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TWO-SCALE MICROSTRUCTURE DYNAMICS

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Wave propagation in materials with embedded two different microstructures is considered. Each microstructure is characterized by its own length scale. The dual internal variables approach is adopted yielding in a Mindlin-type model including both microstructures. Equations of motion for microstructures are coupled with the balance of linear momentum for the macromotion, but not coupled with each other. Corresponding dispersion curves are provided and scale separation is pointed out.

Keywords: Wave propagation; microstructured solids; double microstructure; dual internal variables.

1. Introduction

Modern advanced materials (composites, functionally graded materials, shape memory alloys, ...) are inhomogeneous by definition. Their properties are highly dependent on their composition or the embedded microstructure. This microstructure is characterized by a length scale which is usually smaller than a macroscale. Nevertheless, the influence of microstructure may not be necessary small, especially in dynamics.

The prediction of the dynamical response of advanced materials over multiple scales should include the tracking of microstructural evolution and the load transfer between different constituents. There are different possibilities to describe the microstructure influence. If the microstructure can be prescribed (like in laminates), then the solution can be obtained by using rather simple governing equations for constituents. The medium in this case is piecewise homogeneous but may be sufficiently complex. In another limiting case, where existing microstructure is too random, homogenization methods lead to a rather simple "effective" medium, but the governing equations become much more complex in order to take into account the microstructure influence.

An intermediate approach is the introduction of internal variables, which reflect the influence of the microstructure at the macroscopic level of description. In 1940s, Bridgman proposed an introduction of "a large scale thermodynamic parameter of state".[1] These state parameters, which extend the state space, are called the internal (state) variables.[2–4] Physically, internal variables represent an overall effect of microscopic material structural characteristics.

Internal variables are independent variables and obey a special rate equation. The introduction of internal variables can be beneficial when selected material structural characteristics and their associated dissipations affect the local properties significantly.[5] It is hoped that a few aggregate internal variables will adequately describe the microstructure. The thorough thermomechanical theory with internal variables is presented recently by Maugin.[6,7] The extension of this theory by weakly non-local dual internal variables approach[8] allows describe dynamical influence of a microstructure on the wave propagation in solids.[9–11]

Usually, only one kind of the microstructure is considered. At the same time, the direct numerical simulation of a pulse propagation in periodic laminates with two substructures[12] shows that even simple variation in the order of sublayers leads to significant changes in the response of the whole laminate. The corresponding results are presented in Figs. 1 and 2. The substructure composition is shown in the upper part of each figure. Here the white corresponds to layers of the hardest material and black denotes the softest one, and a material with intermediate hardness is marked by grey. In the given examples, the distinction in composition consists in

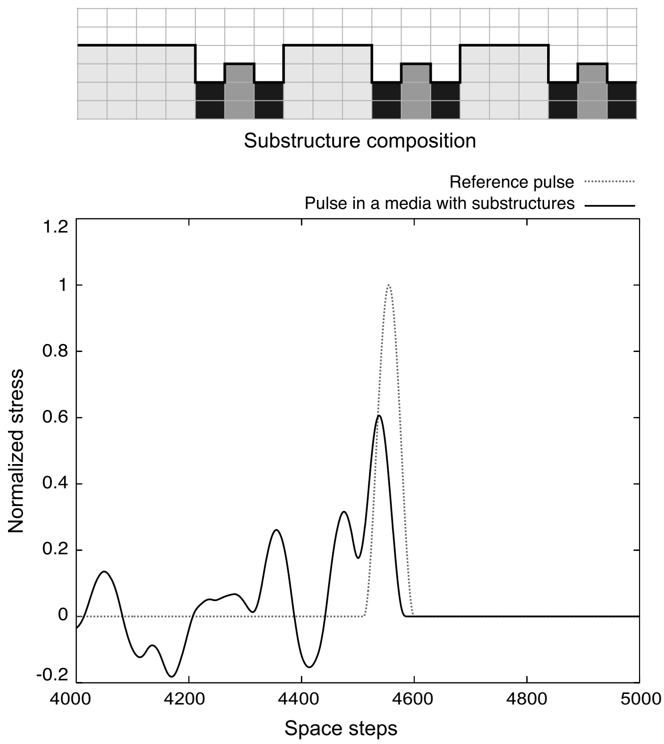


Fig. 1. Pulse shape in "hard-soft-intermediate-soft-hard" double structure laminate.

