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Waves and complexity of microstructured solids

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A complex system as it is understood nowadays is composed by its constituents that interact with each other resulting in emergent properties of the system as a whole. In mechanics the concepts of complexity has been analysed by Engelbrecht [7] with a focus on wave propagation. This theory is based on some cornerstones like the introduction of internal structures at different scales and the nonlinearity of the models which in other words means incorporating intrinsic microstructural and nonlinear effects. In this case complexity means that we have different scales, with several interaction processes which encompass many physically meaningful phenomena. Usually a microstructured body, as we shall see, is modeled as a solid with an internal structure at a different scale, which is apt to describe the mechanical behaviour of solids with dislocations, polycrystalline solids, ceramic composites, granular media, etc. One main aspect of such theories is that they always take into account the nonlinearity of the materials, the nonlocality and the interactions between micro- and macroscales. It is possible, and useful, to develop also models with a hierarchy of microstructures, i.e. a first level micro-structure which contains a second level micro-structure, and it is meaningful also the case of concurrent micro-structures (see Berezovski et al [1]). In this paper we want to analyze the subject, recalling some main results in the theory of complex microstructures, developing new results in the case of multiple microstructures, exploiting hierarchical governing equations and analyzing nonlinear wave propagation, which is crucial to put in evidence the weight of the different scales and the interaction of micro- and macro-structures.

1 Introduction

In this presentation we want to elaborate the idea that complex systems in Continuum Mechanics are strictly related to a more general theory, as briefly described in Maugin [12], that we can obviously call Generalized Continuum Theory. This theory is based on some cornerstones like the introduction of internal structures at different scales and the nonlinearity of the models which in other words means incorporating intrinsic microstructural and nonlinear effects. A typical case in continuum mechanics, among many, is the case of materials with certain microstructure. In this case complexity means that we have different scales, with several interaction processes which encompass many physically meaningful phenomena. The pioneering work of Mindlin [13] is a basic reference, another more recent general treatment can be found in Capriz [2], while many papers have appeared where different particular and less particular cases have been described (see the papers by Engelbrecht, Pastrone, Cermelli, Porubov quoted in the references). Usually a microstructured body, as we shall see, is modeled as a 3D solid with an internal structure at a different scale, which is apt to describe the mechanical behaviour of solids with dislocations, polycrystalline solids, ceramic composites, granular media, etc. One main aspect of such theories is that they always take into account the nonlinearity of the materials, the nonlocality and the interactions between micro- and macroscales. It is possible, and useful, to develop also models with a hierarchy of microstructures, i.e. a first level micro-structure which contains a second level micro-structure, and so on, as done in Casasso and Pastrone [3], Engelbrecht et al [10]. But it is meaningful also the case of concurrent micro-structures (see Berezovski et al [1]). In Section 2 we recall some main results in the theory of complex microstructures, developing new results in the case of multiple microstructures. In Section 3 we exploit hierarchical governing equations and analyze nonlinear wave propagation, which is crucial to put in evidence the weight of the different scales and the interaction of micro- and macro-structures. In Section 4 we analyse similar problems in the case of concurrent microstructures. The presentation in its full form is to be published in *Atti della Accademia delle Scienze di Torino* [6]. To give a simple idea of different scales in solids we refer to Gates et al. [11]: from 10^{-9} m (nanomechanics) over 10^{-6} m (mesomechanics) and 10^{-3} m (micromechanics) to 10^{0} m (structural mechanics).

2 The field equations

The kinetic energy T of a microstructured body is defined as a quadratic form in the velocities $\dot{\mathbf{r}}$, $\dot{\mathbf{d}}_H$, where $\mathbf{r}$ is the position vector describing the macrostructure, $\mathbf{d}_H$ is the director apt to provide a description of some properties of the microstructure as they act at the macroscopic level, dot means derivative with respect to time t while the material point $\mathbf{X}$ is kept fixed, the notation $(\cdot)_{,j} = \partial(\cdot)/\partial X^j$ will mean derivatives with respect to the material coordinates X^i. Here and in the following $H, K, \dots = 1, 2, 3, \dots, n$, where n depends on the type of microstructure we want to model; $i, j = 1, 2, 3$. T is a definite positive quadratic form. Without any loss of generality, we can reduce it to a diagonal form

$$T = \frac{1}{2}\left(\rho\dot{\mathbf{r}}\cdot\dot{\mathbf{r}} + I^{HK}\dot{\mathbf{d}}_H\cdot\dot{\mathbf{d}}_K\right), \qquad (1)$$

where ρ is the mass density and I^{HK} represents the inertia form of the microstructure. If we deal with a Lagrangian formulation, ρ and I are defined on the reference configuration, hence they are functions of $\mathbf{X}$ only.

