limit of the Fourier components of the initial disturbance. Then the dispersion relation may be constructed (for details see [18]):

$$\omega(k) = \Omega_1 k + \frac{1}{6} \epsilon^2 \Omega_3 k^3 + \dots, \quad (16)$$

where ω and k are the frequency and the wavenumber, respectively. For a two-component structure with densities ρ_1 and ρ_2 , and moduli μ_1 and μ_2 , one has the velocities $c_1^2 = \mu_1/\rho_1$, $c_2 = \mu_2/\rho_2$ and impedances $z_1 = (\rho_1 \mu_1)^{1/2}$, $z_2 = (\rho_2 \mu_2)^{1/2}$. Then

$$\Omega_1^2 = \frac{(\theta/\mu_1 + (1-\theta)/\mu_2)^{-1}}{(\theta \rho_1 + (1-\theta) \rho_2)}, \quad (17)$$

$$\Omega_3 = \Omega_3(z_i, c_i, \theta, \Omega_1), \quad (18)$$

where θ denotes the volume fraction of the mixture. The wave equation, corresponding to (16) is:

$$U_{tt} = \Omega_1^2 U_{xx} + \frac{1}{3} \Omega_1 \Omega_3 p^2 u_{xxxx}. \quad (19)$$

From (17) follows that $\Omega_1 < c_1$ and it can be shown [18] that $\Omega_3 < 0$.

3.3 Periodic structures with microinertia

A special case of periodic structures is considered by Wang and Sun [27], who have used a continuum model for macromotion involving also micro-inertia terms in energy densities. Assuming the linear approximate local displacement field, the macro displacement equation of motion yields

$$U_{tt} = \frac{L}{\rho} U_{xx} + \frac{H}{\rho} U_{xxtt}, \quad (20)$$

where

$$L = \frac{\mu_1 \delta_1 \delta_2}{\delta_2 f_1 + \gamma \delta_1 f_2}, \quad (21)$$

$$H = \frac{1}{6} \frac{f_1 f_2 (\gamma \delta_1 - \delta_2) (p f_1^2 - f_2^2)}{(\delta_2 f_1 + \gamma \delta_1 f_2) (p f_1 - f_2)} (d_1 + d_2)^2 \rho_2, \quad (22)$$

$$\rho = \rho_1 f_1 + \rho_2 f_2. \quad (23)$$

Here ρ_1, ρ_2 are the densities, μ_1, μ_2 are the elastic moduli of layers with widths d_1, d_2 , respectively. Further, $\gamma = \mu_1/\mu_2$, $p = \rho_1/\rho_2$ and $\sigma_i = 2(1-\nu_i)/(1-2\nu_i)$, $f_i = d_i/(d_1 - d_2)$ for $i = 1, 2$ while ν_1, ν_2 are the Poisson's ratios.

4 Discussion

The basic model (10) for waves in microstructured materials reflects the following physical phenomena:

- (i) it describes the wave hierarchy in Whitham's sense [28] including two wave operators - one for macrostructure, another for microstructure; if the scale parameter δ is small then the last two terms. i.e. influence of microstructure can be neglected; if δ is large then on contrary, the influence of first two terms, i.e. influence of macrostructure is weaker and the process is governed by the properties of the microstructure;
- (ii) the wave speed in the compound material is affected by the microstructure (1 versus $A \alpha^{-1} B^{-1}$) and clearly only $A = 0$ excludes this dependence.

(iii) 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}).

The other models described in Section 3 are based on weaker assumptions. In order to compare them we list below all the models (scaling see Sect. 2, 3):

(i) continua:

$$U_{TT} = c^2 U_{XX} + \delta (\beta_1 U_{TT} - \gamma U_{XX})_{XX}; \quad (24)$$

(ii) periodic structures

$$U_{TT} = \Omega_1^2 U_{XX} + \frac{1}{6} \Omega_1 \Omega_3 p^2 U_{XXXX}; \quad (25)$$

(iii) lattice theory

$$U_{TT} = c_0^2 U_{XX} - \frac{1}{12} c_0^2 a^2 U_{XXXX} + b U_{XXXXXXXX} + \dots \quad (26)$$

(iv) continua with microinertia

$$U_{TT} = c^2 U_{XX} + h U_{TTXX}. \quad (27)$$

First, the wave speed. Clearly all the models, except lattice theory (26) take the influence of the microstructure into account while the speed is definitely different from c_0 - the wave speed in the macromaterial.