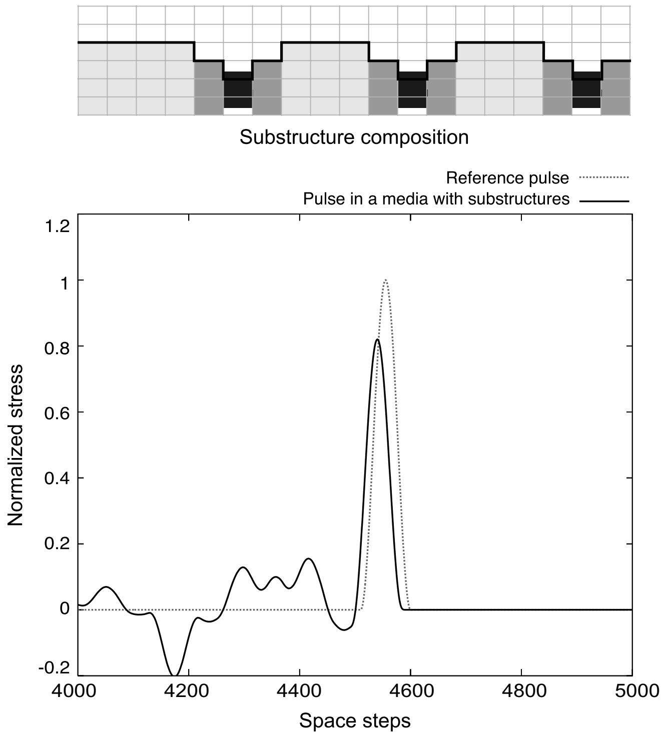


Fig. 2. Pulse shape in "hard-intermediate-soft-intermediate-hard" double structure laminate.

the interchange of soft and intermediate sublayers only. The difference in the corresponding pulse shape is surprisingly large. This example demonstrates the necessity in the investigation of the behavior of materials with at least two microstructures.

In this paper, the influence of a double microstructure is considered on the example of the one-dimensional dispersive wave propagation in microstructured solids. The paper is organized as follows. First, the dispersive wave equations are recalled briefly in the next section. Then the dual internal variable theory for media with a single microstructure is presented in Sec. 3. This theory is extended on the case of double microstructures in Sec. 4. Dispersion curves for both single and double microstructures are given in Sec. 5. In Sec. 6, it is demonstrated how the scales can be separated depending on material parameters. Some conclusions are given in last section.

2. Dispersive Wave Equations

The classical equation of linear elastic wave propagation in homogeneous solids in the one-dimensional case reads

$$u_{tt} = c^2 u_{xx} \,, \tag{1}$$

where u is the displacement, c is the elastic wave speed, and subscripts denote derivatives.

The effect of periodic inhomogeneity (Figs. 1 and 2) manifests itself in slowing down of the propagation and in dispersion of the signal. To describe the dispersion effects, several modifications of the wave equation are proposed for wave propagation in heterogeneous materials. The simplest generalization of the wave Eq. (1) is the linear version of the Boussinesq equation for elastic crystals[13]

$$u_{tt} = c^2 u_{xx} + c^2 l^2 A_{11} u_{xxxx}\,, \tag{2}$$

where l is an internal length parameter and A_{11} is a dimensionless coefficient. Similar equations were obtained using the homogenization of a periodically layered medium[14–16] or using strain gradient theories.[17] Here the dispersive term contains fourth-order space derivative of the displacement.

Another generalization of the wave equation (1) is the Love-Rayleigh equation for rods accounting for lateral inertia (cf. Ref. 18, p. 428)

$$u_{tt} = c^2 u_{xx} + l^2 A_{12} u_{xxtt}\,, \tag{3}$$

where A_{12} is again a dimensionless constant. This equation is derived also by other authors.[19–22] Here the fourth-order mixed derivative of the displacement characterizes the dispersion.