Let us assume that the body admits a generalized stored energy density

$$W = W(\mathbf{r}_{,h}, \mathbf{d}_H, \mathbf{d}_{H,j}, \mathbf{X}). \qquad (2)$$

We can derive the field equations via the usual variational principle, namely requiring that the motions of the body in a certain interval of time $[t_0, t_1]$ will make the energy functional

$$\mathcal{E} = \int_{t_0}^{t_1}\int_{\mathcal{B}}(T - W - W_b)dVdt \qquad (3)$$

stationary in comparison with all admissible motions. The Euler–Lagrange equations read

$$\begin{cases} \left(\dfrac{\partial W}{\partial \mathbf{r}_{,i}}\right)_{,i} - \dfrac{\partial W_b}{\partial \mathbf{r}} = \dfrac{d}{dt}\dfrac{\partial T}{\partial \dot{\mathbf{r}}}, \\ \left(\dfrac{\partial W}{\partial \mathbf{d}_{H,i}}\right)_{,i} - \dfrac{\partial W}{\partial \mathbf{d}_H} - \dfrac{\partial W_b}{\partial \mathbf{d}_H} = \dfrac{d}{dt}\dfrac{\partial T}{\partial \dot{\mathbf{d}}_H}. \end{cases} \qquad (4)$$

In general, from a physical point of view, the microbody forces are different from the macrobody forces, hence we can split W_b in two parts:

$$W_b = W_b^{\text{macro}}(\mathbf{r}, \mathbf{X}) + W_b^{\text{micro}}(\mathbf{d}_H, \mathbf{X}). \qquad (5)$$

3 One dimensional model with hierarchical microstructure

We consider a one-dimensional microstructured model with two different scale levels applied for the microstructure. Instead of the two-scale elastic system, containing both macro- and microstructures, we introduce a material, which is supposed to be a compound of a macrostructure, a first level microstructure and a second level microstructure at a much smaller scale. The last may be interpreted as a nanostructure, to some extent (see [3], [10], [14]).

In Figure 1 we give a sketch of the possible configuration of a solid with two levels microstructures.

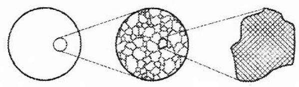

Figure 1: Two-levels microstructure

Therefore, following the model, we deal with three different scalar functions: the one for the macrostructure and two for the microstructures, one for each scale level. The model of a material is the one-dimensional manifold, and we consider the material coordinates in space x and in time t; and the functions $v = v(x, t)$ for the macrostructure, $\varphi = \varphi(x, t)$ and $\psi = \psi(x, t)$ respectively for the first and the second scale level in microscale. The macro body is supposed to be purely elastic, and both the first and second level microstructures satisfy the same generalized elasticity hypothesis as well, therefore the existence of an internal strain energy is assumed.

A particular choice of the strain energy function W defines different nonlinear models, see [3]; in this paper we consider it in the following form:

$$W = \frac{1}{2}\alpha v_x^2 + \frac{1}{3}\beta v_x^3 + A_1\varphi v_x + \frac{1}{2}B_1\varphi^2 + \frac{1}{2}C_1\varphi_x^2 + B\varphi_x\psi + \frac{1}{2}B_2\psi^2 + \frac{1}{2}C_2\psi_x^2. \qquad (6)$$

This function is the generalization of the strain energy function for nonlinear elastic solids with one microstructure level to our case, where the introduction of the cubic term v_x^3 represents the nonlinear behaviour of the matrix.

The field equations can be derived as in [3] via a variational principle:

$$\begin{cases} \rho v_{tt} = \alpha v_{xx} + \left(\beta v_x^2\right)_x + A_1\varphi_x, \\ I_1\varphi_{tt} = C_1\varphi_{xx} - A_1 v_x - B_1\varphi - B\psi_x, \\ I_2\psi_{tt} = C_2\psi_{xx} - A_2\varphi_x - B_2\psi, \end{cases} \qquad (7)$$

where α, β and A_i, B_i, C_i $(i = 1, 2)$ denote material constants.

To obtain the governing equation in dimensionless form, it is necessary to introduce some suitable parameters and constants (see [4]) and two different parameters δ_i, $i = 1, 2$, characterizing the ratio between the microstructure and the wave length L, and ϵ, accounting for small but finite elastic strain magnitude:

$$\delta_1 = (l_1/L)^2, \quad \delta_2 = (l_2/L)^2, \quad \epsilon = v_0 << 1, \quad (8)$$

where v_0 is the intensity of the initial excitation and the values l_1 and l_2 represent the size of the microstructural elements. Introducing the macrostrain $\nu = v_x$ (the term "strain" is used for brevity only; in fact, it is the longitudinal displacement gradient component, while expressions for genuine strains are nonlinear with respect to ν) and the dimensionless variables

$$u = \nu/v_0, \quad X = x/L, \quad T = (c_0/L)t \quad (9)$$

and substituting them into the previous system, we obtain the field equations. The slaving principle [10] can now be used for further transformations. This procedure allows us to write one function in terms of the other; on this way we can obtain the governing equation for the function $u(x,t)$ only:

$$u_{TT} + \alpha_1 u_{XX} + \alpha_2 (u^2)_{XX} + (\alpha_3 u_{XX} + \alpha_4 u_{TT})_{XX} + (\alpha_5 u_{4X} + \alpha_6 u_{TTXX} + \alpha_7 u_{4T})_{XX} = 0, \quad (10)$$

where the α_i are constant coefficients explicitely defined in [4] and in the final remark of this section.