Second, the dispersion. Clearly the basic model (24) takes into account two phenomena: inertia of the microstructure (term U_{TTXX} and velocity in microstructure (term U_{XXXX}). Other models are in this sense less general, paying the attention only to one or another phenomenon. The further analysis should show the accuracy of models (25), (26), and (27). Clearly the sign of U_{XXXX} terms coincides in all the models where it is kept. The double dispersion is also important for describing strain waves in rods [29].

Third, numerical simulation. We have used the finite-volume method [30, 31] that permits to assign all the physical parameters to every volume element in a material.

The wave propagation in metal-ceramic composites is considered. The elastic properties of the metal matrix and ceramic reinforcement are the following [32]: Young

modulus 70 GPa and 420 GPa , Poisson ratio 0.3 and 0.17 , and density 2800 kg/m^3 and 3100 kg/m^3 , respectively. Volume fraction $f = V_c/V$, where V_c is the volume of ceramic particles and V is the total volume is varied. A Gaussian-type excitation was generated at the left boundary of a 2D specimen between 40 and 160 space steps (see Fig. 1)

$$\sigma_0(0, t) = \sigma_0 \sin^2(\pi(t - 2t_r)/2t_r), \quad (28)$$

where $\sigma_0 = 125 \text{ MPa}$ and $t_r = 10$. The initial wave length corresponds to 20 space steps. In Fig. 1 the wavefronts in pure ceramics (Fig. 1a) and in pure metal (Fig. 1b) are shown. The differences in wave speeds are obvious. In case of a metal-ceramic composite, as shown in Fig. 2 for various volume fractions (left column in Fig. 2), the wave speed clearly depends on the density distribution (cf right column in Fig. 2). This supports all those analytical models that foresee such changes (models (24), (25), (27)).

Another example is a case of functionally graded materials [31, 32]. Again a 2D problem is considered, the material is assumed graded along the vertical direction (see Fig. 3) and the excitation (28) is generated at the upper surface. Four possible forms of volume fraction are considered [32]: a) the specimen is composed as a single metal-matrix composite with fixed volume fraction f ; b) a layered structure has different volume fractions for each layer; c) the volume fraction varies following the power law

$$f(z) = f_0(z/h)^b, \quad (29)$$

where z is the vertical coordinate, h is the thickness of the specimen, and b is the parameter defining the variation of particle distribution and equals here 0.25 - high f front; e) the same with $b = 4$ (low f front). The material properties are same as above for the example shown in Figs. 1, 2. Figure 4 shows the normal stress along the centerline of the specimen for the excitation (28) with $t_r = 0.75 \mu\text{s}$. Again, the differences in wave speeds are visible.

The numerical analysis of dispersive effects is in the progress to be compared with solutions of model equations.

The nonlinear effects at macroscale and microscale (cf. [22, 24]) need clearly attention only with dispersive effects taken into account simultaneously. This analysis is also in progress.

Acknowledgements. The support from the Estonian Science Foundation, MIUR COFIN 2000, and ESF NATEMIS Programme is gratefully acknowledged.

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Figure Captions

Figure 1. Wave fronts at $t = 180$: a) pure ceramics; b) pure metal.

Figure 2. Density distribution (left column) and wavefronts at $t = 180$ (right column): a) volume fraction $f = 0.75$; b) $f = 0.50$; c) $f = 0.25$.

Figure 3. Density distribution in a metal-ceramic composite: a) uniform; b) layered; c) graded (high volume fraction front); d) graded (low volume fraction front).

Figure 4. Normal stress distribution along the centerline of a metal-ceramic composite at $3\mu s$ (see legend in Fig.3).