A more general equation combining the two dispersion models gives[16,23,24]

$$u_{tt} = c^2 u_{xx} - c^2 l^2 A_{11} u_{xxxx} + l^2 A_{12} u_{xxtt}\,. \tag{4}$$

An extended model proposed by Engelbrecht and Pastrone[25]

$$u_{tt} = (c^2 - c_A^2) u_{xx} - c^2 l^2 A_{11} u_{xxxx} + l^2 A_{12} u_{xxtt}\,, \tag{5}$$

contains a contribution of the microstructure on a slowing down of the propagation velocity c_A. In its turn, the Maxwell-Rayleigh model of anomalous dispersion[13] introduces in consideration the fourth-order time derivative

$$u_{tt} = c^2 u_{xx} + \frac{l^2 A_{22}}{c^2} (u_{tt} - c^2 u_{xx})_{tt}\,. \tag{6}$$

The fourth-order time derivatives are included also in the "causal" model for the dispersive wave propagation proposed by Metrikine[23]

$$u_{tt} = c^2 u_{xx} - c^2 l^2 A_{11} u_{xxxx} + l^2 A_{12} u_{xxtt} - \frac{l^2}{c^2} A_{22} u_{tttt}\,, \tag{7}$$

and in the model based on the Mindlin theory of microstructure[26] proposed in the form[27]

$$u_{tt} = (c^2 - c_A^2) u_{xx} - p^2 (u_{tt} - c^2 u_{xx})_{tt} + p^2 c_1^2 (u_{tt} - c^2 u_{xx})_{xx}\,. \tag{8}$$

In the last equation, p and pc_1 determine time and length scales of the microstructure, respectively, c_1 can be associated with the wave propagation velocity in the microstructure itself.

The unified equation for dispersion effects accompanying wave propagation in microstructured materials in the one-dimensional case can be represented as

$$u_{tt} = (c^2 - c_A^2)u_{xx} + l^2 P(u_{tt} - c^2 u_{xx})_{xx} + \frac{l^2}{c^2} Q(u_{tt} - c^2 u_{xx})_{tt} + c^2 l^2 R u_{xxxx}\,, \tag{9}$$

where c_A is the velocity shift due to the microstructure, and P, Q and R are dimensionless coefficients. It is clear that the last microstructure model (9) includes all the particular cases (2)–(8).

3. Single Microstructure

The unified model of microstructure (9) can be recovered by means of the dual internal variable approach.[8] In this approach, the internal variable φ is associated with the distributed effect of the microstructure,[2–4] and ψ is the auxiliary internal variable.[8] It is supposed that the free energy depends on the displacement gradient as well as on the internal variable φ and its gradient. In the simplest case, only the contribution of the second internal variable ψ itself is included in the quadratic function of the free energy dependence[10]

$$W = \frac{\rho_0 c^2}{2} u_x^2 + A\varphi u_x + A'\varphi_x u_x + \frac{1}{2}B\varphi^2 + \frac{1}{2}C\varphi_x^2 + \frac{1}{2}D\psi^2\,, \tag{10}$$

where A, A', B, C and D are material parameters. This corresponds to the Mindlin-type microstructure model[28] where the internal variable φ represents microstrain. Accordingly, material parameters A and B have dimension of energy per unit volume (Pa) with the evident multiplication by dimension of length for A' and by its square for C, respectively. The dimension of D will be clear from what follows.

The macrostress σ and microstress η are determined by the corresponding derivatives of the free energy

$$\sigma = \frac{\partial W}{\partial u_x} = \rho_0 c^2 u_x + A\varphi + A'\varphi_x\,, \tag{11}$$

$$\eta = -\frac{\partial W}{\partial \varphi_x} = -A'u_x - C\varphi_x\,, \tag{12}$$

while the interactive internal force τ is

$$\tau = -\frac{\partial W}{\partial \varphi} = -Au_x - B\varphi\,. \tag{13}$$

For the dual internal variable we have, correspondingly,

$$\xi = -\frac{\partial W}{\partial \psi} = -D\psi\,, \quad \zeta = -\frac{\partial W}{\partial \psi_x} = 0\,. \tag{14}$$

It can be checked that the intrinsic dissipation is calculated as[10]

$$\Phi = (\tau - \eta_x)\dot{\varphi} + (\xi - \zeta_x)\dot{\psi} \geq 0\,. \tag{15}$$

The intrinsic dissipation can be vanished with a simple choice of evolution equations for internal variables

$$\dot{\varphi} = R_1(\xi - \zeta_x)\,, \quad \dot{\psi} = -R_1(\tau - \eta_x)\,, \tag{16}$$

where R_1 is an appropriate constant.