The equation (10) above may be considered as a hierarchical equation in terms of u, where two different levels of microstructure are expressed in five different dispersive terms, and the higher order terms contain the parameters of the second level of microstructure.

We have obtained a 6th order PDE that is hardly to be solved explicitly in general case. However, we will find some exact travelling wave solutions of the PDE (10), when the equation can be reformulated in terms of the phase variable $z = x \pm Vt$ in the corresponding ODE and by means of the method introduced by Samsonov in [17], upon the introduction of z and integration twice with corresponding conditions at infinity $|z| \to \infty \Rightarrow u, u' \to 0$ the field equation may be rewritten as the nonlinear ODE of the 4th order:

$$u^{(IV)} + au^{(II)} + bu^2 + cu = 0, \quad (11)$$

where obviously:

$$a = (\alpha_3 + V^2\alpha_4)/\chi; \quad b = \alpha_2/\chi; \; c = (\alpha_1 + V^2)/\chi; \quad \chi = \alpha_5 + V^2\alpha_6 + V^4\alpha_7. \quad (12)$$

Following the method described in [17], the exact solution to the ODE (11) in terms of elliptic functions, containing only poles as the critical singularities, has be found in the following form:

$$u = M\wp^2(x; g_2, g_3) + S\wp(x; g_2, g_3) + K, \quad (13)$$

where the coefficients M, S, K and invariants g_i of the Weierstrass elliptic function $\wp$ are defined in [4].

In the appropriate limit the Weierstrass elliptic function $\wp$ may be further reduced to the elliptic Jacobi *cn* function and, in due course, to the bounded solution u_0 in terms of $\cosh^{-2}$ function, i.e., to *the solitary wave solution*, as follows:

$$u_0 = s\cosh^{-4}(x) + q\cosh^{-2}(x) + p; \quad p = -c/b = -\frac{-18928 + 3640a - 31a^2}{507b}; \quad q = \frac{140(52+a)}{13b}; \; s = -840/b, \quad (14)$$

which has a form of the so called "mexican hat". Figure 3 provides two graphical examples of the solutions for different values of the parameter b.

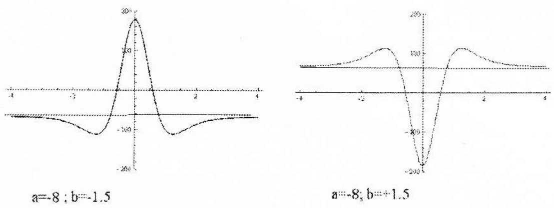

Figure 2: $a = -8$, $b = -1.5$ for the figure on the left, $a = -8$, $b = +1.5$ for the figure on the right.

Remark

The approach used to obtain these solutions is similar to that introduced and grounded in [17], and can be applied to explicitly solve different higher order ODE, e.g., the 5th order KdV and the 5th order mKdV equations.

4 Concurrent microstructures

Instead of a hierarchy of microstructures, one can be interested in concurrent microstructures, as introduced in [1], namely in two, or more, microstructures which act at the same scale level and interact with the macrostructure as well, as illustrated in Figure 3.

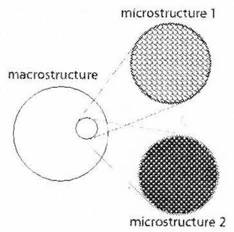

Figure 3: Concurrent microstructures

We can obtain the fields equations as done before just introducing a different expression of the strain energy function, for instance:

$$W = \frac{1}{2}\alpha v_x^2 + \frac{1}{3}\beta v_x^3 + A_1\varphi v_x + A_2\psi v_x + \frac{1}{2}B_1\varphi^2 + \frac{1}{2}C_1\varphi_x^2 + A\varphi\psi + \frac{1}{2}B_2\psi^2 + \frac{1}{2}C_2\psi_x^2, \quad (15)$$

where φ and ψ denote the microstrains of the two concurrent microstructures.