It follows from Eqs. (14) and $(16)_1$ that

$$\dot{\varphi} = -R_1 D\psi\,, \tag{17}$$

and the evolution equation for the dual internal variable can be rewritten in terms of the primary one as the hyperbolic equation

$$\ddot{\varphi} = R_1^2 D(\tau - \eta_x)\,. \tag{18}$$

As a result, we can represent the equations of motion in the form, which includes only the primary internal variable

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + A\varphi_x + A'\varphi_{xx}\,, \tag{19}$$

$$I\varphi_{tt} = C\varphi_{xx} + A'u_{xx} - Au_x - B\varphi\,, \tag{20}$$

where $1/(R_1^2 D)$ can be associated with the internal inertia measure I.

To obtain the higher-order dispersion equation, we can determine the first space derivative of the internal variable from Eq. (20)

$$B\varphi_x = -I\varphi_{ttx} + C\varphi_{xxx} + A'u_{xxx} - Au_{xx}\,. \tag{21}$$

The third mixed derivative φ_{ttx} follows from Eq. (19)

$$A\varphi_{ttx} = (\rho_0 u_{tt} - \rho_0 c^2 u_{xx})_{tt} - A'\varphi_{ttxx}\,. \tag{22}$$

Appeared fourth-order mixed derivative of the internal variable is calculated by means Eq. (20)

$$I\varphi_{ttxx} = C\varphi_{xxxx} + A'u_{xxxx} - Au_{xxx} - B\varphi_{xx}\,, \tag{23}$$

and, in its turn, the fourth-order space derivative is determined again from Eq. (19)

$$A'\varphi_{xxxx} = (\rho_0 u_{tt} - \rho_0 c^2 u_{xx})_{xx} - A\varphi_{xxx}. \tag{24}$$

Collecting all the results (21)–(24) and substituting them into Eq. (19) we arrive at the dispersive wave equation

$$\begin{aligned} u_{tt} = c^2 u_{xx} &+ \frac{C}{B}(u_{tt} - c^2 u_{xx})_{xx} - \frac{I}{B}(u_{tt} - c^2 u_{xx})_{tt} \\ &+ \frac{A'^2}{\rho_0 B} u_{xxxx} - \frac{A^2}{\rho_0 B} u_{xx}\,, \end{aligned} \tag{25}$$

which is nothing else but the general model of the dispersive wave propagation (9) as is easy to see, identifying $A^2 = c_A^2 B\rho_0, A'^2 = c^2 l^2 RB\rho_0, C = l^2 PB, Ic^2 = l^2 QB$.

The formulated model provides the description of wave propagation in materials with microstructure characterized by the single internal length l.[9,10,28,29] The next step is to extend the model to the case of microstructures which are characterized by more than one length scale.

4. Double Microstructure

The generalization of the microstructure model (19)–(20) to the case with two microstructures can be achieved in different ways. The first one is the "hierarchy of microstructures".[30] In this case, the coupling of the corresponding microstructure hierarchy may be represented schematically as follows:

$$\boxed{\text{Macrosystem}} \longrightarrow \boxed{\text{Microstructure1}} \longrightarrow \boxed{\text{Microstructure2}}$$

This means that only the motion of the first microstructure is coupled with the macromotion, and the motion of the second microstructure is coupled with that of the first one. The very same model is presented by Pastrone[31] including nonlinear terms at the macroscopic level.

Another example of possible coupling of macromotion and microstructures can be constructed by means of the representation of the free energy dependence as the sum of two similar contributions (cf. Ref. 32)

$$\begin{aligned} W = {} & \frac{\rho_0 c^2}{2} u_x^2 + A_1 \varphi_1 u_x + A_1' (\varphi_1)_x u_x + \frac{1}{2} B_1 \varphi_1^2 + \frac{1}{2} C_1 (\varphi_1)_x^2 + \frac{1}{2} D_1 \psi_1^2 \\ & + A_2 \varphi_2 u_x + A_2' (\varphi_2)_x u_x + \frac{1}{2} B_2 \varphi_2^2 + \frac{1}{2} C_2 (\varphi_2)_x^2 + \frac{1}{2} D_2 \psi_2^2 \,. \end{aligned} \tag{26}$$

The corresponding stresses are determined as follows:

$$\sigma = \frac{\partial W}{\partial u_x} = \rho_0 c^2 u_x + A_1 \varphi_1 + A_2 \varphi_2 + A_1' (\varphi_1)_x + A_2' (\varphi_2)_x \,, \tag{27}$$

$$\eta_1 = -\frac{\partial W}{\partial (\varphi_1)_x} = -A_1' u_x - C(\varphi_1)_x \,, \quad \zeta_1 = -\frac{\partial W}{\partial (\psi_1)_x} = 0 \,, \tag{28}$$

$$\eta_2 = -\frac{\partial W}{\partial (\varphi_2)_x} = -A_2' u_x - C(\varphi_2)_x \,, \quad \zeta_2 = -\frac{\partial W}{\partial (\psi_2)_x} = 0 \,, \tag{29}$$

as well as the interactive internal forces:

$$\tau_1 = -\frac{\partial W}{\partial \varphi_1} = -A_1 u_x - B_1 \varphi_1 \,, \quad \tau_2 = -\frac{\partial W}{\partial \varphi_2} = -A_2 u_x - B_2 \varphi_2 \,. \tag{30}$$

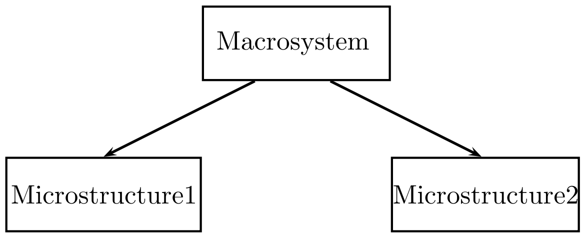
Accordingly, the equations of motion take the form

$$\rho_0 u_{tt} = \rho_0 c^2 u_{xx} + A_1 (\varphi_1)_x + A_2 (\varphi_2)_x + A_1' (\varphi_1)_{xx} + A_2' (\varphi_2)_{xx} \,, \tag{31}$$

$$I_1 (\varphi_1)_{tt} = C_1 (\varphi_1)_{xx} + A_1' u_{xx} - A_1 u_x - B_1 \varphi_1 \,, \tag{32}$$

$$I_2 (\varphi_2)_{tt} = C_2 (\varphi_2)_{xx} + A_2' u_{xx} - A_2 u_x - B_2 \varphi_2 \,. \tag{33}$$

In the considered case, both equations of motion for microstructures are coupled with the balance of linear momentum for the macromotion, but not coupled with each other. This is illustrated as follows:



The doubling of the amount of coefficients in the double microstructure model in comparison to the single microstructure complicates the quantitative analysis of the model. Nevertheless, qualitatively it can be analyzed by dispersion curves.

5. Dispersion Analysis

Dispersion relations are derived by assuming the solutions of Eqs. (31)–(33) in the form of harmonic waves

$$u(x,t) = \hat{u}e^{i(kx-\omega t)}\,, \quad \varphi_1(x,t) = \hat{\varphi}_1 e^{i(kx-\omega t)}\,, \quad \varphi_2(x,t) = \hat{\varphi}_2 e^{i(kx-\omega t)}\,, \tag{34}$$

where k is the wavenumber, ω is the frequency, and $i^2 = -1$. Substituting relations (34) into Eqs. (31)–(33) we get

$$\begin{pmatrix} \rho_0 c^2 k^2 - \rho_0 \omega^2 & -iA_1 k + A_1' k^2 & -iA_2 k + A_2' k^2 \\ iA_1 k + A_1' k^2 & C_1 k^2 - I_1 \omega^2 + B_1 & 0 \\ iA_2 k + A_2' k^2 & 0 & C_2 k^2 - I_2 \omega^2 + B_2 \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{\varphi}_1 \\ \hat{\varphi}_2 \end{pmatrix} = 0\,. \tag{35}$$

Nontrivial solutions of the system of Eq. (35) correspond to the vanished determinant of this system. This leads to the dispersion relation

$$\begin{aligned} &(c^2k^2 - \omega^2)(c_1^2 k^2 - \omega^2 + \omega_1^2)(c_2^2 k^2 - \omega^2 + \omega_2^2) \\ &\quad - ({c'}_{A2}^4 k^4 + c_{A2}^2 \omega_2^2 k^2)(c_1^2 k^2 - \omega^2 + \omega_1^2) \\ &\quad - ({c'}_{A1}^4 k^4 + c_{A1}^2 \omega_1^2 k^2)(c_2^2 k^2 - \omega^2 + \omega_2^2) = 0\,, \end{aligned} \tag{36}$$