Hence the field equations read:

$$\begin{cases} \rho v_{tt} = \alpha v_{xx} + \beta(v_x^2)_x - A_1\varphi_x - A_2\psi_x, \\ I_1\varphi_{tt} = C_1\varphi_{xx} - A_1 v_x - B_1\varphi - A\psi, \\ I_2\psi_{tt} = C_2\psi_{xx} - A_2 v_x - B_2\psi - A\varphi, \end{cases} \quad (16)$$

where α, A_i, B_i, C_i, A_{12} $(i = 1, 2)$ denote material constants.

With the substitution $v_0 u = v_x$, from $(16)_1$ we derive:

$$\rho v_0 u_{tt} = \alpha v_0 u_{xx} + \beta v_0^2(u^2)_{xx} - A_1\varphi_{xx} - A_2\psi_{xx}. \quad (17)$$

Using the slaving principle at the first order approximation, namely, as done before, setting

$$\begin{aligned} \varphi &= \varphi_0 + \delta_1\varphi_1 + \dots, \\ \psi &= \psi_0 + \delta_1\psi_2 + \dots \end{aligned} \quad (18)$$

we obtain from (16), as proved in [6], the 4th order PDE:

$$u_{TT} + \alpha_1 u_{XX} + \beta_1(u^2)_{XX} + \delta_1\left(\alpha_3 u_{XX} + \alpha_4 u_{TT}\right)_{XX} + \delta_2\left(\alpha_5 u_{XX} + \alpha_6 u_{TT}\right)_{XX} = 0, \quad (19)$$

where the coefficients α_i can be explicitly evaluated in terms of the material constants appearing in (16).

Equation (19) is clearly different from (10), since here we have two concurrent microstructures acting at the same level, one is responsible of the term $\delta_1(\dots)$, the second one of the term $\delta_2(\dots)$, but in both cases the order of the derivatives is the 4th. In (10), as remarked, we have a hierarchy of microstructures, at the first level corresponding to 4th order derivatives, the second level to 6th order derivatives. The two terms $\delta_1(\dots)$ and $\delta_2(\dots)$ are coupled through the coefficient A_{12} which appears in both terms. Obviously, if $A_{12} = 0$, the microstructures are independent and the two terms are uncoupled.

Technically, the reason is that in the actual strain energy function (15) does not appear the term $-A_2\varphi_x\psi$ which is in (6), related to the hierarchy of the microstructures in that case, while here we have a "peer" coupling term $A_{12}\varphi\psi$.

Equation (19) is very similar with the DDE (3.16) in Samsonov [17], the meaning of the coefficients being obviously different. Hence we can follow the same procedure. Introducing the phase variable $z = x \pm Vt$ we obtain the 4th order PDE

$$(V^2 + \alpha_1)u^{II} + \beta_1(u^2)^{II} + \delta_1\left(\alpha_3 + V^2\alpha_4\right)u^{IV} + \delta_2\left(\alpha_5 + V^2\alpha_6\right)u^{IV} = 0. \quad (20)$$

By double integration and regrouping the last two terms we obtain the 2nd order ODE

$$\delta_1\left(\alpha_3 + V^2\alpha_4\right) + \delta_2\left(\alpha_5 + V^2\alpha_6\right)u^{II} + \beta_1(u^2) + (V^2 + \alpha_1)u + c_1 z + c_2 = 0. \quad (21)$$

This equation can be formally written, with obvious meaning of the coefficients, as

$$u^{II} + b(u^2) + cu + c_1 z + c_2 = 0. \quad (22)$$

Multiplying by u' and integrating once more we have

$$\frac{1}{2}(u')^2 = -\frac{1}{3}bu^3 - \frac{1}{2}cu^2 - c_2 u - c_1(z + \frac{1}{2}z^2)u + d. \quad (23)$$

In Samsonov [17], Chapter 3 one can find an extensive analysis of equations of this kind and we can apply here his conclusions too, namely that by means of an appropriate choice of the invariants of the elliptic P-functions appearing in the Weierstrass equation associated to (23) and appropriate P-function limits in real axis, equation (23) can admit a discontinuous general travelling wave solution that can be reduced to solitary wave and to *cnoidal* wave solution.

Indeed one can imagine higher order coupling terms introducing in W products of derivatives of φ and ψ, namely terms containing $\varphi_x\psi$, $\psi_x\varphi$, $\varphi_x\psi_x$, but for need of brevity we do not go further in this direction.

5 Conclusions

The problem of the propagation of non linear waves in solids with different internal structural scales is studied. The general model developed in [3] and [14] has been used. In the case of one microstructure a 6th order PDE is obtained and the hierarchy of waves is clearly obtained. Using the same basic model, the case of two concurrent microstructures is studied and by means of the slaving principle one can reach meaningful approximate equations.

This model takes in account interaction between microstructures and macrostructure. We have derived the model equations for single and multiple scales and we have shown that we can obtain analytical solutions, but in many cases numerics are needed. Such an approach demonstrates clearly that complexity appears naturally in Continuum Mechanics, when you deal with microstructures.

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