where parameters

$$c_1^2 = \frac{C_1}{I_1}\,, \quad c_2^2 = \frac{C_2}{I_2}\,, \quad c_{A1}^2 = \frac{A_1^2}{\rho_0 B_1}\,, \quad c_{A2}^2 = \frac{A_2^2}{\rho_0 B_2}\,, \tag{37}$$

$${c'}_{A1}^4 = \frac{{A'}_1^2}{\rho_0 I_1}\,, \quad {c'}_{A2}^4 = \frac{{A'}_2^2}{\rho_0 I_2}\,, \quad \omega_1^2 = \frac{B_1}{I_1}\,, \quad \omega_2^2 = \frac{B_2}{I_2}\,, \tag{38}$$

have been introduced. The parameters c_i and c_{Ai} represent characteristic velocities in microstructures, and ω_i are characteristic frequencies. Dispersion relation (36) can be compared with those derived in Ref. 32 for a slightly different structure of free energy. To reduce the number of coefficients, we use the dimensionless quantities

$$\xi = \frac{ck}{\omega_1}\,, \quad \eta = \frac{\omega}{\omega_1}\,. \tag{39}$$

Introducing them into Eq. (36) yields the dispersion relations in dimensionless form

$$\begin{aligned}(\xi^2-\eta^2)(\gamma_1^2\xi^2-\eta^2+\eta_1^2)(\gamma_2^2\xi^2-\eta^2+\eta_2^2)\\ -(\gamma'^4_{A2}\xi^4+\gamma_{A2}^2\eta_2^2\xi^2)(\gamma_1^2\xi^2-\eta^2+\eta_1^2)\\ -(\gamma'^4_{A1}\xi^4+\gamma_{A1}^2\xi^2)(\gamma_2^2\xi^2-\eta^2+\eta_2^2)=0\,,\end{aligned} \tag{40}$$

where velocity ratios and dimensionless frequencies have been introduced as follows:

$$\gamma_1 = \frac{c_1}{c}\,, \quad \gamma_2 = \frac{c_2}{c}\,, \quad \gamma_{A1} = \frac{c_{A1}}{c}\,, \quad \gamma_{A2} = \frac{c_{A2}}{c}\,, \tag{41}$$

$$\gamma'_{A1} = \frac{c'_{A1}}{c}\,, \quad \gamma'_{A2} = \frac{c'_{A2}}{c}\,, \quad \eta_1 = 1\,, \quad \eta_2 = \frac{\omega_2}{\omega_1}\,. \tag{42}$$

The dispersion curves are shown in Fig. 3. The dispersion relation (40) represents three distinct branches (see Fig. 3). The lower dispersion curve is called acoustical, while the two higher frequency curves are called optical and they reflect internal modes of oscillation.[26] The acoustical curve starts at the origin with a slope $\eta = (1-\gamma_{A1}^2-\gamma_{A2}^2)^{1/2}\xi$, then it approaches $\eta = \gamma_2\xi$ in the short wave limit. The middle optical curve starts at $\eta = \eta_1$ with a slope $\eta = (1-\gamma_{A2}^2)^{1/2}\xi$ and then approaches $\eta = \gamma_1\xi$ in the short wave limit. The second optical curve starts at $\eta = \eta_2$ and approaches $\eta = \xi$. The asymptotical lines $\eta = \xi$, $\eta = \gamma_1\xi$ and $\eta = \gamma_2\xi$ are represented by dashed lines in Fig. 3.

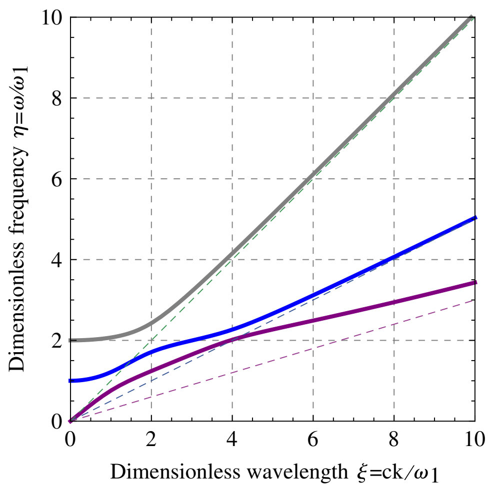


Fig. 3. Dispersion curves of Eq. (40) for $\gamma_{A1} = \gamma_{A2} = 0.4, \gamma_1 = 0.5, \gamma_2 = 0.3, \eta_2 = 2$: solid lines — concurrent microstructure model, dashed lines — asymptotes to dispersion curves.

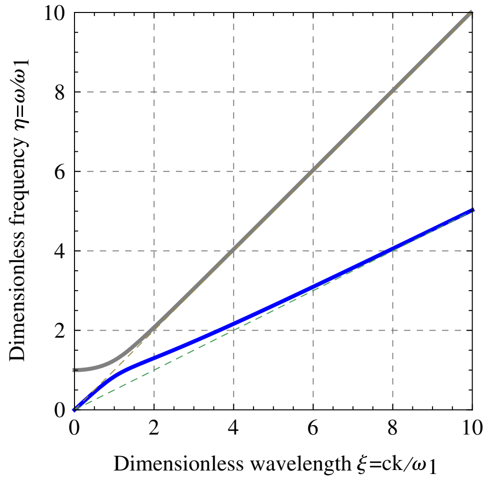


Fig. 4. Dispersion curves for $\gamma_{A1} = 0.4, \gamma_1 = 0.5$: solid lines — microstructure model, dashed lines — asymptotes to dispersion curves.

In the case of single microstructure the picture is more simple. There are two dispersion curves as it is shown in Fig. 4 (see also Ref. 27). As we can see, the presence of the second microstructure changes the behavior of dispersion curves significantly.

6. Scale Separation

To demonstrate the scale separation explicitly, the dimensionless variables should be introduced as follows[32]:

$$U = \frac{u}{U_0}, \quad X = \frac{x}{L}, \quad T = \frac{ct}{L}, \tag{43}$$

where U_0 and L are certain constants (intensity and wavelength of the initial excitation).

To characterize microstructures we also need to introduce scaled microstrains

$$\Phi_1 \equiv \frac{l_1}{L}\varphi_1, \quad \Phi_2 \equiv \frac{l_2}{L}\varphi_2. \tag{44}$$

In terms of dimensionless variables, the equation of motion at the macroscale (31) reads

$$\begin{aligned} U_{TT} = U_{XX} &+ \frac{A_1}{\rho_0 c^2}\frac{l_1}{U_0}(\Phi_1)_X + \frac{A_2}{\rho_0 c^2}\frac{l_2}{U_0}(\Phi_2)_X \\ &+ \frac{A_1'}{\rho_0 c^2 L}\frac{l_1}{U_0}(\Phi_1)_{XX} + \frac{A_2'}{\rho_0 c^2 L}\frac{l_2}{U_0}(\Phi_2)_{XX}, \end{aligned} \tag{45}$$

and the corresponding micromotions are governed by

$$\frac{I_1}{L^2\rho_0}\frac{l_1}{L}(\Phi_1)_{TT} = \frac{C_1}{L^2\rho_0 c^2}\frac{l_1}{L}(\Phi_1)_{XX} + \frac{A_1'}{\rho_0 c^2 L}\frac{U_0}{L}U_{XX} - \frac{A_1}{\rho_0 c^2}\frac{U_0}{L}U_X - \frac{B_1}{\rho_0 c^2}\frac{l_1}{L}\Phi_1\,, \tag{46}$$

and

$$\frac{I_2}{L^2\rho_0}\frac{l_2}{L}(\Phi_2)_{TT} = \frac{C_2}{L^2\rho_0 c^2}\frac{l_2}{L}(\Phi_2)_{XX} + \frac{A_2'}{\rho_0 c^2 L}\frac{U_0}{L}U_{XX} - \frac{A_2}{\rho_0 c^2}\frac{U_0}{L}U_X - \frac{B_2}{\rho_0 c^2}\frac{l_2}{L}\Phi_2\,, \tag{47}$$

respectively.

As it can be seen, contributions of microstructures and their motion can be separated clearly if the difference of their characteristic scales, l_1 and l_2, is large enough.

7. Conclusions

The dual internal variable concept applied to the analysis of the influence of a double microstructure on wave propagation in solids shows that the evolution equations for each microstrain are hyperbolic in the reversible nondissipative case. The solution of the evolution equations is non-trivial even for zero initial and boundary conditions for internal variables due to the coupling with the macromotion equation. The influence of a microstructure depends on the values of material parameters characterizing the microstructure.

It is clear that different kinds of microstructure models can be constructed by means of the combination of simple microstructure models considered above. Nonlinear terms may be introduced at any level of description as well as at the coupling.

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